Activity Report Bordeaux - Sud-Ouest 2019

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List of Inria's Research Teams

Team Auctus

Designing the collaborative robotics cells of the future

Inria teams are typically groups of researchers working on the definition of a common project, and objectives, with the goal to arrive at the creation of a project-team. Such project-teams may include other partners (universities or research institutions).

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Robotics and Smart environments

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Team Auctus

Creation of the Project-Team: 2020 April 01

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1. Team, Visitors, External Collaborators

Research Scientists

David Daney [Team leader, Inria, Researcher, HDR]
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Pierre Laguillaumie [Univ de Poitiers, PhD Student]
Jessica Colombel [Inria Larsen, PhD Student]
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Nicolas Simonazzi [Orange, PhD Student, granted by CIFRE]

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Administrative Assistant

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2. Overall Objectives

2.1. Overall Objectives

The project of the Auctus team is to design the collaborative robotics cells of the future.

The robotics community still tends to separate the cognitive (HRI) and physical (pHRI) aspects of human/robot interaction. One of the main challenges is to characterize the task as well as mechanical, physiological and cognitive capacities of humans in the form of physical constraints or objectives for the design of cobotized workstations. This design is understood in a large sense: the choice of the robot's architecture (cobot, exoskeleton, etc.), the dimensional design (human/robot workspace, trajectory calculation, etc.), the coupling mode (comanipulation, teleoperation, etc.) and control. The approach then requires the contributions of the human and social sciences to be considered in the same way as those of exact sciences. The topics considered are broad, ranging from cognitive sciences, ergonomics, human factors, biomechanics and robotics.

The first challenge is to evaluate the hardship at work, the well-being of the operators and, further upstream, their cognitive state which impacts their sensorimotor strategy for performing a task. In industry, the ergonomic analysis of the task is carried out by an ergonomist based on direct but often ad hoc observations. However, the context is changing: the digitization of factories, through the installation of on-site sensors, allows longitudinal observation of machines and humans. The information available can thus allow us to rethink the way in which the evaluation of activities is carried out. Currently, an emerging subdomain named *ergonomic robotics* adapts the available ergonomic evaluation criteria (RULA, REBA, etc.). However, they are related to the (quasi-static) posture of the operator, which limits the understanding of human motor strategies over a long period of time. Similarly, kinematic or biomechanical analysis may tend to see humans as a high-performance machine to be optimized. This may make sense for a top-level athlete, but repeating actions in the industry over a day, months or years of work means that a temporary change of posture, possibly poorly rated according to usual ergonomic criteria, can in fact be a good long-term strategy. These questions make a direct link between motor and cognitive aspects that can be reflected in particular strategies as the fatigue or the expertise (manual and cognitive). This approach has not been widely explored in robotics to determine the right criteria to adapt the behavior of a cobot.

The second challenge is to define a methodology to link the analysis of the task and the human movements it induces to the robot design. Indeed, as we have been able to verify on several occasions in the context of industrial projects, between the ergonomist, expert in task analysis and psychology, and the robotician, expert in mechanics, control and computer science, there is a significant conceptual distance that makes it very difficult to analyze needs and define the specifications of the technical solution. To fill these methodological gaps, it is necessary, on the basis of case studies, to better define the notion of tasks in the context of a human/robot coupling and to establish a typology of this type of interaction by taking into account, with as much details as possible, the different physical and cognitive constraints and their potential psychological, organizational or ethical impacts.

The third challenge is related to the need to think about the control laws of collaborative robots in terms of human/robot coupling. The effectiveness of this coupling requires an ability to predict future human actions. This prediction should make the interaction more intuitive but also aims at an optimal coupling from the point of view of “slow” phenomena such as fatigue. The major challenge is therefore to move from reactive to predictive control laws, integrating a human prediction model, both in terms of movement strategies and decision strategies. Beyond the great computational complexity of predictive approaches, obtaining prediction models is an ambitious challenge. It is indeed necessary to learn models that are quite complex in terms of the physical realities they can account for and quite simple from a computational point of view.

3. Research Program

3.1. Analysis and modelling of human behavior

3.1.1. Scientific Context

The purpose of this axis is to provide metrics to assess human behavior. We place ourselves here from the point of view of the human being and more precisely of the industrial operator. We assume the following working hypotheses: the operator’s task and environmental conditions are known and circumscribed; the operator is trained in the task, production tools and safety instructions; the task is repeated with more or less frequent intervals. We focus our proposals on assessing:

- the physical and cognitive fragility of operators in order to meet assistance needs;
- cognitive biases and physical constraints leading to a loss of operator safety;
- ergonomic, performance and acceptance of the production tool.

In the industrial context, the fields that best answer these questions are work ergonomics and cognitive sciences. Scientists typically work on 4 axes: physiological/biomechanical, cognitive, psychological and sociological. More specifically, we focus on biomechanical, cognitive and psychological aspects, as described by the ANACT [24], [26]. The aim here is to translate these factors into metrics, optimality criteria or constraints in order to implement them in our methodologies for analysis, design and control of the collaborative robot.

To understand our desired contributions in robotics, we must review the current state of ergonomic workstation evaluation, particularly at the biomechanical level. The ergonomist evaluates the gesture through the observation of workstations and, generally, through questionnaires. This requires long periods of field observation, followed by analyses based on ergonomic grids (e.g. RULA [42], REBA [32], LUBA [37], OWAS [36], ROSA [60],...). Until then, the use of more complex measurement systems was reserved for laboratories, particularly biomechanical laboratories. The appearance of inexpensive sensors such as IMUs (Inertial Measurement Units) or RGB-D cameras makes it possible to consider a digitalized, and therefore objective, observation of the gesture, postures and more generally of human movement. Thanks to these sensors, which are more or less intrusive, it is now possible to permanently install observation systems on production lines. This completely changes paradigms and opens the door to longitudinal observations. It should be noted that this is comparable to the evolution of maintenance, which becomes predictive.

On the strength of this new paradigm, *ergonomic robotics* has recently taken an interest in this type of evaluation to adapt the robot’s movements in order to reduce ergonomic risk scores. This approach complements the more traditional approaches that only consider the performance of the action produced by the human in interaction with the robot. However, we must go further. Indeed, the ergonomic criteria are based on the principle that the comfort positions are distant from the human articular stops. In addition, the notation must be compatible with an observation of the human being through the eye of the ergonomist. In practice, evaluations are inaccurate and subjective [63]. Moreover, they are made for quasi-static human positions without taking into account the evolution of the person’s physical, physiological and psychological state. The repetition of gestures, the solicitation of muscles and joints is one of the questions that must complete these analyses. One of the methods used by ergonomists to limit biomechanical exposures is to increase variations in motor stress by rotating tasks [61]. However, this type of extrinsic method is not always possible in the industrial context [40].

One of Auctus' objectives is to show how, through a cobot, the operator's environment can be varied to encourage more appropriate motor strategies. To do so, we must focus on a field of biomechanics that studies the intrinsic variability of the motor system allowed by the joint redundancy of the human body. This motor variability refers to the natural alternation of postures, movements and muscle activity observed in the individual to respond to a requested task [61]. This natural variation leads to differences between the motor coordinates used by individuals, which evokes the notion of motor strategy [33].

As shown by the cognitive dimension of ergonomics (see above), we believe that some of these motor strategies are a physically quantifiable reflection of the operator's cognitive state. For example, fatigue [57] and its anticipation or the manual expertise (dexterous and cognitive) of the operator which allows him to anticipate his movements over long periods of time in order to preserve his body, his performance and his pain.

3.1.2. Methodology

How can we observe, understand and quantify these human motor strategies to better design and control the behavior of the cobotic assistant? When we study the systems of equations considered (kinematic, static, dynamic, musculoskeletal), several problems appear and explain our methodological choices:

- the large dimensions of the problems to be considered, due to joint, muscle and placement redundancy,
- the variabilities of the parameters, for example: physiological (consider not an operator, but a set of operators), geometric (consider a set of possible placements of the operator) and static (consider a set of forces that the operator must produce);
- the uncertainties of measurement, model approximation.

The idea is to start from a description of redundant workspaces (geometric, static, dynamic...). To do this, we use set theory approaches, based on interval analysis [3], [48], which allow us to respond to the uncertainties and variability issues previously mentioned. In addition, one of the advantages of these techniques is that they allow the results to be certified, which is essential to address safety issues. Some members of the team has already achieved success in mechanical design for performance certification and robot design [44]. The adaptation of these approaches allows us to obtain a mapping of ergonomic and efficient movements in which we can project the operators' motor strategies and thus define a metric quantifying the sensorimotor commands chosen with regard to the cognitive criteria studied.

It is therefore necessary to:

- propose new indices linking different types of performance (ergonomic biomechanical robotics, but also influence of fatigue, stress, level of expertise on the evolution of performance);
- divide the gesture into homogeneous phases: this process is complex and depends on the type of index used and the techniques used. We are exploring several ways: inverse optimal control, learning methods, or the use of techniques from signal processing.
- develop interval extensions of the identified indices. These indices are not necessarily the result of a direct model, and algorithms need to be developed or adapted (calculation of manipulability, UCM, etc.).
- Aggregate proposals into a dedicated interval analysis library (use of and contribution to the existing ALIAS-Inria and the open source IBEX library).

The originality and contribution of the methodology is to allow an analysis taking into account in the same model the measurement uncertainties (important for on-site use of analytical equipment), the variability of tasks and trajectories, and the physiological characteristics of the operators.

Other avenues of research are being explored, particularly around the inverse optimal control [49] which allows us to project human movement on the basis of performance indices and thus to offer a possible interpretation in the analysis of behaviors.

We also use automatic classification techniques: 1) to propose cognitive models that will be learned experimentally 2) for segmentation or motion recognition, for example by testing Reservoir Computing [34] approaches.

3.2. Operator / robot coupling

3.2.1. Scientific Context

Thanks to the progress made in recent years in the field of p-HRI (Physical Human-Robot Interaction), robotic systems are beginning to operate in the same workspace as humans, which is profoundly changing industrial issues and allowing a wide variety of human-robot coupling solutions to be considered to perform the same task [25]. Different types of interactions exist. They can be classified in different ways: according to the degree of autonomy of the robot and its proximity to the user [31] with particularities for “wearable robots” [30], [29], or for collaborative robotics [62], or according to the role of the human being [58]. From a cognitive point of view, classifications are more concerned with autonomy, the complexity of information processing and the type of communication and representation of the human being by the robot [47], [64].

We proposed a classification of cobotic systems according to the configuration of the schema of interactions between humans, robots and the environment [45], [55].

The parameters of the coupling being numerous and complex, the determination of the most appropriate type of coupling for a type of problem is an open problem [50], [2], [46], [41]. The traditional approach consists in trying to identify and classify the various possible options and to select the one that seems most relevant with regard to the feasibility, efficiency, budget envelope and acceptability of the operator. One of the main objectives of our research project is to define a typology of cobots or cobotic systems in order to specify the methodology for developing the best solution: what are the criteria for defining the best robotic architecture, what type of coupling, what autonomy of the robot, what role for the operator, what risks for the human, what overall performance? These are the key issues that need to be addressed. To meet this methodological need, we propose an approach guided by experience on use cases obtained thanks to our industrial partners.

3.2.2. Methodology

Task analysis and human behavior modelling, discussed in the previous sections, should help to characterize the different types of coupling and interaction modalities, their advantages and disadvantages, in order to assist in the decision-making process. One of the ideas we would like to develop is to try to break down the task into a sequence of elementary gestures corresponding to simple motor actions performed in a clearly identified context and to evaluate for each of them the degree of feasibility in automatic mode or in robot assistance mode. The assessment must take into account a large number of parameters that relate to physical interactions, human-robot communication, reliability and human factors, including acceptability and impact on the valuation or devaluation of the operator’s work. Concerning the evaluation of human factors, we have already begun to work on the subject within the more general framework of human systems interactions by operating Bayesian networks, drawing inspiration from the work of [28], [56].

The adoption of assessment criteria for a single domain (e. g. robotics or ergonomics) cannot guarantee that the performance of this coupling will be maximized. From design to evaluation, cross-effects must be constantly considered:

- impact of the cobot design on the user’s performance: intuitiveness, adaptation to intra- and inter-individual variations, affordance, stress factors (noise, vibrations,...), fatigue factors (control laws, necessary attention,...) and motivation factors (effectiveness, efficiency, aesthetics,...);
- impact of user performance on cobot exploitation: risks of human error (attention error, perseveration, circumvention of procedures, syndrome outside the loop) [28].

In addition to purely physical assistance, some cobotic systems are designed to assist the operator in his decision-making. The issues of trust, acceptance, sharing of representations and co-construction of a shared awareness of the situation are then to be addressed [59].

3.3. Design of cobotic systems

3.3.1. Architectural design

Is it necessary to cobotize, robotize or assist the human being? Which mechanical architecture meets the task challenges (a serial cobot, a specific mechanism, an exoskeleton)? What type of interaction (H/R cohabitation, comanipulation, teleoperation)? These questions are the first requests from our industrial partners. For the moment, we have few comprehensive methodological answers to provide them. Choosing a collaborative robot architecture is a difficult problem [38]. It is all the more when the questions are approached from both a cognitive ergonomics and robotics perspective. There are indeed major methodological and conceptual differences in these areas. It is therefore necessary to bridge these representational gaps and to propose an approach that takes into consideration the expectations of the robotician to model and formalize the general properties of a cobotic system as well as those of the ergonomist to define the expectations in terms of an assistance tool.

To do this, we propose a user-centered design approach, with a particular focus on human-system interactions. From a methodological point of view, this requires first of all the development of a structured experimental approach aimed at characterizing the task to be carried out through a “system” analysis but also at capturing the physical markers of its realization: movements and efforts required, ergonomic stress. This characterization must be done through the prism of the systematic study of the exchange of information (and their nature) by humans in their performance of the considered task. On the basis of these analyses, the main challenge is to define a decision support tool for the choice of the robotic architecture and for the specifications of the role assigned to the robot and the operator as well as their interactions.

The evolution of the chosen methodology is for the moment empirical, based on the user cases regularly treated in the team (see sections on contracts and partnerships).

It can be summarized for the moment as:

- identify difficult jobs on industrial sites. This is done through visits and exchanges with our partners (manager, production manager, ergonomist...);
- select some of them, then observe the human in its ecological environment. Our tools allow us to produce a motion analysis, currently based on ergonomic criteria. In parallel we carry out a physical evaluation of the task in terms of expected performance and an evaluation of the operator by means of questionnaires.
- Synthesize these first results to deduce the robotic architectures to be initiated, the key points of human-robot interaction to be developed, the difficulties in terms of human factors to be taken into account.

In addition, the different human and task analyses take advantage of the different expertise available within the team. We would like to gradually introduce the evaluation criteria presented above. Indeed, the team has already worked on the current dominant approach: the use of a virtual human to design the cobotic cell through virtual tools [1]. However, the very large dimensions of the problems treated (modelling of the body’s ddl and the constraints applied to it) makes it difficult to carry out a certified analysis. We then choose to go through the calculation of the body’s workspace, representing its different performances, which is not yet done in this field. The idea here is to apply set theory approaches, using interval analysis and already discussed in section 3.1.2. The goal is then to extend to intervals the constraints played in virtual reality during the simulation. This would allow the operator to check his trajectories and scenarios not only for a single case study but also for sets of cases. For example, it can be verified that, regardless of the bounded sets of simulated operator physiologies, the physical constraints of a simulated trajectory are not violated. Thus, the assisted design tools certify cases of use as a whole. Moreover, the intersection between the human and robot workspaces provides the necessary constraints to certify the feasibility of a task. This allows us to better design a cobotic system to integrate physical constraints. In the same way, we will look for ways in which human cognitive markers can be included in this approach.

Thus, we summarize here the contributions of the other research axes, from the analysis of human behavior in its environment for an identified task, to the choice of a mechanical architecture, via an evaluation of torque and interactions. All the previous analyses provide design constraints. This methodological approach is perfectly integrated into an Appropriate Design approach used for the dimensional design of robots, again based on interval analysis. Indeed, to the desired performance of the human-robot couple in relation to a task, it is sufficient to add the constraints limiting the difficulty of the operator's gesture as described above. The challenges are then the change of scale in models that symbiotically consider the human-robot pair, the uncertain, flexible and uncontrollable nature of human behavior and the many evaluation indices needed to describe them.

3.3.2. Control design

The control laws of collaborative robots from the major robot manufacturers differ little or not at all from the existing control laws in the field of conventional industrial robotics. Security is managed a posteriori, as an exception, by a security PLC / PC. It is therefore not an intrinsic property of the controller. This quite strongly restricts the possibilities of physical interaction [0] and collaboration and leads to sub-optimal operation of the robotic system. It is difficult in this context to envision real human-robot collaboration. Collaborative operation requires, in this case, a control calculation that integrates safety and ergonomics as a priori constraints.

The control of truly collaborative robots in an industrial context is, from our point of view, underpinned by two main issues. The first is related to the macroscopic adaptation of the robot's behaviour according to the phases of the production process. The second is related to the fine adaptation of the degree and/or nature of the robot's assistance according to the ergonomic state of the operator. If this second problem is part of a historical dynamic in robotics that consists in placing safety constraints, particularly those related to the presence of a human being, at the heart of the control problem [31] [43], [35], it is not approached from the more subtle point of view of ergonomics where the objective cannot be translated only in terms of human life or death, but rather in terms of long-term respect for their physical and mental integrity. Thus, the simple and progressive adoption by a human operator of the collaborative robot intended to assist him in his gesture requires a self-adaptation in the time of the command. This self-adaptation is a fairly new subject in the literature [51], [52].

At the macroscopic level, the task plan to be performed for a given industrial operation can be represented by a finite state machine. In order not to increase the human's cognitive load by explicitly asking him to manage transitions for the robot, we propose to develop a decision algorithm to ensure discrete transitions from one task (and the associated assistance mode) to another based on an online estimate of the current state of the human-robot couple. The associated scientific challenge requires establishing a link between the robot's involvement and a given working situation. To do so, we propose an incremental approach to learning this complex relationship. The first stage of this work will consist in identifying the general and relevant control variables to conduct this learning in an efficient and reusable way, regardless of the particular method of calculating the control action. Physically realistic simulations and real word experiments will be used to feed this learning process.

In order to handle mode transitions, we propose to explore the richness of the multi-tasking control formalism under constraints [39] in order to ensure a continuous transition from one control mode to another while guaranteeing compliance with a certain number of control constraints. Some of these constraints are based on ergonomic specifications and are dependent on the state of the robot and of the human operator, which, by nature, is difficult to predict accurately. We propose to exploit the interval analysis paradigm to efficiently formulate ergonomic constraints robust to the various existing uncertainties.

Purely discrete or reactive adaptation of the control law would make no sense given the slow dynamics of certain physiological phenomena such as fatigue. Thus, we propose to formulate the control problem as a predictive problem where the impact of the control decision at a time t is anticipated at different time horizons. This requires a prediction of human movement and knowledge of the motor variability strategies it employs. This prediction is possible on the basis of the supervision at all times of the operational objectives (task in progress) in the short term. However, it requires the use of a virtual human model and possibly a dynamic simulation to quantify the impact of these potential movements in terms of performance, including ergonomics. It is impractical to use a predictive command with simulation in the loop with an advanced virtual manikin model. We therefore propose to adapt the prediction horizon and the complexity of the corresponding model in order to guarantee a reasonable computational complexity.

[0] In the ISO TS 15066 technical specification on collaborative robotics, human-robot physical interaction is allowed but perceived as a situation to be avoided.

The planned developments require both an approach to modelling human sensorimotor behaviour, particularly in terms of accommodating fatigue via motor variability, and validating related models in an experimental framework based on observation of movement and quantification of ergonomic performance. Experimental developments must also focus on the validation of proposed control approaches in concrete contexts. To begin with, the Woobot project related to gesture assistance for carpenters (Nassim Benhahib's thesis) and a collaboration currently being set up with Safran on assistance to operators in shrink-wrapping tasks (manual knotting) in aeronautics are rich enough background elements to support the research conducted. Collaborative research projects with PSA will also soon provide a larger set of contexts in which the proposed research can be validated.

4. Application Domains

4.1. Factory 4.0

The 4th industrial revolution (factory 4.0) is characterized by the integration of digital technologies into the production process, in order to meet the challenge of customizing services and products. This agility requires making manufacturing and maintenance lines flexible and versatile. This capacity for adaptation is the characteristic of the human being, which puts him at the center of the production apparatus. However, this can no longer be done at the expense of their health and well-being. How then can we reconcile the enhancement of our manual and analytical expertise, the ever desired increase in productivity and manufacturing quality, while reducing the hardship at work? Collaborative robotics, which we are seeking to build, is one of the central solutions to meet this societal challenge. By assisting humans in their most dangerous and painful tasks, it complements or replaces them in their phases of physical and cognitive fragility.

More generally, we are interested in workstation cobotization, in the manufacturing and assembly industry but also in the construction and craft industries. The application areas are related to regional needs in aeronautics, including maintenance, water and waste treatment. In most of these cases, it is possible to define the tasks, evaluate the stakes and added value of our work.

5. Highlights of the Year

5.1. Highlights of the Year

- Jean-Marc Salotti has been elected Member of the International Academy of Astronautics
- The startup Touch Sensity [0] has been created by Ganna Pugach.

6. New Software and Platforms

6.1. HuMoSoft

Human Motion Analysis Software

KEYWORDS: Movement analysis - 3D movement

FUNCTIONAL DESCRIPTION: HuMoSoft is based on the ROS platform. The acquisition data can come from different depth sensors, for example Kinect, via the Nuitrack JDK. An extended Kalman filter has been implemented, and motion analysis uses the RULA method.

- Authors: Jessica Colombel and David Daney
- Contact: Sylvain Pion
- URL: https://gitlab.inria.fr/auctus/kombos-server

[0] http://touchsensity.com/

6.2. KCADL

Kinematic Chain Appropriate Design Library

KEYWORDS: Interval analysis - Uncertainty - Kinematics

FUNCTIONAL DESCRIPTION: Software for the modelling and analysis of imprecise serial kinematic chains. Chain objects are built by iteratively adding rigid-body segments with associated joint connections (e.g., fixed, revolute, prismatic). Several standard options are provided to model each segment (e.g., Denavit-Hartenberg parameters, transformation matrices, twists). Each option accepts interval and non-interval arguments, allowing to model the uncertainties and variabilities of imprecise serial kinematic chains and also the conventional precise serial kinematic chains. Forward Kinematic (FK) and Inverse Kinematic (IK) solvers are available for Chain objects. The FK solver computes an outer bound of the set of poses associated with a set of joint configurations. The IK solver computes an outer bound of the set of joint configurations associated with a set of poses.

- Participant: Joshua Pickard
- Contact: Joshua Pickard
- Publication: hal-02367664, version 1
- URL: https://gitlab.inria.fr/auctus/kinematic-chain-appropriate-design-library

6.3. AUCTUS-MOVER

AUCTUS panda MOVER project

KEYWORDS: Automatic control - Variability

FUNCTIONAL DESCRIPTION: Software for controlling the Franka Emika Panda robot to study human motor variabilities. Consists of a torque-based controller for the Franka Emika Panda collaborative robot with the following actuation modes: auto mode - the robot follows a predefined trajectory, manual mode - the robot is in a constrained gravity compensation mode (the constraints may be adapted online). A graphical interface allows the operator to switch between modes. Software for calibrating the robot with respect to the Optitrack motion capture system is also included.

- Contact: Joshua Pickard
- URL: https://gitlab.inria.fr/auctus/auctuspanda/tree/mover_project

6.4. AUCTUS-RT

AUCTUS - Redunancy Tubes

KEYWORD: Variability

FUNCTIONAL DESCRIPTION: Software for modelling and analyzing human motor variabilities along a path. Currently used to study the redundant motions associated with the upper limb. Anatomical constraints for the shoulder, elbow, and wrist may be customized for a human subject using: maximal and minimal bounding regression equations, spherical polygon constraints. A constrained imprecise kinematic model of the subject is obtained and the task redundancies and joint redundancies associated with the constrained imprecise kinematic model are able to be evaluated via branch-and-bound exploration to determine achievable and non-achievable redundant motions of the human. For n redundant degrees-of-freedom, this provides an n-dimensional redundant workspace describing the human's capabilities. Along a path, this provides an (n+1)-dimensional redundant workspace tube.

- Contact: Joshua Pickard
- URL: https://gitlab.inria.fr/auctus/redundancy-tubes

6.5. WoobotSim

KEYWORDS: Robotics - Dynamic Analysis

FUNCTIONAL DESCRIPTION: WoobotSim is a simulator that reports the dynamics of the parties involved in an industrial task implying a strong interaction between a machine tool, an operator and a handled object, it also offers the possibility to add a cobot as an actor. Developed on Matlab, this simulator allows to visualize the efforts exchanged by the participants during the task, as well as the dynamics of the object being manipulated. For the specific case of woodworking shaper. It includes a wood cutting model. A model of task control by the craftsman and a model of the robot.

- Contact: Nassim Benhabib

6.6. Arcol

The Arcol platform provides technical support for the short, medium and long term experimental developments carried out within the framework of Auctus' scientific and dissemination activities.

These technological developments are essentially software related in the context of human motion capture and real-time control of collaborative robots. Arcol aims at easing their implementation, deployment, documentation and support.

Implementations include:

- a software component for online estimation of the state of one or more human "subjects" of a collaborative robotics experiment; ǐsualization tool for replaying a number of simulated experiments;
- an integrating architecture allowing the simple addition of hardware components (sensors, robots,...) and the configuration of an experiment by describing the hardware components included, the nature of the treatments to be performed and the history files (logs) to be constituted.

To date the work done is:

- help and realization of an experimental setup for the study of the motor variability of a user ;
- assistance and realization of an experimental setup for the study of the interaction wrenches during a machining task of a piece of wood in an industrial context ;
- implementation and deployment of a method for using Inria integration tools for the team's code ;
- development of a solution allowing to simply interface the ROS framework with the Unity3D software, in a modular and easily deployable experimentation perspective.

7. New Results

7.1. Posture and motion capture by smart textile

The objective of Postex is to design an intelligent textile jacket, without the use of additional sensors, to determine an operator's posture.

Since 2017, we offer an innovative solution based on the electrical properties of a conductive stretch fabric that is used in the manufacture of an intelligent garment. We use Electrical Impedance Tomography (EIT) to identify fabric deformations. A neural network is used to correlate the different postures and movements measured using a reference device with the electric field measured in the intelligent textile.

By 2018, we had successfully identified the movements of an elbow and then filed a patent under the number FR1860192. In 2019, we identified the shoulder and worked on the design of the fabric parts. In order to valorize the technology, the Touch Sensity startup was created at the end of 2019.

7.2. Set-based evaluation of robot capabilities

Set-based approaches allow to model serial mechanisms with varying levels of geometric uncertainties. The Kinematic Chain Appropriate Design Library (KCADL) has been created for the purpose of modelling imprecise serial kinematic chains and provides numerous certified methods, implemented using the IBEX interval analysis library, for analyzing the capabilities of these modelled mechanisms. The KCADL software provides a set of public routines to build arbitrary serial mechanisms by incrementally adding rigid-body segments with associated parent-child uncertainties. Efficient Forward Kinematic (FK) and Inverse Kinematic (IK) solvers have been formulated and integrated into the software. These solvers are fully compatible with set-based inputs and are capable of handling sets of poses or sets of joint configurations. In addition to the FK and IK solvers, analysis routines which are applicable to imprecise kinematic chains with set-based inputs are also implemented in the software (e.g., evaluating the mechanism's: force/velocity/acceleration capabilities, precision). These routines provide offline analysis and design tools as well as online real-time capable tools for reliably evaluating current and future capabilities.

7.3. Redundancy tube

A set-based approach for modelling the human upper-limb and its complex articular constraints as a 7-degree-of-freedom (dof) constrained imprecise kinematic chain is formulated and implemented in the AUCTUS-RT software. This software allows to easily customize the geometric parameters and articular constraints. This permits to adapt the upper-limb model to each unique human subject and may also be used to model sets of human subjects. Various visualization tools are available for Python and Matlab to aid in the selection of appropriate articular constraints. When given a task with m redundant dofs and the desired workspace resolution, the software is capable of computing certified inside and outside regions of the (m+1)-dimensional redundant workspace associated with the task and upper-limb model. When a temporal dimension is added to the task description, the redundant workspace varies over time and produces a tube of redundant motions, which we refer to as the redundancy tube. The software accepts spatial-temporal task descriptions and allows to compute the full redundancy tube or slices of the tube. Furthermore, the software allows to model individual and/or sets of trajectories to describe tasks exactly or with varying level of uncertainties. Much effort has been put into improving the efficiency of the redundancy tube evaluations and parallel computing, both locally and non-locally via PlaFRIM, using OpenMP is supported. The AUCTUS-RT software is currently being used for the ongoing study of human motor-variabilities for the AUCTUS Mover project.

Related publications: [16]

7.4. Mover project

The Mover project is an experiment-based project to evaluate and study the links between human motor-variability, expertise, and fatigue associated with repetitive tasks. A wireloop game serves as the experimental task where a human subject is tasked with moving a metal ring along a fixed conductive wire while trying to maximize a score which is a function of the task time and the number of ring-wire contacts. To more easily study motor-variabilities, the wireloop ring is actively constrained by a collaborative robot (the Frank Emika Panda), allowing to isolate desired task variabilities and easily modify the task (e.g., through applied disturbances, changes in robot stiffness, task guidance). A preliminary version of the experiment is currently being developed to test all aspects of the project (i.e., experimental protocol, robot control, motion capture, human modelling, and redundancy tube evaluation). All experimental aspects of the project will be finalized before March 2020.

7.5. Interactions with a chatbot

In the context of the CIFRE Orange PhD work by Nicolas Simonazzi under the supervision of Jean-Marc Salotti and with the objective of analyzing and identifying emotions during interactions with a chatbot, a first experiment was conducted. It involved a user, the use of a smartphone, viewing videos and asking questions about the content of the video and the feeling of the user just after the answer. The collected data were numerous: the accuracy of the answers to the questions, the emotional feeling (choice of emoticons by the user) as well as the real-time measurements of the accelerometer of the smartphone. An analysis of the data was carried out with Russell's relatively simple emotional model as an explanatory framework based on two variables, the positive or negative valence of the emotion, and the degree of excitement. The experimental results showed that there was a slight correlation between the valence indicated by the user, the accuracy of the answers to the questions and the accelerations of the smartphone. However, it was hoped that the videos would have an impact on the valence, because their content had an intrinsic valence, but it proved impossible to find a correlation with the valence indicated by the user, probably due to a lack of the user engagement and also because of the focus on the questions that followed and the accuracy of the answers. A new experimental protocol is currently being studied with a priori more impactful videos (likely to produce an emotion with a greater degree of excitement).

Related publications:[10], [19]

7.6. Prediction of human error in robotics

The INRS provides a database of accidents at work, from which we can extract those concerning robotics. Many accidents are due to a deterioration of situational awareness. However, as there are many different causes and human factors are not well understood, it is very difficult for experts to provide probabilistic risk assessments. We proposed to simplify the problem by classifying the accidents according to the main demons that degrade the consciousness of the situation (Endsley model) and to use a Bayesian approach with the Noisy-Or nodes. We had already tried such an interpretation in the field of aeronautics. We propose to extend it to the field of robotics. Even if the approach remains empirical and approximate, it is possible to infer general probabilities of risk of human error leading to accidents and to deduce actions to reduce risks.

Related publications: [18]

7.7. Securing industrial operators with collaborative robots: simulation and experimental validation for a carpentry task

In this work, a robotic assistance strategy is developed to improve the safety in an artisanal task that involves a strong interaction between a machine-tool and an operator. Wood milling is chosen as a pilot task due to its importance in carpentry and its accidentogenic aspect.

In order to analyze the wood milling task, a wood shaping training was conducted in collaboration with a carpentry learning institute which allowed to collect information related to the task (perceived effort, position of the operator, accident circumstances).

To analyze the human-machine interaction, a formalization of the problem as a dynamic exchange of spatial forces inspired by the grasping theory has been performed. This theory presents structural similarities with the studied task. Based on this formalization, a behavior simulator of the system "wood + human + tool" has been developed.

To propose a credible and a realistic assistance solution, accidentogenic situations are simulated (see Woobot-sim). Based on the observation made with these simulations, the use of a collaborative robot to secure wood instability cases has been explored and validated by an experiment. An operational space damping behaviour appears to be the most appropriate solution to improve safety in the studied cases.

The experiment was designed to reproduce two cases of instability during a carpentry milling task based on the entry and exit of the tool into and out of a wood node. For safety reasons, the experiment is performed on a safe but tangible simulation of the task. We then show how a robot ((Franka Emika's Panda, 7-DOF)) controlled in torque can instantly stabilize the wood to avoid an accident without modifying the carpenter's sensations.

Related publications: [22]

7.8. A software architecture for the control of a 7 dof robot for the conduct of several experiment

The Franka Emika Panda robot is a 7 dof robot. Using the Robot Operating System (ROS), an experimental setup has been built to exploit this robot. The experimental setup consists in:

- the Panda robot;
- several RGBD sensors (Kinects);
- a safety laser scanner.

Dedicated algorithms have been developed to exploit the capacities of the Kinects to visualize the environment surrounding the robot and compute the distance to the closest obstacle. Several Kinects can be used simultaneously. Specific drivers have been developed to exploit the data given by the laser scanner to also determine the closest distance between a human and a robot.

Within the framework of Arcol (see 6.6) A software architecture has been developed to ease the development of different controllers. The robot can be controlled in joint position, velocity and torque using standard state-of-the-art control technique or constrained convex optimization methods. Trajectories can be easily defined, played, and modified at run time. The robot can be simulated using the GAZEBO dynamic simulator or run on the real robot with similar behaviours. All this software architecture works on a real-time patched computer.

7.9. Modulation of the robot velocity capabilities according to the distance to a human

Using the setup described in 7.8, a controller has been defined to constrain the robot maximum velocity according to the distance to a human. The aim of this work is to be able to use the robot optimally at all time. When a human comes near the robot workspace, the robot must stop to avoid any dangerous interaction. Several strategies exist to reduce the robot velocity as a function of the distance to the human. In this work, the goal is to determine the maximum deceleration capabilities of the robot in real time and determine if the robot has the capacity to stop before a contact. If not, the maximum allowable joint velocities of the robot are reduced. When the human reaches the robot workspace, these joint velocities must be null to ensure safety. Simply reducing the joint velocity of the robot without modulating the trajectory would induce a bad tracking of the robot task. Hence, the trajectory is updated in real time to take into account the capacities of the robot. This work has been submitted for publication at the ICRA 2020 conference.

Related publications: [23]

7.10. Human motion analysis in ecological environment

The estimation of human motion from sensors that can be used in an ecological environment is an important issue being it for home assistance for frail people or for human/robot interaction in industrial contexts. We are continuing our work on data fusion from RGB-D sensors using extended Kalman filters. The original approach uses a biomechanical model of the person to obtain anthropomorphically constrained joint angles to make their estimation physically coherent. In addition, we propose a method for the optimal adjustment of the covariance matrices of the extended Kalman filter. The proposed approach was tested with six healthy subjects performing 4 rehabilitation tasks. The accuracy of the joint estimates was evaluated with a reference stereophotogrammetric system. Our results show that an affordable RGB-D sensor can be used for simple home rehabilitation when using a constrained biomechanical model. This work has led to the writing of an article now in submission to the MBEC (Medical & Biological Engineering & Computing).

In a second step, we compared the joint centre estimates obtained with the new Kinect 3 (Azure Kinect) sensor, the Kinect 2 (Kinect for Windows) and a reference stereophotogrammetric system. Regardless of the system used, we have shown that our algorithm improves the body tracker data. This study also shows the importance of defining good heuristics to merge the data according to the body tracking operation. This study is submitted for publication at ICRA 2020.

7.11. Human motion decomposition

The aim of the work is to find ways of representing human movement in order to extract meaningful physical and cognitive information.

After the realization of a state of the art on human movement, several methods are compared: principal component analysis (PCA), Fourier series decomposition and inverse optimal control.

These methods are used on a signal comprising all the angles of a walking human being. PCA makes it possible to understand the correlations between the different angles during the trajectory. Fourier series decomposition methods are used for a harmonic analysis of the signal. Finally, inverse optimal control sets up a modeling of the engine control to highlight qualitative properties characteristic of the whole motion. These three methods are tested, combined and compared on data from the EWalk database (http://gamma.cs.unc.edu/GAIT/#EWalk) in order to test emotion recognition based on these decompositions and simple classifiers.

7.12. New method for cobotic task evaluation

Two industrial studies allowed us improving our methodology for cobotic task evaluation.

- Thanks to the partnership with Suez and the work of ENSC student Nina Docteur under Auctus supervision, there are several interesting results: first, the methodological approach has been reinforced. There was a detailed analysis of an accident-prone gesture (the pipe cover raising), meetings with field agents, supervisory teams, discussions with SUEZ ergonomic expert and field observations. Second, there was a theoretical framework - a model - for the general evaluation of a cobotic task, as well as the exploration of rules for evaluating the components of this model. Five main components have been proposed for the evaluation: bio-mechanics, cognitics, usability, hedonism and social impact. An important difficulty was to mix every component and to unify the evaluation. In order to mature the model, it has been decided to carry on the partnership with a PhD work.
- The PORTAGE project (Plateforme de RoboTisation et d'Automatisation GénériquE de bâtis industriels) involves AKKA Technologies, Ez-Wheel, IIDRE and IMS laboratory. It aims at developing semi-autonomous solutions for moving heavy structures within industrial environments (e.g. aircraft industry). Our contributions is concerned with human-robot interactions, and especially accounting for real-life constraints of operators' job within their industrial environment, and translate them into design choices and requirements for the to-be-developed robotic solution. In order to identify relevant elements from the work situation, three Human Factors models have been used: Reason's model [54], Situation Awareness model [27], and Skill Rule Knowledge (SRK) model [53]. The Reason's model details the different layers to explain accidents, notably in the aircraft industry. These layers gather equipment, procedure, training, management, policies and even psychological precursors of the operator. Therefore, this model allows investigations on potential latent causes of accident in complement with "obvious" patent causes usually more easily identified. The Situation Awareness model of Endsley describes cognitive mechanisms involved in a given situation for a person when performing actions, based on 1) the perception of elements of the current situation, 2) the understanding of the current situation, and 3) the projection of the future status of the situation. This model leads to identifying 8 daemons where situation awareness can be deteriorated, potentially resulting in accidents. The SRK model describes the decision process of an operator (or any person) performing a given task, based on his/her familiarity with this task. This model, coupled with the Situation Awareness model, can be leveraged to identify elements to be accounted when developing collaborative robots in industrial environments.

7.13. Situation awareness analysis

Baptiste Prébot, PhD student under the direction of Jean-Marc Salotti developed a methodology to analyze and assess representation sharing and situation awareness in groups of humans, possibly involving robots or artificial intelligence systems. An experiment has been carried out with two persons and a vehicle. The first person was assigned the role of mission control and the second person the role of an astronaut driving a vehicle using a real driving interface but in a simulated environment (surface of Mars in virtual reality). The two persons were located in different rooms and could communicate only by voice. Mission control had to guide the driver to a specific location. Every minute, the experiment was stopped and the two persons were asked to make a cross on a map corresponding to what they believe was the location of the vehicle. Comparisons of crosses on the maps, including ground truth locations, enabled us to determine the exactness of the localization and the degree of correct sharing of the situation. This experiment helped us better understanding communication and sharing issues, which are particularly relevant for the design of tasks and procedures for robotic operations.

Related publications:[12], [13], [9]

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral collaboration with SAFRAN EP

An industrial collaboration has been initiated with SAFRAN EP (Villemur-sur-Tarn) on the analysis of manual industrial activities for the improvment of working conditions in highly demanding tasks. Vincent Padois and Jean-Marc Salotti have supervised the internship of Gaëlle Lannuzel who was focusing on knot tying activities for electrical cables. A CIFRE PhD thesis is being discussed to pursue this work.

8.2. Bilateral collaboration with SUEZ

A contract has been signed with Suez (see 7.12) for a 6-month internship under Auctus supervision (David Daney and jean-Marc Salotti). The objective was the development of a new method to improve strenuous manual activities and an implementation of the method for the specific activity of pipe cover raising. This study has been performed by Nina Doctor, ENSC student (recruitment February - September 2019).

8.3. Bilateral collaboration with PSA

An industrial collaboration has been initiated with PSA on the synthesis and dynamic analysis of shared workspaces for safety in collaborative robotics. A CIFRE PhD thesis has been approved by ANRT and will start in February 2020.

9. Partnerships and Cooperations

9.1. Regional Initiatives

9.1.1. Woobot

The main objective of Woobot is to propose a methodology for designing and controlling a collaborative robotic system to assist and secure an operator's actions. The system must preserve the health and sensory expertise of the operator while guaranteeing his or her mobility. Motivated by a pilot case from carpentry, the determination of the behavior of the collaborative robot will be based on a human-centered approach and based on a precise ergonomic analysis of the task and the biomechanical performances and needs of the operator. Two scientific issues are important: the choice of the system architecture (type of collaborative robot, number of degrees of freedom, level of redundancy with respect to the task, type of interaction of the collaborative robot with the task and/or the human...), and the behavior of the collaborative robot that must be implemented in the control. To answer these questions, it is then necessary to consider in the same formalism the human and task constraints from the point of view of:

- of the performance necessary for the task (cutting forces, trajectories);
- of the operator's biomechanical performance (kinematics -i.e. dexterity; static -i.e. manipulability and human dynamics).
- ergonomic (task, work environment, human posture).

Other partners: Région Nouvelle-Aquitaine, BTP CFA Blanquefort [0], Aerospline [0]

9.1.2. Portage

The global objective of this project is to develop a semi-autonomous carrier dedicated to the transport of heavy structures in industrial factories. The Auctus team has been assigned the role of task analysis and human systems interactions analysis in order to determine the best interface, to improve ergonomics, to reduce risks and to account for acceptability. A postdoctoral student, Charles Fage, has been recruited for the first year of the study.

A 2-years contract (2019-2021) has been signed with AKKA Technologies as part of a consortium, which included two other companies, IIDRE and Ez-Wheel, and another research team from IMS laboratory.

9.2. European Initiatives

Program: COVR (https://safearoundrobots.com/)

Project acronym: HARRY[2]

Project title: **H**ighly s**A**fe **R**obot integ**R**ation for the industr**Y** throug**H** an **A**dvanced cont**R**ol and monito**R**ing strateg**Y**

Duration: 2019/07 – 2020/03

Coordinator: Vincent Padois

Other partners: RoBioSS [0], PPRIME (Poitiers, France), Fuzzy Logic Robotics [0] (Paris France)

Abstract: he objective of the HARRY2 project is to attain more advanced workspace sharing capabilities through fully exploiting the collaborative possibilities defined by ISO TS 15066. We will achieve this by:

- Developing PLC software and motion controllers using robot-agnostic industrially-rated components to ease and standardize the development of safe robotic applications with workspace sharing.
- Integrating state-of-the-art energy-based control algorithms using these industrial hardware components, so that safety is no longer treated as an exception but considered as a constraint when computing the control solution in real-time.
- Enabling the use of high-level and intuitive teaching interfaces reducing robot programming time and difficulty.
- Developing a systematic and practical methodology for quantitative safety evaluation.

9.3. International Initiatives

9.3.1. Inria International Partners

- Vincent Padois is collaborating with Alessandro Saccon from TU Eindhoven regarding research activities on the modeling and control of robots physically interacting with their environments and more specifically on impact models for such interactions. A ICRA 2020 paper has been submitted based on this collaboration [21].
- Jean-Marc Salotti worked with Ephraim Suhir, Departments of Mechanical and Materials Engineering and Electrical and Computer Engineering, Portland State University. Ephraim Suhir is a world expert in systems reliability. He and Jean-Marc Salotti worked on human-in-the-loop issues and published a paper in an IEEE conference [14].

[0] http://www.btpcfa-aquitaine.fr
[0] https://www.aerospline.eu
[0] https://www.pprime.fr/?q=fr/robioss
[0] https://www.flr.io

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events: Organisation

Jessica was member of the organizing committee of the Young Researchers' Day in Robotics 2019 (Journée Jeunes Chercheurs en Robotique) in Vittel, France the 14th October.

10.1.2. Member of the Conference Program Committees

- Journées Nationales de la Recherche en Robotique (JNRR) 2019. [David Daney, scientific Program Committee member]
- 44ème Congrès de la Sociéte de Biomécanique [Vincent Padois, scientific committee member]
- IROS 2019 (IEEE/RSJ International Conference on Intelligent Robots and Systems) [Vincent Padois, associate editor]
- ICRA 2020 (IEEE/RAS International Conference on Robotics and Automation) [Vincent Padois, associate editor]

10.1.3. Reviewer Activities: conferences

- ICRA 2020 (IEEE International Conference on Robotics and Automation) [Vincent Padois, David Daney, Lucas Joseph]
- IROS 2019 (IEEE/RSJ International Conference on Intelligent Robots and Systems) [David Daney, Vincent Padois, Jessica Colombel]
- ECC 2019 (European Control Conference) [Vincent Padois]
- 44ème Congrès de la Sociéte de Biomécanique [Vincent Padois]
- IEEE International Workshop on Metrology for Aerospace, Torino, June 2019 [Jean-Marc Salotti]
- CableCon 2019 @ 15th IFToMM World Congress, June 30 – July 4, 2019, Krakow, Poland [David Daney]

10.1.4. Reviewing Activities: journal

- ASME Journal of Mechanisms and Robotics [David Daney, Joshua Pickard]
- Mechanism and Machine Theory [David Daney]
- IEEE Robotics and Automation Letters [Vincent Padois, Jessica Colombel]
- IEEE Transactions on Human-Machine Systems [Vincent Padois]
- IEEE Transactions on Robotics [Vincent Padois]
- Acta Astronautica [Jean-Marc Salotti]
- Foresight [Jean-Marc Salotti]
- Behavioural Brain Research [jean-Marc Salotti]
- Computer Aided Geometric Design [Joshua Pickard]

10.1.5. Talks / Invited Talks

- David Daney – "Designing the collaborative robotics cells", Eighth International Congress on Design and Modeling of Mechanical Systems (CMSM'19), March 18-20, 2019 Hammamet, Tunisia.
- David Daney – "Concevoir les cellules de robotique collaborative du futur", Colloque Augmentation de l'Humain, Talence, 28-29 mars 2019
- Vincent Padois – "Sécurité et Robotique collaborative: n'oublions pas la commande!" – États Généraux de la Robotique – 2019/03/07

- Lucas Joseph – “HARRY2: développement d’un contrôleur de robot industriel répondant à des contraintes de sécurité basées sur un critère énergétique” – Journée GDR Robotique “GT3 - GT6”: “Conception et contrôle pour la manipulation sûre et flexible” – 2019/09/27– CEA LIST Centre Nano-Innov-Palaiseau
- Vincent Padois – “Quelques problématiques sous-jacentes en Robotique collaborative” – Journées Nationales de la Recherche en Robotique – 2019/10/15
- Nassim Benhabib – “Methodology for designing and controlling a collaborative robotic system to assist and secure an operator’s gestures” – Journées Nationales de la robotique Humanoïde) – 2019/11/{25,26} – LAAS, Toulouse
- Lucas Joseph, Vincent Padois – “HARRY2: développement d’un contrôleur de robot industriel répondant à des contraintes de sécurité basées sur un critère énergétique” – Launch of the ANR LabCom MACH4 between Iteca and PPrime – 2019/11/7 – Poitiers, France
- Joshua Pickard – “Appropriate Synthesis of a Crank-Rocker Linkage” World Congress of the International Federation for the Promotion of Mechanism and Machine Science (IFToMM), June 30 - July 4, 2019, Krakow, Poland
- Joshua Pickard – “Redundancy Tubes: Modelling Individual and Group Range-of-Motions Along a Path” 44 ème congres societe de biomecanique 28-30 octobre 2019, Poitiers, France

10.1.6. Leadership within the Scientific Community

- Vincent Padois is, together with Olivier Stasse from LAAS, the co-animator of GT7 “Humanoid Robotics” of the CNRS “Groupement de Recherche en Robotique” (GDR). The role of animator consists in organizing regular workshops in humanoid robotics with the members of the French research community in this domain. It also consists in reporting strategic elements to the GDR in order to better organize the structure of research in Robotics in France.

10.1.7. Scientific Expertise

- Vincent Padois is a reviewer for the 2nd European COVR call.
- Vincent Padois and David Daney are reviewers for the best PhD thesis award of GDR Robotique.
- David Daney is an expert of “Robot Boost” Nouvelle-Aquitain’s progam.
- Jean-Marc Salotti and David Daney are official animators of the Humans Systems Interactions AESE DAS (Strategic Activities Domain of the Aerospace Valley Pole), which gathers all regional actors concerned with human factors, human systems interactions, and collaborative robotics mainly in the aerospace sector, but not limited to that domain. At least 2 daily workshops are organized each year for the members of the group in order to focus on a specific issue. Jean-Marc Salotti and David Daney are also solicited to examine regional projects linked to the DAS in order to provide advice and eventually to participate to the labelling process of the pole.
- The Auctus team is involved in the “Aquitaine robotics” cluster, which brings together robotics players in Nouvelle-Aquitaine. David Daney and Jean-Marc Salotti respectively represent Inria and Ensc on the board of directors. David Daney is a member of the executive board. David Daney and Jean-Marc Salotti are respectively president and vice-president of the labelling committee which promotes all robotics projects for the Nouvelle-Aquitaine region.

10.1.8. Research Administration

- Sylvain Pion represents the Auctus team in the CUMI-R (Comité des Utilisateurs des Moyens Informatiques) committee of Inria Bordeaux.
- Jean-Marc Salotti participated to the Inria Committee directed by Clair Poignard and dedicated to the selection of research candidates for delegations, PhD and Postdoctoral positions.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

Master: Jean-Marc Salotti, Intelligence Artificielle, 103,5h éqTD, M1, Ecole Nationale Supérieure de Cognitique / Bordeaux INP, France

Master: Jean-Marc Salotti, Facteurs Humains et Ingénierie Cognitique, 15h éqTD, M1, Ecole Nationale Supérieure de Cognitique / Bordeaux INP, France

Master: Jean-Marc Salotti, Interactions Hommes Robots, 15h éqTD, M2, Ecole Nationale Supérieure de Cognitique / Bordeaux INP, France. In this course, all students have practical works involving cobotic systems: programming NAOs and UR3 (Universal Robots) and testing an exoskeleton.

Master: David Daney, Interactions Hommes Robots, 2h éqTD, M2, Ecole Nationale Supérieure de Cognitique / Bordeaux INP, France.

Master: David Daney, Mathématiques pour la robotique, 30h éqTD, M2, Enseirb/Ensc, Bordeaux INP, France.

Master: David Daney, Décision, 7h éqTD, M2, Ecole Nationale Supérieure de Cognitique / Bordeaux INP, France.

Master: Vincent Padois, Literature review - What, Why and How?, 20h éqTD, M2, Enseirb/Ensc, Bordeaux INP, France.

Master: Vincent Padois, Enjeux technologiques de la maintenance aéronautique, 6h éqTD, M1, Enseirb-Matmeca, Bordeaux INP, France.

Master: Vincent Padois, Maintenance du futur - Cours introductif, 2h éqTD, M1, ENSPIMA, Bordeaux INP, France.

Master: Nassim Benhabib, Interactions Hommes Robots, 15h éqTD, M2, ENSC, Bordeaux INP, France.

Master: Jessica Colombel, Robot Operating System, 10h éqTD, M2, Enseirb/Ensc, Bordeaux INP, France.

Master: Charles Fage, Cognitive Disabilities and Assistive Technologies, , M2, Master de Sciences cognitives et Ergonomie, Université de Bordeaux, France.

Master: Charles Fage, Human-Computer Interactions, 15h éqTD, M1, Master de Sciences cognitives et Ergonomie, Université de Bordeaux, France.

Licence: Charles Fage, Disabilities Management and Ethics, 15h éqTD, L2, Licence de MIASHS, Université de Bordeaux, France.

Licence: Charles Fage, Alternative and Augmentative Communication, 15h éqTD, 2ème année, Institut de formation en ergothérapie de Bordeaux, France.

Licence: Charles Fage, Autism and Developmental Disorders, 15h éqTD, 2ème année, Institut de formation en ergothérapie de Bordeaux, France.

Licence: Charles Fage, Aging and Assistive Technologies, 15h éqTD, 2ème année, Institut de formation en ergothérapie de Bordeaux, France.

10.2.2. Supervision

PhD: Jonathan Savin, "Modeling motion variability using virtual humans for the ergonomic evaluation of work stations", Sorbonne Université, 2019/11/22, Philippe Bidaud (Onera / Sorbonne Université) and Jacques Marsot (INRS) and Vincent Padois;

PhD: José Pedro Pontes, "Optimization and adaptation of robot locomotion in varying conditions: an evolutionnary approach", Sorbonne Université, 2019/3/12, Stéphane Doncieux (Sorbonne Université) and Vincent Padois and Cristina Santos (U. Minho, Portugal);

PhD in progress: Quoc Bach Hoa (Thèse ED SMAER, Paris), "Biomechanically plausible simulations of healthy and altered human locomotion", September 2017–, Vincent Padois and Faiz Ben Amar (Sorbonne Université)

PhD in progress: Nassim Benhabib (Inria / Région NA – Woobot project), “Méthodologie de conception et de commande d’un système robotique collaboratif pour assister et sécuriser les gestes d’un opérateur”, November 2018 – , David Daney and Vincent Padois;

PhD in progress: Jessica Colombel (Inria), “Analyse du mouvement humain pour l’assistance à la personne”, February 2019 – , François Charpillet and David Daney (Inria Nancy Grand-Est);

PhD in progress: Nicolas Simonazzi (CIFRE Orange), “Analyse comportementale et détection des émotions dans le cadre de l’utilisation de chat-bots en ligne”, May 2018 –, Jean-Marc Salotti;

PhD in progress: Baptiste Prébot (DGA), “Partage des représentations et de la conscience de situation”, January 2017 –, Jean-Marc Salotti and Bernard Claverie (ENSC, IMS laboratory;

PhD in progress: Olfa Jema (Cotutelle Université de Sousse, Tunisie), “Analyse du mouvement humain”, December 2017 –, Lotfi Romdhane, Sami Bennour, David Daney;

PhD in progress: Pierre Laguillaumie (Thèse laboratoire PPRIME), “Méthodologie pour la mise en œuvre d’un robot collaboratif de nouvelle génération prenant en compte la sécurité et le confort biomécanique de l’opérateur en situation de travail”, March 2018 – Jean-Pierre Gazeau and Vincent Padois.

10.2.3. Juries

Vincent Padois:

- HdR: Adrien Escande, “Numerical Optimization and Motion Generation in Robotics”, Université de Montpellier, 2019/2/25;
- PhD: Nolwenn Briquet-Kerestedjian, Reviewer, “Impact detection and classification for safe physical Human-Robot Interaction under uncertainties”, Université Paris-Saclay, 2019/7/10;
- PhD: Kai Pfeiffer, Examinor, “Efficient Kinematic and Algorithmic Singularity Resolution for Multi-Contact and Multi-Level Constrained Dynamic Robot Control”, Université de Montpellier, 2019/12/4;
- PhD: Sonny Tarbouriech, Reviewer, “An energetic approach to safety in robotic manipulation”, Sorbonne Université, 2019/12/5.

David Daney:

- PhD: Mathias Bordon, Examinor, “Modélisation et calibration pour une numérisation robotisée”, 2019/06/06, École Normale Supérieure Paris-Saclay
- PhD: Thomas Le Mézo, Reviewer, “Bracketing largest invariant sets of dynamical systems; An application to drifting underwater robots in ocean currents”, 2019/12/05, ENSTA Bretagne;
- PhD: Étienne Picard, Reviewer, “Modeling and robust control of cable-driven parallel robots for industrial applications”, 2019/12/17, Université Bretagne Loire .

Jean-Marc Salotti:

- PhD: Damien L’Haridon, Reviewer,“Décision collective optimisée en milieu extrême: application aux situations inconnues en vol spatial habité”, ISAE - Université de Toulouse, 2019/05/02
- PhD: Vanessa Haykal, Reviewer,“Modélisation des séries temporelles par apprentissage profond”, Université de Tours, 2019/12/02;

10.3. Popularization

10.3.1. Interventions

- “Collaborative Robotics” – Demonstration at the 2019 Fête de la Sciences by Lucas Joseph – Cap Sciences, Bordeaux

- “Tame a robot” with Thymios II – Animation by Jessica Colombel at Fête de la Science, Université de Lorraine, Nancy, October 2019.
- Fage, C. “Communication Alternative et Améliorée – Aider les enfants et adultes avec difficultés de communication”. Invited Oral Presentation at the Interphase Association (Autism care) by Charles Fage, Bordeaux, December 2019.

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Project-Team CAGIRE

Computational AGility for internal flows sImulations and compaRisons with Experiments

IN COLLABORATION WITH: Laboratoire de mathématiques et de leurs applications (LMAP)

IN PARTNERSHIP WITH:
CNRS

Université de Pau et des Pays de l'Adour

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Numerical schemes and simulations

Table of contents

Project-Team CAGIRE

Creation of the Team: 2011 June 01, updated into Project-Team: 2016 May 01

Keywords:

Computer Science and Digital Science:

A6.1.1. - Continuous Modeling (PDE, ODE)
A6.2.1. - Numerical analysis of PDE and ODE
A6.2.7. - High performance computing
A6.5. - Mathematical modeling for physical sciences
A6.5.2. - Fluid mechanics

Other Research Topics and Application Domains:

B4. - Energy
B4.2. - Nuclear Energy Production
B5.2.1. - Road vehicles
B5.2.3. - Aviation
B5.2.4. - Aerospace

1. Team, Visitors, External Collaborators

Research Scientists

Pascal Bruel [Team leader, CNRS, Researcher, HDR]
Rémi Manceau [Team leader, CNRS, Senior Researcher, HDR]
Vincent Perrier [Inria, Researcher]

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Enrique Gutierrez Alvarez [Inria, Post-Doctoral Fellow]
Franck Mastrippolito [CNRS, Post-Doctoral Fellow]

Administrative Assistant

Sylvie Embolla [Inria, Administrative Assistant]

2. Overall Objectives

2.1. Turbulent flows with complex interactions

This interdisciplinary project brings together researchers coming from different horizons and backgrounds (applied mathematics and fluid mechanics), who gradually elaborated a common vision of what should be the simulation tools for fluid dynamics of tomorrow. Our applications will be focused on wall bounded turbulent flows, featuring complex phenomena such as aeroacoustics, hydrodynamic instabilities, phase change processes, complex walls, buoyancy or localized relaminarization. Because such flows are exhibiting a multiplicity of time and length scales of fluctuations resulting from complex interactions, their simulation is extremely challenging. Even if various methods of simulation (DNS [0]) and turbulence modeling(RANS [0], LES [0], hybrid RANS-LES) are available and have been significantly improved over time, none of them does satisfy all the needs encountered in industrial and environmental configurations. We consider that all these methods will be useful in the future in different situations or regions of the flow, if combined in the same simulation in order to benefit from their respective advantages wherever relevant, while mutually compensating their known limitations. It will thus lead to a description of turbulence at widely varying scales in the computational domain, hence the name *multi-scale simulations*. For example, the RANS mode may extend throughout regions where turbulence is sufficiently close to equilibrium, leaving to LES or DNS the handling of regions where large-scale coherent structures are present. However, a considerable body of work is required to:

- Establish the behavior of the different types of turbulence modeling approaches when combined with high order discretization methods.
- Elaborate relevant and robust switching criteria between models, similar to error assessments used in automatic mesh refinement, but based on the physics of the flow, in order to adapt on the fly the scale of resolution from one extreme of the spectrum to another (say from the Kolmogorov scale to the geometrical scale, i.e., from DNS to RANS).
- Ensure a high level of accuracy and robustness of the resulting simulation tool to address a large range of flow configurations, i.e., from a generic lab-scale geometry for validation to practical systems of interest of our industrial partners.

But the best agile modeling and high-order discretization methods are useless without the recourse to high performance computing (HPC) to bring the simulation time down to values compatible with the requirement of the end users. Therefore, a significant part of our activity will be devoted to the proper handling of the constantly evolving supercomputer architectures. But even the best ever simulation library is useless if it is not disseminated and increasingly used by the CFD community as well as our industrial partners. In that respect, the significant success of the low-order finite volume simulation suite OpenFOAM [0] or the more recently proposed SU2 [0] from Stanford are considered as examples of quite successful dissemination stories that could be, if not followed, but at least considered as a source of inspiration. Our natural inclination though will be to promote the use of the library in direction of our present and future industrial and academic partners, with a special interest on the SMEs active in the highly competitive and strategic economical sectors of energy production and aerospace propulsion. Indeed, these sectors are experiencing a revolution of the entire design process especially for complex parts with an intimate mix between simulations and additive manufacturing (3D printing) processes in the early stages of the design process. For large companies, such as General Electric or Safran (co-developing the CFM Leap-1 engines with 3D printed fuel nozzles), as well as medium-size companies such as Aerojet Rocketdyne, this is a unique opportunity to reduce the duration and hence the cost of development of their systems, while preserving if not strengthening their capability of designing innovative components that cannot be produced by classical manufacturing processes. On the other hand, for the small companies of this sector, this may have a rather detrimental

[0]Direct numerical simulation
[0]Reynolds-averaged Navier-Stokes
[0]Large-eddy simulation
[0]http://www.openfoam.com
[0]http://su2.stanford.edu/

effect on their competitiveness since their capability of mastering both these new manufacturing processes and advanced simulation approaches is far more limited. Thus, through our sustained direct (EDF, Turbomeca, PSA group, AD Industrie, Dassault Aviation) or indirect (European programs: WALLTURB, KIAI, IMPACT-AE, SOPRANO; ANR program MONACO_2025) partnership with different companies, we are able to identify relevant generic configurations, from our point of view of scientists, to serve as support for the development of our approach. This methodological choice was motivated by the desire to lead an as efficient as possible transfer activity, while maintaining a clear distinction between what falls within our field of competence of researchers and what is related to the development of their products by our industrial partners. The long-term objective of this project is to develop, validate, promote and transfer an original and effective approach for modeling and simulating generic flows representative of flow configurations encountered in the field of energy production and aeronautical/automotive propulsion. Our approach will be combining mesh (h) + turbulence model (m) + discretization order (p) agility. This will be achieved by:

- Contributing to the development of new turbulence models.
- Improving high order numerical methods, and increasing their efficiency in the constantly evolving High Performance Computing context.
- Developing experimental tools.

Concerning applications, our objective are :

- To reinforce the long term existing partnership with industrial groups active in the sector of energy production and aeronautical/automotive propulsion, and the other European partners involved in the same European projects as we are.
- To consolidate and develop partnership with SMEs operating in the aeronautical sector.

3. Research Program

3.1. The scientific context

3.1.1. Computational fluid mechanics: modeling or not before discretizing ?

A typical continuous solution of the Navier-Stokes equations at sufficiently large values of the Reynolds number is governed by a wide spectrum of temporal and spatial scales closely connected with the turbulent nature of the flow. The term deterministic chaos employed by Frisch in his enlightening book [46] is certainly conveying most adequately the difficulty in analyzing and simulating this kind of flows. The broadness of the turbulence spectrum is directly controlled by the Reynolds number defined as the ratio between the inertial forces and the viscous forces. This number is not only useful to determine the transition from a laminar to a turbulent flow regime, it also indicates the range of scales of fluctuations that are present in the flow under consideration. Typically, for the velocity field and far from solid walls, the ratio between the largest scale (the integral length scale) and the smallest one (Kolmogorov scale) is proportional to $Re_t^{3/4}$ per dimension, where $Re_t^{3/4}$ is the turbulent Reynolds number, based on the length and velocity scales of the largest turbulent eddies. In addition, for internal flows, viscous effects near the solid walls yield a scaling proportional to Re_τ per dimension, where Re_τ is the friction Reynolds number. The smallest scales play a crucial role in the dynamics of the largest ones, which implies that an accurate framework for the computation of turbulent flows must take into account all the scales, which can lead to unrealistic computational costs in real-world applications. Thus, the usual practice to deal with turbulent flows is to choose between an a priori modeling (in most situations) or not (low Re number and rather simple configurations) before proceeding to the discretization step, followed by the simulation itself. If a modeling phase is on the agenda, then one has to choose again among the above-mentioned variety of approaches. The different simulation options and their date of availability for high-Reynolds-number applications are illustrated in Fig. 1: simulation of turbulent flows can be achieved either by directly solving the Navier-Stokes equations (DNS) or by first applying to the equations a statistical averaging (RANS), a spatial filtering (LES), or a combination of these two operators (hybrid RANS/LES). The new terms brought about by the operator have to be modeled. From a computational point of view, the RANS approach is the least demanding, which explains why historically it has been the workhorse in both the academic and the industrial sectors, and it remains the standard approach nowadays for industrial design, except for very specific applications. It has permitted quite a substantial progress in the understanding of various phenomena such as turbulent combustion or heat transfer. Its inherent inability to provide a time-dependent information has led to promote in the last decade the recourse to either LES or DNS to supplement if not replace RANS. By simulating the large scale structures while modeling the smallest ones, assumed more isotropic, LES proved to be quite a breakthrough to fully take advantage of the increasing power of computers to study complex flow configurations. At the same time, DNS was gradually applied to geometries of increasing complexity (channel flows with values of Re_τ multiplied by 45 during the last 30 years, jets, turbulent premixed flames, among many others), and proved to be a formidable tool to **(i)** improve our knowledge on turbulent flows and **(ii)** test (i.e., validate or invalidate) and improve the modeling hypotheses inherently associated to the RANS and LES approaches. From a numerical point of view, due to the steady nature of the RANS equations, numerical accuracy is generally not ensured via the use of high-order schemes, but rather on careful grid convergence studies. In contrast, the high computational cost of LES or DNS makes necessary the use of highly-accurate numerical schemes in order to optimize the use of computational resources.

To the noticeable exception of the hybrid RANS-LES modeling, which is not yet accepted as a reliable tool for industrial design, as mentioned in the preamble of the Go4hybrid European program [0], a turbulence model represents turbulent mechanisms in the same way in the whole flow. Thus, depending on its intrinsic strengths and weaknesses, accuracy will be a rather volatile quantity, strongly dependent on the flow configuration. For instance, RANS is perfectly suited to attached boundary layers, but exhibits severe limitations in massively-separated flow regions. Therefore, the turbulence modeling and industrial design communities waver between the desire to continue to rely on the RANS approach, which is unrivaled in terms of computational cost, but is still not able to accurately represent all the complex phenomena; and the temptation to switch to LES, which outperforms RANS in many situations, but is prohibitively expensive in high-Reynolds number wall-bounded flows. In order to account for the limitations of the two approaches and to combine them for significantly improving the overall performance of the models, the hybrid RANS-LES approach has emerged during the last two decades as a viable, intermediate way, and we are definitely inscribing our project in this innovative field of research, with an original approach though, based on temporal filtering (Hybrid temporal LES, HTLES) rather than spatial filtering, and a systematic and progressive validation process against experimental data produced by the team.

3.1.2. Computational fluid mechanics: high order discretization on unstructured meshes and efficient methods of solution

All the methods considered in the project are mesh-based methods: the computational domain is divided into cells, that have an elementary shape: triangles and quadrangles in two dimensions, and tetrahedra, hexahedra, pyramids, and prisms in three dimensions. If the cells are only regular hexahedra, the mesh is said to be structured. Otherwise, it is said to be unstructured. If the mesh is composed of more than one sort of elementary shape, the mesh is said to be hybrid. In the project, the numerical strategy is based on discontinuous Galerkin methods. These methods were introduced by Reed and Hill [57] and first studied by Lesaint and Raviart [53]. The extension to the Euler system with explicit time integration was mainly led by Shu, Cockburn and their collaborators. The steps of time integration and slope limiting were similar to high-order ENO schemes, whereas specific constraints given by the finite-element nature of the scheme were gradually solved for scalar conservation laws [41], [40], one dimensional systems [39], multidimensional scalar conservation laws [38], and multidimensional systems [42]. For the same system, we can also cite the work of [45], [50], which is slightly different: the stabilization is made by adding a nonlinear term, and the time integration is implicit. In contrast to continuous Galerkin methods, the discretization of diffusive operators is not straightforward. This is due to the discontinuous approximation space, which does not fit well with the space function in which the diffusive system is well posed. A first stabilization was proposed by Arnold [31]. The first application of discontinuous Galerkin methods to Navier-Stokes equations was proposed in [36] by mean of a mixed

[0] https://cordis.europa.eu/project/rcn/109107/factsheet/en

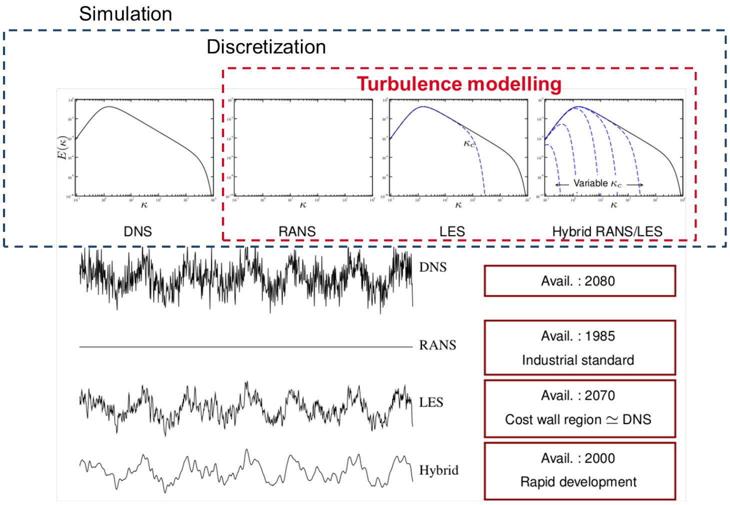

Figure 1. Schematic view of the different nested steps for turbulent flow simulation: from DNS to hybrid RANS-LES. The approximate dates at which the different approaches are or will be routinely used in the industry are indicated in the boxes on the right (extrapolations based on the present rate of increase in computer performances).

formulation. Actually, this first attempt led to a non-compact computational stencil, and was later proved to be unstable. A compactness improvement was made in [37], which was later analyzed, and proved to be stable in a more unified framework [32]. The combination with the $k - \omega$ RANS model was made in [35]. As far as Navier-Stokes equations are concerned, we can also cite the work of [48], in which the stabilization is closer to the one of [32], the work of [54] on local time stepping, or the first use of discontinuous Galerkin methods for direct numerical simulation of a turbulent channel flow done in [43]. Discontinuous Galerkin methods became very popular because:

- They can be developed for any order of approximation.
- The computational stencil of one given cell is limited to the cells with which it has a common face. This stencil does not depend on the order of approximation. This is a pro, compared for example with high-order finite volumes, for which the number of neighbors required increases with the order of approximation.
- They can be developed for any kind of mesh, structured, unstructured, but also for aggregated grids [34]. This is a pro compared not only with finite-difference schemes, which can be developed only on structured meshes, but also compared with continuous finite-element methods, for which the definition of the approximation basis is not clear on aggregated elements.
- p-adaptivity is easier than with continuous finite elements, because neighboring elements having a different order are only weakly coupled.
- Upwinding is as natural as for finite volumes methods, which is a benefit for hyperbolic problems.
- As the formulation is weak, boundary conditions are naturally weakly formulated. This is a benefit compared with strong formulations, for example point centered formulation when a point is at the intersection of two kinds of boundary conditions.

For concluding this section, there already exists numerical schemes based on the discontinuous Galerkin method, which proved to be efficient for computing compressible viscous flows. Nevertheless, there remain many things to be improved, which include: efficient shock capturing methods for supersonic flows, high-order discretization of curved boundaries, low-Mach-number behavior of these schemes and combination with second-moment RANS closures. Another aspect that deserves attention is the computational cost of discontinuous Galerkin methods, due to the accurate representation of the solution, calling for a particular care of implementation for being efficient. We believe that this cost can be balanced by the strong memory locality of the method, which is an asset for porting on emerging many-core architectures.

3.1.3. Experimental fluid mechanics: a relevant tool for physical modeling and simulation development

With the considerable and constant development of computer performance, many people were thinking at the turn of the 21st century that in the short term, CFD would replace experiments, considered as too costly and not flexible enough. Simply flipping through scientific journals such as Journal of Fluid Mechanics, Combustion and Flame, Physics of Fluids or Journal of Computational Physics or through websites such that of Ercoftac [0] is sufficient to convince oneself that the recourse to experiments to provide either a quantitative description of complex phenomena or reference values for the assessment of the predictive capabilities of models and simulations is still necessary. The major change that can be noted though concerns the content of the interaction between experiments and CFD (understood in the broad sense). Indeed, LES or DNS assessment calls for the experimental determination of temporal and spatial turbulent scales, as well as time-resolved measurements and determination of single or multi-point statistical properties of the velocity field. Thus, the team methodology incorporates from the very beginning an experimental component that is operated in strong interaction with the modeling and simulation activities.

3.2. Research directions

3.2.1. Boundary conditions

3.2.1.1. Generating synthetic turbulence

A crucial point for any multi-scale simulation able to locally switch (in space or time) from a coarse to a fine level of description of turbulence, is the enrichment of the solution by fluctuations as physically meaningful as possible. Basically, this issue is an extension of the problem of the generation of realistic inlet boundary conditions in DNS or LES of subsonic turbulent flows. In that respect, the method of anisotropic linear forcing (ALF) we have developed in collaboration with EDF proved very encouraging, by its efficiency, its generality and simplicity of implementation. So, it seems natural, on the one hand, to extend this approach to the compressible framework and to implement it in AeroSol. On the other hand, we shall concentrate (in cooperation with EDF R&D in Chatou in the framework of a the CIFRE PhD of V. Duffal) on the theoretical link between the local variations of the scale of description of turbulence (e.g. a sudden variations in the size of the time filter) and the intensity of the ALF forcing, transiently applied to promote the development of missing fluctuating scales.

3.2.1.2. Stable and non reflecting boundary conditions

In aerodynamics, and especially for subsonic computations, handling inlet and outlet boundary conditions is a difficult issue. A significant amount of work has already been performed for second-order schemes for Navier-Stokes equations, see [56], [59] and the huge number of papers citing it. On the one hand, we believe that decisive improvements are necessary for higher-order schemes: indeed, the less dissipative the scheme is, the worse impact have the spurious reflections. For this purpose, we will first concentrate on the linearized Navier-Stokes system, and analyze the way to impose boundary conditions in a discontinuous Galerkin framework with a similar approach as in [47]. We will also try to extend the work of [60], which deals with Euler equations, to the Navier-Stokes equations.

[0] http://www.ercoftac.org

3.2.2. Turbulence models and model agility

3.2.2.1. Extension of zero-Mach models to the compressible system

We shall develop in parallel our multi-scale turbulence modeling and the related adaptive numerical methods of AeroSol. Without prejudice to methods that will be on the podium in the future, a first step in this direction will be to extend to a compressible framework the continuous temporal hybrid RANS/LES method we have developed up to now in a Mach zero context.

3.2.2.2. Study of wall flows with and without mass or heat transfer at the wall: determination and validation of relevant criteria for hybrid turbulence models

In the targeted application domains, turbulence/wall interactions and heat transfer at the fluid-solid interface are physical phenomena whose numerical prediction is at the heart of the concerns of our industrial partners. For instance, for a jet engine manufacturer, being able to properly design the configuration of the cooling of the walls of its engine combustion chamber in the presence of thermoacoustic instabilities is based on the proper identification and a thorough understanding of the major mechanisms that drive the dynamics of the parietal transfer. Our objective is to take advantage of our analysis, experimental and computational tools to actively participate in the improvement of the collective knowledge of such kind of transfer. The flow configurations dealt with from the beginning of the project are those of subsonic, single-phase impinging jets or JICF (jets in crossflow) with the possible presence of an interacting acoustic wave. The issue of conjugate heat transfer at the wall will be also gradually investigated. The existing switchover criteria of the hybrid RANS/LES models will be tested on these flow configurations in order to determine their domain of validity. In parallel, the hydrodynamic instability modes of the JICF will be studied experimentally and theoretically (in cooperation with the SIAME laboratory) in order to determine the possibility to drive a change of instability regime (e.g., from absolute to convective) and thus to propose challenging flow conditions that would be relevant for the setting-up of an hybrid LES/DNS approach aimed at supplementing the hybrid RANS/LES approach.

3.2.2.3. Improvement of turbulence models

The production and subsequent use of DNS (AeroSol library) and experimental (MAVERIC bench) databases dedicated to the improvement of the physical models is a significant part of our activity. In that respect, our present capability of producing in-situ experimental data for simulation validation and flow analysis is clearly a strongly differentiating mark of our project. The analysis of the DNS and experimental data produced make the improvement of the hybrid RANS/LES approach possible. Our hybrid temporal LES (HTLES) method has a decisive advantage over all other hybrid RANS/LES approaches since it relies on a well-defined time-filtering formalism. This feature greatly facilitates the proper extraction from the databases of the various terms appearing in transport equations obtained at the different scales involved (e.g. from RANS to LES). But we would not be comprehensive in that matter if we were not questioning the relevance of any simulation-experiment comparisons. In other words, a central issue is the following question: are we comparing the same quantities between simulations and experiment? From an experimental point of view, the questions to be raised will be, among others, the possible difference in resolution between the experiment and the simulations, the similar location of the measurement points and simulation points, the acceptable level of random error associated to the necessary finite number of samples. In that respect, the recourse to uncertainty quantification techniques will be advantageously considered.

3.2.3. Development of an efficient implicit high-order compressible solver scalable on new architectures

As the flows simulated are very computationally demanding, we will maintain our efforts in the development of AeroSol in the following directions:

- Efficient implementation of the discontinuous Galerkin method.
- Implicit methods based on Jacobian-Free-Newton-Krylov methods and multigrid.
- Porting on heterogeneous architectures.
- Implementation of models.

3.2.3.1. Efficient implementation of the discontinuous Galerkin method

In high-order discontinuous Galerkin methods, the unknown vector is composed of a concatenation of the unknowns in the cells of the mesh. An explicit residual computation is composed of three loops: an integration loop on the cells, for which computations in two different cells are independent, an integration loop on boundary faces, in which computations depend on data of one cell and on the boundary conditions, and an integration loop on the interior faces, in which computations depend on data of the two neighboring cells. Each of these loops is composed of three steps: the first step consists in interpolating data at the quadrature points; the second step in computing a nonlinear flux at the quadrature points (the physical flux for the cell loop, an upwind flux for interior faces or a flux adapted to the kind of boundary condition for boundary faces); and the third step in projecting the nonlinear flux on the degrees of freedom.

In this research direction, we propose to exploit the strong memory locality of the method (i.e., the fact that all the unknowns of a cell are stocked contiguously). This formulation can reduce the linear steps of the method (interpolation on the quadrature points and projection on the degrees of freedom) to simple matrix-matrix product which can be optimized. For the nonlinear steps, composed of the computation of the physical flux on the cells and of the numerical flux on the faces, we will try to exploit vectorization.

3.2.3.2. Implicit methods based on Jacobian-Free-Newton-Krylov methods and multigrid

For our computations of the IMPACT-AE project, we have used explicit time stepping. The time stepping is limited by the CFL condition, and in our flow, the time step is limited by the acoustic wave velocity. As the Mach number of the flow we simulated in IMPACT-AE was low, the acoustic time restriction is much lower than the turbulent time scale, which is driven by the velocity of the flow. We hope to have a better efficiency by using time implicit methods, for using a time step driven by the velocity of the flow.

Using implicit time stepping in compressible flows in particularly difficult, because the system is fully nonlinear, such that the nonlinear solving theoretically requires to build many times the Jacobian. Our experience in implicit methods is that the building of a Jacobian is very costly, especially in three dimensions and in a high-order framework, because the optimization of the memory usage is very difficult. That is why we propose to use a Jacobian-free implementation, based on [52]. This method consists in solving the linear steps of the Newton method by a Krylov method, which requires Jacobian-vector product. The smart idea of this method is to replace this product by an approximation based on a difference of residual, therefore avoiding any Jacobian computation. Nevertheless, Krylov methods are known to converge slowly, especially for the compressible system when the Mach number is low, because the system is ill-conditioned. In order to precondition, we propose to use an aggregation-based multigrid method, which consists in using the same numerical method on coarser meshes obtained by aggregation of the initial mesh. This choice is driven by the fact that multigrid methods are the only one to scale linearly [61], [62] with the number of unknowns in term of number of operations, and that this preconditioning does not require any Jacobian computation.

Beyond the technical aspects of the multigrid approach, which is challenging to implement, we are also interested in the design of an efficient aggregation. This often means to perform an aggregation based on criteria (anisotropy of the problem, for example) [55]. To this aim, we propose to extend the scalar analysis of [63] to a linearized version of the Euler and Navier-Stokes equations, and try to deduce an optimal strategy for anisotropic aggregation, based on the local characteristics of the flow. Note that discontinuous Galerkin methods are particularly well suited to h-p aggregation, as this kind of methods can be defined on any shape [34].

3.2.3.3. Porting on heterogeneous architectures

Until the beginning of the 2000s, the computing capacities have been improved by interconnecting an increasing number of more and more powerful computing nodes. The computing capacity of each node was increased by improving the clock speed, the number of cores per processor, the introduction of a separate and dedicated memory bus per processor, but also the instruction level parallelism, and the size of the memory cache. Even if the number of transistors kept on growing up, the clock speed improvement has flattened since the mid 2000s [58]. Already in 2003, [49] pointed out the difficulties for efficiently using the biggest clusters: "While these super-clusters have theoretical peak performance in the Teraflops range, sustained performance with real applications is far from the peak. Salinas, one of the 2002 Gordon Bell Awards was able to sustain 1.16 Tflops on ASCI White (less than 10% of peak)." From the current multi-core architectures, the trend is now to use many-core accelerators. The idea behind many-core is to use an accelerator composed of a lot of relatively slow and simplified cores for executing the most simple parts of the algorithm. The larger the part of the code executed on the accelerator, the faster the code may become. Therefore, it is necessary to work on the heterogeneous aspects of computations. These heterogeneities are intrinsic to our computations and have two sources. The first one is the use of hybrid meshes, which are necessary for using a locally-structured mesh in a boundary layer. As the different cell shapes (pyramids, hexahedra, prisms and tetrahedra) do not have the same number of degrees of freedom, nor the same number of quadrature points, the execution time on one face or one cell depends on its shape. The second source of heterogeneity are the boundary conditions. Depending on the kind of boundary conditions, user-defined boundary values might be needed, which induces a different computational cost. Heterogeneities are typically what may decrease efficiency in parallel if the workload is not well balanced between the cores. Note that heterogeneities were not dealt with in what we consider as one of the most advanced work on discontinuous Galerkin on GPU [51], as only straight simplicial cell shapes were addressed. For managing at best our heterogeneous computations on heterogeneous architectures, we propose to use the execution runtime StarPU [33]. For this, the discontinuous Galerkin algorithm will be reformulated in terms of a graph of tasks. The previous tasks on the memory management will be useful for that. The linear steps of the discontinuous Galerkin methods require also memory transfers, and one issue consists in determining the optimal task granularity for this step, i.e. the number of cells or face integrations to be sent in parallel on the accelerator. On top of that, the question of which device is the most appropriate to tackle such kind of tasks is to be discussed.

Last, we point out that the combination of shared-memory and distributed-memory parallel programming models is better suited than only the distributed-memory one for multigrid, because in a hybrid version, a wider part of the mesh shares the same memory, therefore making a coarser aggregation possible.

These aspects will benefit from a particularly stimulating environment in the Inria Bordeaux Sud Ouest center around high-performance computing, which is one of the strategic axes of the center.

3.2.3.4. Implementation of turbulence models in AeroSol and validation

We will gradually insert models developed in research direction 3.2.2.1 in the AeroSol library in which we develop methods for the DNS of compressible turbulent flows at low Mach number. Indeed, due to its formalism based on temporal filtering, the HTLES approach offers a consistent theoretical framework characterized by a continuous transition from RANS to DNS, even for complex flow configurations (e.g. without directions of spatial homogeneity). As for the discontinuous Galerkin method available presently in AeroSol, it is the best suited and versatile method able to meet the requirements of accuracy, stability and cost related to the local (varying) level of resolution of the turbulent flow at hand, regardless of its complexity. The first step in this direction was taken in 2017 during the internship of Axelle Perraud, who has implemented a turbulence model (k-ω-SST) in the Aerosol library.

3.2.4. Validation of the simulations: test flow configurations

To supplement whenever necessary the test flow configuration of MAVERIC and apart from configurations that could emerge in the course of the project, the following configurations for which either experimental data, simulation data or both have been published will be used whenever relevant for benchmarking the quality of our agile computations:

- The impinging turbulent jet (simulations).
- The ORACLES two-channel dump combustor developed in the European projects LES4LPP and MOLECULES.
- The non reactive single-phase PRECCINSTA burner (monophasic swirler), a configuration that has been extensively calculated in particular with the AVBP and Yales2 codes.
- The LEMCOTEC configuration (monophasic swirler + effusion cooling).
- The ONERA MERCATO two-phase injector configuration provided the question of confidentiality of the data is not an obstacle.

- Rotating turbulent flows with wall interaction and heat transfer.
- Turbulent flows with buoyancy.

4. Application Domains

4.1. Aeronautics

Cagire is presently involved in studies mainly related to:

- The combustion chamber wall: the modelling, the simulation and the experimentation of the flow around a multiperforated plate representative of a real combustion chamber wall are the three axes we have been developing during the recent period. The continuous improvement of our in-house test facility Maveric is also an important ingredient to produce our own experimental validation data for isothermal flows. For non-isothermal flows, our participation in the EU funded program Soprano will be giving us access to non-isothermal data produced by Onera.
- The flow around airfoils: the modelling of the turbulent boundary layer has been for almost a century a key issue in the aeronautics industry. However, even the more advanced RANS models face difficulties in predicting the influence of pressure gradients on the development of the boundary layer. A main issue is the reliability of the modelling hypotheses, which is crucial for less conservative design. One of the technological barriers is the prediction of the flow in regimes close to the edge of the flight domain (stall, buffeting, unsteady loads) when the boundary layer is slowed down by an adverse pressure gradient. This is the subject of the CIFRE PhD thesis of Gustave Sporschill, started in 2018, in collaboration with Dassault Aviation.

4.2. Power stations

R. Manceau has established a long term collaboration (4 CIFRE PhD theses in the past, 2 ongoing) with the R & D center of EDF of Chatou, for the development of refined turbulence models in the in-house CFD code of EDF, Code_Saturne :

- The prediction of heat transfer in fluid and solid components is of major importance in power stations, in particular, nuclear power plants. Either for the thermohydraulics of the plenum or in the study of accidental scenarii, among others, the accurate estimation of wall heat transfer, mean temperatures and temperature fluctuations are necessary for the evaluation of relevant thermal and mechanical design criteria. The PhD thesis (CIFRE EDF) of G. Mangeon is dedicated to the development of relevant RANS models for these industrial applications.
- Moreover, the prediction of unsteady hydrodynamic loadings is a key point for operating and for safety studies of PWR power plants. Currently, the static loading is correctly predicted by RANS computations but when the flow is transient (as, for instance, in Reactor Coolant Pumps, due to rotor/stator interactions, or during operating transients) or in the presence of large, energetic, coherent structures in the external flow region, the RANS approach is not sufficient, whereas LES is still too costly for a wide use in industry. This issue constitutes the starting point of the just-started PhD thesis (CIFRE EDF) of Vladimir Duffal.

4.3. Automotive propulsion

- The engine (underhood) compartment is a key component of vehicle design, in which the temperature is monitored to ensure the effectiveness and safety of the vehicle, and participates in 5 to 8% of the total drag and CO2 emissions. Dimensioning is an aerodynamic and aerothermal compromise, validated on a succession of road stages at constant speed and stopped phases (red lights, tolls, traffic jam). Although CFD is routinely used for forced convection, state-of-the-art turbulence models are not able to reproduce flows dominated by natural convection during stopped phases, with a Rayleigh number of the order of 10^{10}, such that the design still relies on costly, full-scale, wind tunnel experiments. This technical barrier must be lifted, since the ambition of the PSA group is to reach a *full digital design of their vehicles in the 2025 horizon*, i.e., to almost entirely rely on CFD. This issue is the focus of the ongoing PhD thesis (CIFRE PSA) of S. Jameel, supervised by R. Manceau, and also a part of the ANR project MONACO_2025 described in section 9.2.2.

- The Power & Vehicles Division of IFPEN co-develops a CFD code to simulate the internal flow in a spark-ignition engine, in order to provide the automotive industry with tools to optimize the design of combustion engines. The RANS method, widely used in the industry, is not sufficiently reliable for quantitative predictions, and is only used as a tool to qualitatively compare different geometries. On the other hand, LES provides more detailed and accurate information, but at the price of a CPU cost unafordable for daily use in the industry. Therefore, IFPEN aims at developing the hybrid RANS/LES methodology, in order to combine the strengths of the two approaches. The PhD thesis of Hassan Afailal, co-supervised by Rémi Manceau, is focused on this issue.

5. Highlights of the Year

5.1. Highlights of the Year

5.1.1. R. Manceau, new Cagire team leader

After having taken over the responsibility of the team since its creation, Pascal Bruel, 59, has decided this year to hand over the reins! After consultation, Inria's management has appointed Remi Manceau as the new head of the Cagire team as of 18 November 2019.

6. New Software and Platforms

6.1. AeroSol

KEYWORD: Finite element modelling

FUNCTIONAL DESCRIPTION: The AeroSol software is a high order finite element library written in C++. The code has been designed so as to allow for efficient computations, with continuous and discontinuous finite elements methods on hybrid and possibly curvilinear meshes. The work of the team CARDAMOM (previously Bacchus) is focused on continuous finite elements methods, while the team Cagire is focused on discontinuous Galerkin methods. However, everything is done for sharing the largest part of code we can. More precisely, classes concerning IO, finite elements, quadrature, geometry, time iteration, linear solver, models and interface with PaMPA are used by both of the teams. This modularity is achieved by mean of template abstraction for keeping good performances. The distribution of the unknowns is made with the software PaMPA , developed within the team TADAAM (and previously in Bacchus) and the team Castor.

NEWS OF THE YEAR: In 2019, the following points were addressed in AeroSol

*Update, documentation, and wiki for the test case

*exact solution of Riemann problem and exact Godunov solver

*Development of Droplet model, and of a Baer and Nunziato diphasic model.

*Beginning of implementation of eddy viscosity models (k-epsilon, Spalart-Almarras) turbulence models.

*Add the possibility of mesh dependent data (for example, a flow computed by AeroSol with the Euler system) for being used as input for another model (e.g. advection of droplets within this flow). This feature is used also for wall distance for turbulent models.

*Penalization problems, with single core mesh adaptation was merged in the master branch.

*Improvements of PETSc usage: possibility of solving linear problems that are not of size nvar, usage of MUMPS LU solver through PETSc.

*Interfacing with SLEPc for solving eigenvalues and eigenvectors problems.

*High order visualization based on GMSH.

*Beginning of interfacing with PARMMG for parallel mesh adaptation.

*Clean of warning, error messages, etc...

- Participants: Benjamin Lux, Damien Genet, Mario Ricchiuto, Vincent Perrier, Héloïse Beaugendre, Subodh Madhav Joshi, Christopher Poette, Marco Lorini, Jonathan Jung and Enrique Gutierrez Alvarez
- Partner: BRGM
- Contact: Vincent Perrier

7. New Results

7.1. A parameter free pressure based approach for simulating flows at all Mach

Participant: Pascal Bruel.

The latest version of the pressure-correction algorithm developed in the last years in close partnership with Prof. E. Dick (Ghent University, Belgium) and Dr. Y. Moguen (UPPA, France) has been published this year [14]. Beyond its promotion [25], future efforts will be directed towards its extension to reacting single phase flows.

7.2. Simulation of a jet in a supersonic cross-flow

Participant: Pascal Bruel.

In our joint work, published this year with our Kazakh colleagues [10], we have focused on detailing the vortical patterns present in the structure of a sonic jet injected normally into a supersonic crossflow. Such a generic flow configuration is considered to feature some prominent characteristics encountered in propulsion system based on supersonic combustion (scramjet). A critical pressure ratio value beyond which new vortical structures are appearing has been evidenced. Contacts have been taken with ONERA to have access to their experimental database which is much more developed than the one we had access to so far. Some specific adaptation will have to be conducted though, in order to adapt the simulation to the slightly different flow configuration considered by ONERA.

7.3. Experiments and simulations related to flows over aerial tanks

Participant: Pascal Bruel.

These results have been obtained in the framework of the cooperation with the National University of Córdoba (Argentina).

- Predicting the pressure loads produced by the atmospheric wind flow over a cylindrical vertical tank

  Pressure distributions obtained using different RANS turbulence models were compared with experimental data obtained in wind tunnel tests for a tank with a closed roof. We have considered a flat shape and a conical roof of 25 degrees. Combinations of aspect ratios equal to 0.5, 1 and 2, and Reynolds numbers equal to 250000, 290000 and 340000 were simulated. The results of the numerical model were compared with those obtained in experimental tests in a wind tunnel of the atmospheric boundary layer using a rigid tank model. We have worked to obtain a stable atmospheric boundary layer in the complete domain using the correct boundary conditions for the implemented RANS models. After that, we have developed numerical simulations for the flow around the tanks inside the atmospheric boundary layer. These results have been published in [17].
- Studying the interaction of a wall with the flow around two cylinders arranged in tandem

For this configuration, the cylinders were immersed in a flow with a boundary layer profile at a subcritical Reynolds number (Re=10000). The three-dimensional transient turbulent flow around the cylinders was simulated numerically using the SAS turbulence model. The effects of wake interference due to both the proximity between the cylinders and their position with respect to the wall were examined through the values of drag, lift and pressure coefficients. The details of the flow fields in the near wake of the cylinders were also studied. The results were compared with experimental and numerical results reported in the literature, and with the case of a single cylinder near a wall. These results have been published in [15]. In parallel, a specific test section for the team's Maveric test facility has been developed. It gives the possibility to accommodate wall mounted cylinder(s) that represent a scaled down version of real horizontal tanks. The objective here is to generate validation data. Particle image velocimetry (PIV) measurements have been carried out during the 1-month stay of Mauro Grioni in Pau in September 2019.

- Simulating the effects of explosions on liquid fuel storage tanks.

  The fast release of energy in explosive processes produces intense shock waves (blast waves). The interaction of these waves with obstacles such as tanks can be extremely destructive. As a first step towards the full simulation of a blast wave with a tank, we have studied the capabilities of OpenFOAM to simulate a blast wave. The numerical results were compared in a cylindrical configuration with the analytical solution provided by the Sedov theory. A special attention has been paid to evaluate the influence of the reconstruction functions in the Euler flux (Kurganov scheme) on the numerical results. The predicted position and velocity of the generated shock wave as well as the pressure jump and its evolution behind the shock were in good agreement with their theoretical counterparts. These results have been published in [16].

7.4. A density-based numerical flux for high order simulation of low Mach flows with acoustics

Participants: Pascal Bruel, Jonathan Jung, Vincent Perrier.

The topic dealt with concerns acoustic computations in low Mach number flows with density based solvers. For ensuring a good resolution of the low Mach number base flow, a scheme able to deal with stationary low Mach number flows is necessary. Previously proposed low Mach number fixes have been tested with acoustic computations. Numerical results prove that they are not accurate for acoustic computations. The issues raised with acoustic computations with low Mach number fixes were studied and a new scheme has been developed, in order to be accurate not only for steady low Mach number flows, but also for acoustic computations. These results have been published in [12].

7.5. Conjugate heat transfer with different fluid-solid physical properties: a new elliptic blending second-moment closure

Participants: Rémi Manceau, Gaëtan Mangeon.

Our approach to model the wall/turbulence interaction, based on Elliptic Blending, was successfully applied to flows with standard thermal boundary conditions at the walls [11]. However, Conjugate Heat Transfer, which couples fluid and solid domains, are particularly challenging for turbulence models. We have developed an innovative model, the Elliptic Blending Differential Flux Model, to account for the influence of various wall thermal boundary conditions on the turbulent heat flux and the temperature variance. An assessment of this new model in Conjugate Heat Transfer has been performed for several values of fluid-solid thermal diffusivity and conductivity ratios. A careful attention is paid to the discontinuity of the dissipation rate associated with the temperature variance at the fluid-solid interface. The analysis is supported by successful comparisons with Direct Numerical Simulations [30].

7.6. Eddy-viscosity models sensitized to buoyancy effects for predicting natural convection flows

Participants: Rémi Manceau, Saad Jameel.

Eddy-viscosity turbulence models have been sensitized to the effects of buoyancy, in order to improve the prediction in natural convection flows. The approach extends in a linear way the constitutive relations for the Reynolds stress and the turbulent heat flux, in order to account for the anisotropic influence of buoyancy. The novelty of this work involves the buoyancy extension applied to two very different eddy-viscosity models, which leads to encouraging results for the highly challenging case of the differentially heated vertical channel [27], [22].

7.7. Development and validation of an improved HTLES approach

Participants: Rémi Manceau, Vladimir Duffal, Hassan Afailal, Franck Mastrippolito, Pascal Bruel.

The HTLES (hybrid temporal LES) approach, developed by the team, has been improved by introducing shielding functions and an internal consistency constraint to enforce the RANS behavior in the near-wall regions [18]. The influence of the underlying closure model was studied by applying HTLES to two RANS models: the k-ω SST and the BL-v2/k. The validation, carried out using two different solvers, Code_Saturne (collaboration with EDF) and Converge-CFD (collaboration with IFPEN), encompassed different type of internal flows: channel, periodic hill, internal combustion engines (in fixed position and with a moving piston), jet in crossflow [21], [9]. The robustness of HTLES to grid coarsening and the accuracy of the predictions at a reduced numerical cost compared to LES was demonstrated. Notably, the capacity of HTLES to provide information on velocity and pressure temporal fluctuations at the wall was assessed, offering a cost-saving alternative to LES to predict unsteady loads. One of the major limitation of HTLES, i.e., the fact that it is based on statistically averaged quantities, which are challenging to estimate in non-stationary flows, has been removed, by approximating the statistical average by a Dynamic Temporal Filter.

7.8. Compact WENO, positivity preserving stabilization of discontinuous Galerkin methods

Participant: Vincent Perrier.

Jointly with Alireza Mazaheri (NASA Langley) and Chi Wang Shu, we have developed a compact WENO stabilization that moreover ensures the positivity of physical quantities. The work was published in [13].

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

- EDF: "Advanced modelling of heat transfer for industrial configurations with or without accounting of the solid wall", contract associated to the PhD thesis of Gaëtan Mangeon
- EDF: "Hybrid RANS/LES modelling for unsteady loadings in turbulent flows", contract associated to the PhD thesis of Vladimir Duffal
- IFPEN: "3D simulation of non-reactive internal aerodynamics of spark-ignition engines using an hybrid RANS/LES method", contract associated to the PhD thesis of Hassan Al Afailal
- PSA: ""Turbulence modelling in the mixed and natural convection regimes in the context of automotive applications", contract associated to the PhD thesis of Saad Jameel.

8.2. Bilateral Grants with Industry

- EDF (Cifre PhD grant): "Advanced modelling of heat transfer for industrial configurations with or without accounting of the solid wall", PhD student: Gaëtan Mangeon
- EDF (Cifre PhD grant): "Hybrid RANS/LES modelling for unsteady loadings in turbulent flows", PhD student: Vladimir Duffal
- IFPEN (PhD grant): "3D simulation of non-reactive internal aerodynamics of spark-ignition engines using an hybrid RANS/LES method", PhD sutdent: Hassan Al Afailal
- PSA (Cifre PhD grant): "Turbulence modelling in the mixed and natural convection regimes in the context of automotive applications", PhD student: Saad Jameel.
- Dassault Aviation (Cifre PhD grant): "Amélioration des modèles pour la turbulence. Applications à la prédiction des écoulements aérodynamiques.", PhD student: Gustave Sporschill.

9. Partnerships and Cooperations

9.1. Regional Initiatives

9.1.1. SEIGLE

Participants: Enrique Gutierrez Alvarez, Jonathan Jung, Vincent Perrier.

SEIGLE means "Simulation Expérimentation pour l'Interaction de Gouttes Liquides avec un Ecoulement fortement compressible". It is a 3-year program which has started since October 2017 and was funded by Régional Nouvelle-Aquitaine, ISAE-ENSMA, CESTA and Inria. The interest of understanding aerodynamic mechanisms and liquid drops atomization is explained by the field of applications where they play a key role, specially in the new propulsion technologies through detonation in the aerospace as well as in the securities field. The SEIGLE project was articulated around a triptych experimentation, modeling and simulation. An experimental database will be constituted. It will rely on a newly installed facility (Pprime), similar to a supersonic gust wind tunnel/ hypersonic from a gaseous detonation tube at high pressure. This will allow to test modeling approaches (Pprime / CEA) and numerical simulation (Inria / CEA) with high order schemes for multiphasic compressible flows, suitable for processing shock waves in two-phase media.

9.1.2. HPC scalable ecosystem

Participants: Jonathan Jung, Vincent Perrier, [A two-year Post-doc starting in 2019 or 2020].

HPC scalable ecosystem is a 3-year program funded by Région Nouvelle-Aquitaine (call 2018), Airbus, CEA-CESTA, University of Bordeaux, INRA, ISAE-ENSMA and Inria. A two-year post-doc will be hired in 2019 or 2020. The objective is to extend the prototype developed in [44] to high order (discontinuous Galerkin) and non-reactive diffusive flows in 3d. The same basis will be developed in collaboration with Pprime for WENO based methods for reactive flows.

9.2. National Initiatives

9.2.1. GIS Success

Participant: Pascal Bruel.

We are members of the CNRS GIS Success (Groupement d'Intérêt Scientifique) organised around two of the major CFD codes employed by the Safran group, namely AVBP and Yales2. This year, the evaluation of the capability of the compressible module of Yales2 has started.

9.2.2. ANR MONACO_2025

Participant: Rémi Manceau.

The ambition of the MONACO_2025 project, coordinated by Rémi Manceau, is to join the efforts made in *two different industrial sectors* in order to tackle the industrial simulation of transient, turbulent flows affected by buoyancy effects. It brings together two academic partners, the project-team Cagire hosted by the university of Pau, and the institute Pprime of the CNRS/ENSMA/university of Poitiers (PPRIME), and R&D departments of two industrial partners, the PSA group and the EDF group, who are major players of the automobile and energy production sectors, respectively.

- The main **scientific objective** of the project is to make a breakthrough in *the unresolved issue* of the modelling of turbulence/buoyancy interactions in transient situations, within the continuous hybrid RANS/LES paradigm, which consists in preserving a computational cost compatible with industrial needs by relying on statistical approaches where a fine-grained description of the turbulent dynamics is not necessary. The transient cavity flow experiments acquired during MONACO_2025 will provide the partners and the scientific community with *an unrivalled source of knowledge* of the physical mechanisms that must be accounted for in turbulence models.
- The main **industrial objective** is *to make available computational methodologies* to address dimensioning, reliability and security issues in buoyancy-affected transient flows. It is to be emphasized that such problems are *not tackled using CFD at present in the industry*. At the end of MONACO_2025, a panel of methodologies, ranging from simple URANS to sophisticated hybrid model based on improved RANS models, will be evaluated in transient situations, against the dedicated cavity flow experiments and a real car underhood configuration. This final benchmark exercise will form *a decision-making tool* for the industrial partners, and will thus pave the way towards high-performance design of low-emission vehicles and highly secure power plants. In particular, the project is in line with the *Full Digital 2025 ambition*, e.g., the declared ambition of the PSA group to migrate, within the next decade, to a design cycle of new vehicles nearly entirely based on CAE (computer aided engineering), without recourse to expensive full-scale experiments.

9.3. European Initiatives

9.3.1. FP7 & H2020 Projects

9.3.1.1. SOPRANO

Participants: Pascal Bruel, Rémi Manceau, Franck Mastrippolito.

Topic: MG-1.2-2015 - Enhancing resource efficiency of aviation

Project acronym: SOPRANO

Project title: Soot Processes and Radiation in Aeronautical inNOvative combustors

Duration: 01/09/2016 - 31/08/2020

Coordinator: SAFRAN

Other partners:

- France: CNRS, CERFACS, INSA Rouen, SAFRAN SA, Snecma SAS, Turbomeca SA.
- Germany: DLR, GE-DE Gmbh, KIT, MTU, RRD,
- Italy: GE AVIO SRL, University of Florence
- United Kingdom: Rolls Royce PLC, Imperial College of Science, Technology and Medecine, Loughborough University.

Abstract: For decades, most of the aviation research activities have been focused on the reduction of noise and NOx and CO2 emissions. However, emissions from aircraft gas turbine engines of non-volatile PM, consisting primarily of soot particles, are of international concern today. Despite the lack of knowledge toward soot formation processes and characterization in terms of mass and size, engine manufacturers have now to deal with both gas and particles emissions. Furthermore, heat transfer understanding, that is also influenced by soot radiation, is an important matter for the improvement of the combustor's durability, as the key point when dealing with low-emissions combustor architectures is to adjust the air flow split between the injection system and the combustor's walls. The SOPRANO initiative consequently aims at providing new elements of knowledge, analysis and improved design tools, opening the way to: • Alternative designs of combustion systems for future aircrafts that will enter into service after 2025 capable of simultaneously reducing gaseous pollutants and particles, • Improved liner lifetime assessment methods. Therefore, the SOPRANO project will deliver more accurate experimental and numerical methodologies for predicting the soot emissions in academic or semi-technical combustion systems. This will contribute to enhance the comprehension of soot particles formation and their impact on heat transfer through radiation. In parallel, the durability of cooling liner materials, related to the walls air flow rate, will be addressed by heat transfer measurements and predictions. Finally, the expected contribution of SOPRANO is to apply these developments in order to determine the main promising concepts, in the framework of current low-NOx technologies, able to control the emitted soot particles in terms of mass and size over a large range of operating conditions without compromising combustor's liner durability and performance toward NOx emissions.

In the SOPRANO project, our objective is to complement the experimental (ONERA) and LES (CERFACS) work by RANS computations of the flow around a multiperforated plate, in order to build a database making possible a parametric study of mass, momentum and heat transfer through the plate and the development of multi-parameter-dependent equivalent boundary conditions. Franck Mastrippolito, the post-doc recruited by mid-january 2019, performed simulations aimed at reproducing the experiment of ONERA Toulouse carried out in the same workpackage. The configuration is that of an effusion plate with a gyration angle of 90 degrees and the turbulence model is EBRSM. Franck presented his results in October 2019 during the ITR meeting in Florence (Italy).

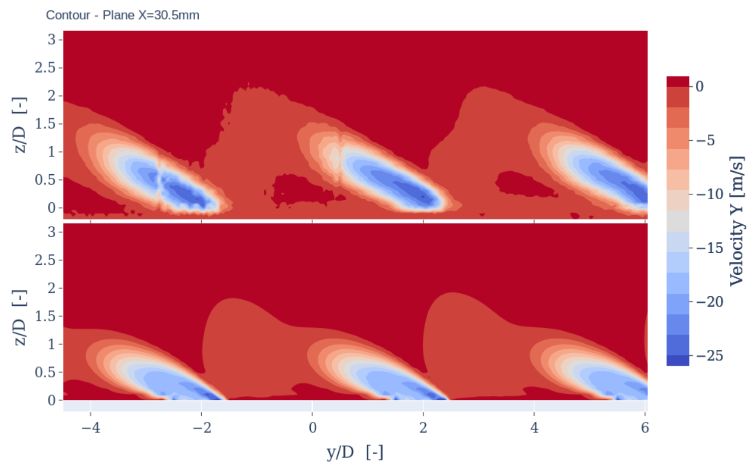

Figure 2. Simulation of the ONERA SOPRANO configuration: example of experimental (top) vs numerical (bottom) results concerning the mean velocity field.

9.4. International Initiatives

9.4.1. Informal International Partners

- Institute of Mathematics and Mathematical Modelling, Almaty, Kazakhstan
  Participant: Pascal Bruel.

  Collaboration with Drs A. Beketaeva and A. Naïmanova for the RANS simulations of a supersonic jet in crossflow configuration for a wide range of pressure ratio ([10]). This year, Pascal Bruel spent two weeks in Almaty in the framework of this partnership.
- University of Evora, Evora, Portugal
  Participant: Pascal Bruel.

  Collaboration with Dr. P. Correia related this year to the partial rewriting of a Fortran code implementing a pressure-based approach for simulating low Mach flows as well as to the promotion of such a pressure-based approach ([25]). This year, Pascal Bruel spent 5 days in Evora in the framework of this partnership.
- University of Ghent, Ghent, Belgium
  Participant: Pascal Bruel.

  Collaboration with Prof. E. Dick related to the development and the promotion of a pressure-based approach for simulating low Mach and all-Mach flows. ([25], [14])

9.4.2. Participation in International Programs

- National University of Córdoba (UNC), Córdoba, Argentina: ECOS-Sud A17A07 project
  Participant: Pascal Bruel.

  2019 was the second year of this project devoted to the simulations of the wind around aerial fuel tanks and related experiments. Pascal Bruel spent two weeks at UNC in the framework of this project.

9.5. International Research Visitors

- Prof. Sergio Elaskar (2 weeks) and PhD student Mauro Grioni (1 month) from University of Córdoba (Argentina) visited the team in the framework of the A17A07 Ecos-Sud project.
- Dr. Paulo Correia from University of Evora spent two weeks in the team in May 2019.

9.5.1. Visits of International Scientists

9.5.1.1. Internships

Mauricio Garcia Zulch from Chile spent 3 months in the team.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Member of the Organizing Committees

- Organizer and scientific chair of the mini-symposium "Numerical method for multi-scale fluid problems" at ICIAM 2019 [JJ].

10.1.2. Journal

10.1.2.1. Member of the Editorial Boards

- Visualization of Mechanical Processes [PB]
- Advisory Board of International Journal of Heat and Fluid Flow [RM]
- Advisory Board of Flow, Turbulence and Combustion [RM]

10.1.2.2. Reviewer - Reviewing Activities

During 2019, the team members reviewed papers for the following journals:

- AIAA Journal [PB, RM]
- Computer & Fluids [RM]
- Int. J. Heat Fluid Flow [RM]
- Journal of Computational Physics [JJ]
- J. Hydr. Res. [RM]
- Physics of Fluids [FM]
- Phys. Rev. Fluids [RM]
- SIAM Journal on Scientific Computing [VP]

10.1.3. Invited Talks

- J. Jung [19]
- R. Manceau [20]

10.1.4. Leadership within the Scientific Community

- Rémi Manceau co-organizes the activities of the Special Interest Group 15 (Turbulence modelling) of ERCOFTAC (European Research Community on Flow, Turbulence and Combustion) as a member of the Steering Committee. The main activity of this group in 2019 was the organization of a workshop in Ljubljana, Slovenia.
- Rémi Manceau coordinates the ANR Project MONACO_2025, a 4-year project started in 2018. The partners are: the institute PPrime, PSA Group and EDF.

10.1.5. Scientific Expertise

- Evaluation of one Ecos Sud project [PB]

10.1.6. Research Administration

- Co-responsible for the organisation of the LMAP seminar of Mathematics and their Applications [JJ].
- Member of the LMAP council [JJ, PB].
- Member of the IPRA research federation scientific council [RM].
- Vincent Perrier is a member of the CUMI-R.
- Vincent Perrier is a member of the CDT, in charge of the evaluation of software projects at the Inria Bordeaux center.
- Vincent Perrier is an elected member of the Inria evaluation committee, and member of the board. [0]
- Vincent Perrier is a member of the CT3-Num committee of Pau University, in charge of managing the computing resources and projects at Pau University.

[0] https://www.inria.fr/en/inria-evaluation-committee

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

Licence : [JJ], Descriptive statistical, 24h, L1 - MIASHS, Université de Pau et des Pays de l'Adour, Pau, France.

Licence : [JJ], Scientific computing, 40.5h, L2 - Informatic, Université de Pau et des Pays de l'Adour, Pau, France.

Licence : [JJ], Numerical analysis for vectorial problems, 33.75h, L2 - Mathematics, Université de Pau et des Pays de l'Adour, Pau, France.

Master : [JJ], Data analysis, 68h25, M1 - GP, Université de Pau et des Pays de l'Adour, Pau, France.

Master : [JJ], Tools for scientific computing, 48h75, M1 - MMS-MSID, Université de Pau et des Pays de l'Adour, Pau, France.

Master : [JJ], Finite volume methods for hyperbolic systems, 15h, Master ANEDP, ENS, Casablanca, Maroc.

Master: [VP], Numerical analysis of PDE 1, Master MMS, Pau.

Master : "Turbulence modelling" (in English), 27h30, M2 - International Master program Turbulence, Université de Poitiers/Ecole centrale de Lille, France. [RM]

Eng. 3 : "Industrial codes for CFD" (in English), 12h30, 3rd year of engineering school (M2), ENSMA, Poitiers, France. [RM]

Eng. 3 : "Advanced physics–Turbulence modelling for CFD", 16h, 3rd year of engineering school (M2), ENSGTI, France. [RM]

10.2.2. Supervision

- PhD in progress : Puneeth Bikkanahally Muni Reddy, "Modelling turbulent flows in natural convection regimes using hybrid RANS-LES approaches, UPPA, October 2018, Rémi Manceau.
- PhD in progress : Gaëtan Mangeon, "Advanced modelling of heat transfer for industrial configurations with or without accounting of the solid wall", UPPA, February 2017, Rémi Manceau.
- PhD in progress : Vladimir Duffal, "Hybrid RANS/LES modelling for unsteady loadings in turbulent flows", UPPA, November 2017, Rémi Manceau.
- PhD in progress : Hassan Al Afailal: "3D simulation of non-reactive internal aerodynamics of spark-ignition engines using an hybrid RANS/LES method", September 2017, Rémi Manceau.
- PhD in progress Saad Jameel : "Turbulence modelling in the mixed and natural convection regimes in the context of automotive applications", UPPA, February 2017, Rémi Manceau.
- PhD in progress : Gustave Sporschill, "Amélioration des modèles pour la turbulence. Applications à la prédiction des écoulements aérodynamiques", UPPA, May 2018, Rémi Manceau.

10.2.3. Juries

The participation in the following thesis juries is noted ("referee" in a French doctoral thesis jury is more or less equivalent to an external opponent in an Anglo-Saxon like PhD jury):

- Thomas Kaiser, "Impact of flow rotation on flame dynamics and hydrodynamic stability", University of Toulouse (France), 31 January 2019. Supervisor: T. Poinsot [PB, Referee].
- Joao Rodrigo Andrade, "Spectral analysis of the turbulent energy cascade and the development of a novel nonlinear subgrid-scale model for large-eddy simulation", Universidade Federale de Uberlândia (Brazil) and University of Lille (France), 27 March 2019. Supervisors: A. S. Neto, G. Mompean and R.L. Thompson [RM, Referee]
- Adithya Ramanathan Krishnan, "Explicit algebraic subfilter scale modeling for DES-like methods and extension to variable density flows", University of Aix-Marseille 3 April 2019. Supervisor: P. Sagaut [RM, Referee]
- Benjamin Lorendeau, "Amélioration des performances via un parallélisme multi-niveaux sur un code CFD en maillages non structurés", University of Bordeaux (France), 16 December 2019. Supervisor: E. Jeannot [PB, Referee]

11. Bibliography

Major publications by the team in recent years

[1] P. BRUEL, S. DELMAS, J. JUNG, V. PERRIER.*A low Mach correction able to deal with low Mach acoustics*, in "Journal of Computational Physics", 2019, vol. 378, p. 723–759, https://hal.inria.fr/hal-01953424

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[6] J.-M. HÉRARD, J. JUNG.*An interface condition to compute compressible flows in variable cross section ducts*, in "Comptes Rendus Mathématiques", February 2016 [*DOI :* 10.1016/J.CRMA.2015.10.026], https://hal.inria.fr/hal-01233251

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Publications of the year

Articles in International Peer-Reviewed Journal

[9] A. H. AFAILAL, J. GALPIN, A. VELGHE, R. MANCEAU.*Development and validation of a hybrid temporal LES model in the perspective of applications to internal combustion engines*, in "Oil & Gas Science and Technology - Revue d'IFP Energies nouvelles", 2019, vol. 74, 56 [*DOI :* 10.2516/OGST/2019031], https://hal-ifp.archives-ouvertes.fr/hal-02162596

[10] A. BEKETAEVA, P. BRUEL, A. Z. NAIMANOVA.*Detailed Comparative Analysis of Interaction of a Supersonic Flow with a Transverse Gas Jet at High Pressure Ratios*, in "Technical Physics / Zhurnal Tekhnicheskoi Fiziki", October 2019, vol. 64, n° 10, p. 1430-1440 [*DOI :* 10.1134/S1063784219100049], https://hal.inria.fr/hal-02373910

[11] S. BENHAMADOUCHE, I. AFGAN, R. MANCEAU.*Numerical simulations of flow and heat transfer in a wall-bounded pin matrix*, in "Flow, Turbulence and Combustion", 2019 [*DOI :* 10.1007/S10494-019-00046-8], https://hal.archives-ouvertes.fr/hal-02179021

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Invited Conferences

[19] J. JUNG.*Quelques applications des mathématiques au centre Inria de Bordeaux Sud-Ouest*, in "Septième journée des Sciences de l'Ingénieur", Casablanca, Morocco, June 2019, https://hal.inria.fr/hal-02283149

[20] R. MANCEAU.*Modelling of turbulent natural convection (keynote lecture)*, in "16th ERCOFTAC SIG15 Workshop on Modelling of wall bounded turbulent natural convection", Ljubljana, Slovenia, Jozef Stefan Institute (IJS), October 2019, https://hal.archives-ouvertes.fr/hal-02319389

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Project-Team CARDAMOM

Certified Adaptive discRete moDels for robust simulAtions of CoMplex flOws with Moving fronts

IN COLLABORATION WITH: Institut de Mathématiques de Bordeaux (IMB)

IN PARTNERSHIP WITH:
Institut Polytechnique de Bordeaux

Université de Bordeaux

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Numerical schemes and simulations

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Project-Team CARDAMOM

Creation of the Team: 2015 January 01, updated into Project-Team: 2016 June 01

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2. Overall Objectives

2.1. Overall Objectives

CARDAMOM is a joint team of Inria Bordeaux - Sud-Ouest, University of Bordeaux and Bordeaux Inst. Nat. Polytechnique) and IMB (Institut de Mathématiques de Bordeaux – CNRS UMR 5251, University of Bordeaux). CARDAMOM has been created on January 1st, 2015 (https://team.inria.fr/cardamom/). The CARDAMOM project aims at providing a robust modelling strategy for engineering applications involving complex flows with moving fronts. The term front here denotes either an actual material boundary (e.g. multiple phases), a physical discontinuity (e.g. shock waves), or a transition layer between regions with completely different dominant flow behaviour (e.g. breaking waves). These fronts introduce a multi-scale behaviour. The resolution of all the scales is however not feasible in certification and optimization cycles, and not necessary in many engineering applications, while in others it is enough to model the average effect of small scales on large ones (closure models). We plan to develop application-tailored models obtained by a tight combination of *asymptotic PDE* (Partial Differential Equations) modelling, *adaptive high order PDE discretizations*, and a *quantitative certification* step assessing the sensitivity of outputs to both model components (equations, numerical methods, etc) and random variations of the data. The goal is to improve parametric analysis and design cycles, by increasing both accuracy and confidence in the results thanks to improved physical and numerical modelling, and to a quantitative assessment of output uncertainties. This requires a research program mixing of PDE analysis, high order discretizations, Uncertainty Quantification (UQ), robust optimization, and some specific engineering know how. Part of these scientific activities started in the BACCHUS and MC2 teams. CARDAMOM harmonizes and gives new directions to this know how.

2.2. Scientific context and challenges

The objective of this project is to provide improved analysis and design tools for engineering applications involving fluid flows, and in particular flows with moving fronts. In our applications *a front is either an actual material interface, or a well identified and delimited transition region in which the flow undergoes a change in its dominant macroscopic character*. One example is the certification of wing de anti-icing systems, involving the predictions of ice formation and detachment, and of ice debris trajectories to evaluate the risk of downstream impact on aircraft components [89], [30]. Another application, relevant for space reentry, is the study of transitional regimes in high altitude gas dynamics in which extremely thin layers appear in the flow which cannot be analysed with classical continuous models (Navier-Stokes equations) used by engineers [35], [61]. An important example in coastal engineering is the transition between propagating and breaking waves, characterized by a strong local production of vorticity and by dissipative effects absent when waves propagates [37]. Similar examples in energy and material engineering provide the motivation of this project.

All these application fields involve either the study of new technologies (e.g. new design/certification tools for aeronautics [44], [55], [73], [30] or for wave energy conversion [53]), or parametric studies of complex environments (e.g. harbour dynamics [63], or estuarine hydrodynamics [28]), or hazard assessment and prevention [57]. In all cases, computationally affordable, quick, and accurate numerical modelling is essential to improve the quality of (or to shorten) design cycles and allow performance level enhancements in early stages of development [93]. The goal is to afford simulations over very long times with many parameters or to embed a model in an alert system.

In addition to this, even in the best of circumstances, the reliability of numerical predictions is limited by the intrinsic randomness of the data used in practice to define boundary conditions, initial conditions, geometry, etc. This uncertainty, related to the measurement errors, is defined as *aleatory*, and cannot be removed, nor reduced. In addition, physical models and the related Partial Differential Equations (PDEs), feature a structural uncertainty, since they are derived with assumptions of limited validity and calibrated with manipulated experimental data (filtering, averaging, etc ..). These uncertainties are defined as *epistemic*, as they are a deficiency due to a lack of knowledge [42], [82]. Unfortunately, measurements in fluids are delicate and expensive. In complex flows, especially in flows involving interfaces and moving fronts, they are sometimes impossible to carry out, due to scaling problems, repeatability issues (e.g. tsunami events), technical issues (different physics in the different flow regions) or dangerousness (e.g. high temperature reentry flows, or combustion). Frequently, they are impractical, due to the time scales involved (e.g. characterisation of oxidation processes related to a new material micro-/meso- structure [46]). This increases the amount of uncertainties associated to measurements and reduces the amount of information available to construct physical/PDE models. These uncertainties play also a crucial role when one wants to deal with numerical certification or optimization of a fluid based device. However, this makes the required number of flow simulations grow as high as hundreds or even thousands of times. The associated costs are usually prohibitive. So the real challenge is to be able to construct an accurate and computationally affordable numerical model handling efficiently uncertainties. In particular, this model should be able to take into account the variability due to uncertainties, those coming from the certification/optimization parameters as well as those coming from modelling choices.

To face this challenge and provide new tools to accurately and robustly modelize and certify engineering devices based on fluid flows with moving fronts, we propose a program mixing scientific research in asymptotic PDE analysis, high order adaptive PDE discretizations and uncertainty quantification.

2.3. Our approach

A standar way a certification study may be contacted can be described as two box modelling. The first box is the physical model itself, which is composed of the 3 main elements: PDE system, mesh generation/adaptation, and discretization of the PDE (numerical scheme). The second box is the main robust certification loop which contains separate boxes involving the evaluation of the physical model, the post-processing of the output, and the exploration of the spaces of physical and stochastic parameters (uncertainties). There are some known

interactions taking place in the loop which are a necessary to exploit as much as possible the potential of high order methods [66] such as e.g. $h-$/$p-$/$r-$ adaptation in the physical model w.r.t. some post-processed output value, or w.r.t. some sort of adjoint sensitivity coming from the physical parameter evolution box, etc.
As things stand today, we will not be able to take advantage of the potential of new high order numerical techniques and of hierarchical (multi-fidelity) robust certification approaches without some very aggressive adaptive methodology. Such a methodology, will require interactions between e.g. the uncertainty quantification methods and the adaptive spatial discretization, as well as with the PDE modelling part. Such a strategy cannot be developed, let alone implemented in an operational context, without completely disassembling the scheme of the two boxes, and letting all the parts (PDE system, mesh generation/adaptation, numerical scheme, evalutaion of the physical model, the post processing of the output, exploration of the spaces of physical and stochastic parameters) interact together. This is what we want to do in CARDAMOM . We have the unique combination of skills which allows to explore such an avenue: PDE analysis, high order numerical discretizations, mesh generation and adaptation, optimization and uncertainty quantification, specific issues related to the applications considered.

Our strength is also our unique chance of exploring the interactions between all the parts. We will try to answer some fundamental questions related to the following aspects

- What are the relations between PDE model accuracy (asymptotic error) and scheme accuracy, and how to control, en possibly exploit these relations to minimize the error for a given computational effort ;
- How to devise and implement adaptation techniques ($r-$, $h-$, and $p-$) for time dependent problems while guaranteeing an efficient time marching procedure (minimize CPU time at constant error) ;
- How to exploit the wide amount of information made available from the optimization *and* uncertainty quantification process to construct a more aggressive adaptation strategy in physical, parameter, and stochastic space, and in the physical model itself ;

These research avenues related to the PDE models and numerical methods used, will allow us to have an impact on the applications communities targeted which are

- Aeronautics and aerospace engineering (de-anti icing systems, space re-entry) ;
- Energy engineering (organic Rankine cycles and wave energy conversion) ;
- Material engineering (self healing composite materials) ;
- Coastal engineering (coastal protection, hazard assessment etc.).

The main research directions related to the above topics are discussed in the following section.

3. Research Program

3.1. Variational discrete asymptotic modelling

In many of the applications we consider, intermediate fidelity models are or can be derived using an asymptotic expansion for the relevant scale resolving PDEs, and eventually considering some averaged for of the resulting continuous equations. The resulting systems of PDEs are often very complex and their characterization, e.g. in terms of stability, unclear, or poor, or too complex to allow to obtain discrete analogy of the continuous properties. This makes the numerical approximation of these PDE systems a real challenge. Moreover, most of these models are often based on asymptotic expansions involving small geometrical scales. This is true for many applications considered here involving flows in/of thin layers (free surface waves, liquid films on wings generating ice layers, oxide flows in material cracks, etc). This asymptotic expansion is nothing else than a discretization (some sort of Taylor expansion) in terms of the small parameter. The actual discretization of the PDE system is another expansion in space involving as a small parameter the mesh size. What is the interaction between these two expansions ? Could we use the spatial discretization (truncation error) as means of filtering undesired small scales instead of having to explicitly derive PDEs for the large scales ? We will investigate in depth the relations between asymptotics and discretization by :

- comparing the asymptotic limits of discretized forms of the relevant scale resolving equations with the discretization of the analogous continuous asymptotic PDEs. Can we discretize a well understood system of PDEs instead of a less understood and more complex one ? ;
- study the asymptotic behaviour of error terms generated by coarse one-dimensional discretization in the direction of the “small scale”. What is the influence of the number of cells along the vertical direction, and of their clustering ? ;
- derive equivalent continuous equations (modified equations) for anisotropic discretizations in which the direction is direction of the “small scale” is approximated with a small number of cells. What is the relation with known asymptotic PDE systems ?

Our objective is to gain sufficient control of the interaction between discretization and asymptotics to be able to replace the coupling of several complex PDE systems by adaptive strongly anisotrotropic finite elemient approximations of relevant and well understood PDEs. Here the anisotropy is intended in the sense of having a specific direction in which a much poorer (and possibly variable with the flow conditions) polynomial approximation (expansion) is used. The final goal is, profiting from the availability of faster and cheaper computational platforms, to be able to automatically control numerical *and* physical accuracy of the model with the same techniques. This activity will be used to improve our modelling in coastal engineering as well as for de-anti icing systems, wave energy converters, composite materials (cf. next sections).

In parallel to these developments, we will make an effort in to gain a better understanding of continuous asymptotic PDE models. We will in particular work on improving, and possibly, simplifying their numerical approximation. An effort will be done in trying to embed in these more complex nonlinear PDE models discrete analogs of operator identities necessary for stability (see e.g. the recent work of [70], [72] and references therein).

3.2. High order discretizations on moving adaptive meshes

We will work on both the improvement of high order mesh generation and adaptation techniques, and the construction of more efficient, adaptive high order discretisation methods.
Concerning curved mesh generation, we will focus on two points. First propose a robust and automatic method to generate curved simplicial meshes for realistic geometries. The untangling algorithm we plan to develop is a hybrid technique that gathers a local mesh optimization applied on the surface of the domain and a linear elasticity analogy applied in its volume. Second we plan to extend the method proposed in [26] to hybrid meshes (prism/tetra).

For time dependent adaptation we will try to exploit as much as possible the use of $r-$adaptation techniques based on the solution of some PDE system for the mesh. We will work on enhancing the results of [29] by developing more robust nonlinear variants allowing to embed rapidly moving objects. For this the use of non-linear mesh PDEs (cf e.g. [80], [85], [38]), combined with Bezier type approximations for the mesh displacements to accommodate high order curved meshes [26], and with improved algorithms to discretize accurately and fast the elliptic equations involved. For this we will explore different type of relaxation methods, including those proposed in [71], [75], [74] allowing to re-use high order discretizations techniques already used for the flow variables. All these modelling approaches for the mesh movement are based on some minimization argument, and do not allow easily to take into account explicitly properties such as e.g. the positivity of nodal volumes. An effort will be made to try to embed these properties, as well as to improve the control on the local mesh sizes obtained. Developments made in numerical methods for Lagrangian hydrodynamics and compressible materials may be a possible path for these objectives (see e.g. [49], [91], [90] and references therein). We will stretch the use of these techniques as much as we can, and couple them with remeshing algorithms based on local modifications plus conservative, high order, and monotone ALE (or other) remaps (cf. [27], [58], [92], [47] and references therein).

The development of high order schemes for the discretization of the PDE will be a major part of our activity. We will work from the start in an Arbitrary Lagrangian Eulerian setting, so that mesh movement will be easily accommodated, and investigate the following main points:

- the ALE formulation is well adapted both to handle moving meshes, and to provide conservative, high order, and monotone remaps between different meshes. We want to address the issue of cost-accuracy of adaptive mesh computations by exploring different degrees of coupling between the flow and the mesh PDEs. Initial experience has indicated that a clever coupling may lead to a considerable CPU time reduction for a given resolution [29]. This balance is certainly dependent on the nature of the PDEs, on the accuracy level sought, on the cost of the scheme, and on the time stepping technique. All these elements will be taken into account to try to provide the most efficient formulation ;
- the conservation of volume, and the subsequent preservation of constant mass-momentum-energy states on deforming domains is one of the most primordial elements of Arbitrary Lagrangian-Eulerian formulations. For complex PDEs as the ones considered here, of especially for some applications, there may be a competition between the conservation of e.g. mass, an the conservation of other constant states, as important as mass. This is typically the case for free surface flows, in which mass preservation is in competitions with the preservation of constant free surface levels [29]. Similar problems may arise in other applications. Possible solutions to this competition may come from super-approximation (use of higher order polynomials) of some of the data allowing to reduce (e.g. bathymetry) the error in the preservation of one of the competing quantities. This is similar to what is done in super-parametric approximations of the boundaries of an object immersed in the flow, except that in our case the data may enter the PDE explicitly and not only through the boundary conditions. Several efficient solutions for this issue will be investigated to obtain fully conservative moving mesh approaches:
- an issue related to the previous one is the accurate treatment of wall boundaries. It is known that even for standard lower order (second) methods, a higher order, curved, approximation of the boundaries may be beneficial. This, however, may become difficult when considering moving objects, as in the case e.g. of the study of the impact of ice debris in the flow. To alleviate this issue, we plan to follow on with our initial work on the combined use of immersed boundaries techniques with high order, anisotropic (curved) mesh adaptation. In particular, we will develop combined approaches involving high order hybrid meshes on fixed boundaries with the use of penalization techniques and immersed boundaries for moving objects. We plan to study the accuracy obtainable across discontinuous functions with $r-$adaptive techniques, and otherwise use whenever necessary anisotropic meshes to be able to provide a simplified high order description of the wall boundary (cf. [69]). The use of penalization will also provide a natural setting to compute immediate approximations of the forces on the immersed body [73], [76]. An effort will be also made on improving the accuracy of these techniques using e.g. higher order approaches, either based on generalizations of classical splitting methods [59], or on some iterative Defect Correction method (see e.g. [40]) ;
- the proper treatment of different physics may be addressed by using mixed/hybrid schemes in which different variables/equations are approximated using a different polynomial expansion. A typical example is our work on the discretization of highly non-linear wave models [54] in which we have shown how to use a standard continuous Galerkin method for the elliptic equation/variable representative of the dispersive effects, while the underlying hyperbolic system is evolved using a (discontinuous) third order finite volume method. This technique will be generalized to other classes of discontinuous methods, and similar ideas will be used in other context to provide a flexible approximation. Such mathods have clear advantages in multiphase flows but not only. A typical example where such mixed methods are beneficial are flows involving different species and tracer equations, which are typically better treated with a discontinuous approximation. Another example is the use of this mixed approximation to describe the topography with a high order continuous polynomial even in discontinuous method. This allows to greatly simplify the numerical treatment of the bathymetric source terms ;

- the enhancement of stabilized methods based on some continuous finite element approximation will remain a main topic. We will further pursue the study on the construction of simplified stabilization operators which do not involve any contributions to the mass matrix. We will in particular generalize our initial results to higher order spatial approximations using cubature points, or Bezier polynomials, or also hierarchical approximations. This will also be combined with time dependent variants of the reconstruction techniques initially proposed by D. Caraeni [39], allowing to have a more flexible approach similar to the so-called $\mathrm{P}^{\mathrm{n}}\mathrm{P}^{\mathrm{m}}$ method [52], [84]. How to localize these enhancements, and to efficiently perform local reconstructions/enrichment, as well as $p-$adaptation, and handling hanging nodes will also be a main line of work. A clever combination of hierarchical enrichment of the polynomials, with a constrained approximation will be investigated. All these developments will be combined with the shock capturing/positivity preserving construction we developed in the past. Other discontinuity resolving techniques will be investigated as well, such as face limiting techniques as those partially studied in [56] ;
- time stepping is an important issue, especially in presence of local mesh adaptation. The techniques we use will force us to investigate local and multilevel techniques. We will study the possibility constructing semi-implicit methods combining extrapolation techniques with space-time variational approaches. Other techniques will be considered, as multi-stage type methods obtained using Defect-Correction, Multi-step Runge-Kutta methods [36], as well as spatial partitioning techniques [65]. A major challenge will be to be able to guarantee sufficient locality to the time integration method to allow to efficiently treat highly refined meshes, especially for viscous reactive flows. Another challenge will be to embed these methods in the stabilized methods we will develop.

3.3. Coupled approximation/adaptation in parameter and physical space

As already remarked, classical methods for uncertainty quantification are affected by the so-called Curse-of-Dimensionality. Adaptive approaches proposed so far, are limited in terms of efficiency, or of accuracy. Our aim here is to develop methods and algorithms permitting a very high-fidelity simulation in the physical and in the stochastic space at the same time. We will focus on both non-intrusive and intrusive approaches.

Simple non-intrusive techniques to reduce the overall cost of simulations under uncertainty will be based on adaptive quadrature in stochastic space with mesh adaptation in physical space using error monitors related to the variance of to the sensitivities obtained e.g. by an ANOVA decomposition. For steady state problems, remeshing using metric techniques is enough. For time dependent problems both mesh deformation and re-meshing techniques will be used. This approach may be easily used in multiple space dimensions to minimize the overall cost of model evaluations by using high order moments of the properly chosen output functional for the adaptation (as in optimization). Also, for high order curved meshes, the use of high order moments and sensitivities issued from the UQ method or optimization provides a viable solution to the lack of error estimators for high order schemes.

Despite the coupling between stochastic and physical space, this approach can be made massively parallel by means of extrapolation/interpolation techniques for the high order moments, in time and on a reference mesh, guaranteeing the complete independence of deterministic simulations. This approach has the additional advantage of being feasible for several different application codes due to its non-intrusive character.
To improve on the accuracy of the above methods, intrusive approaches will also be studied. To propagate uncertainties in stochastic differential equations, we will use Harten's multiresolution framework, following [25]. This framework allows a reduction of the dimensionality of the discrete space of function representation, defined in a proper stochastic space. This reduction allows a reduction of the number of explicit evaluations required to represent the function, and thus a gain in efficiency. Moreover, multiresolution analysis offers a natural tool to investigate the local regularity of a function and can be employed to build an efficient refinement strategy, and also provides a procedure to refine/coarsen the stochastic space for unsteady problems. This strategy should allow to capture and follow all types of flow structures, and, as proposed in [25], allows to formulate a non-linear scheme in terms of compression capabilities, which should allow to handle non-smooth problems. The potential of the method also relies on its moderate intrusive behaviour, compared to e.g. spectral Galerkin projection, where a theoretical manipulation of the original system is needed.

Several activities are planned to generalize our initial work, and to apply it to complex flows in multiple (space) dimensions and with many uncertain parameters.

The first is the improvement of the efficiency. This may be achieved by means of anisotropic mesh refinement, and by experimenting with a strong parallelization of the method. Concerning the first point, we will investigate several anisotropic refinement criteria existing in literature (also in the UQ framework), starting with those already used in the team to adapt the physical grid. Concerning the implementation, the scheme formulated in [25] is conceived to be highly parallel due to the external cycle on the number of dimensions in the space of uncertain parameters. In principle, a number of parallel threads equal to the number of spatial cells could be employed. The scheme should be developed and tested for treating unsteady and discontinuous probability density function, and correlated random variables. Both the compression capabilities and the accuracy of the scheme (in the stochastic space) should be enhanced with a high-order multidimensional conservative and non-oscillatory polynomial reconstruction (ENO/WENO).

Another main objective is related to the use of multiresolution in both physical and stochastic space. This requires a careful handling of data and an updated definition of the wavelet. Until now, only a weak coupling has been performed, since the number of points in the stochastic space varies according to the physical space, but the number of points in the physical space remains unchanged. Several works exist on the multiresolution approach for image compression, but this could be the first time i in which this kind of approach would be applied at the same time in the two spaces with an unsteady procedure for refinement (and coarsening). The experimental code developed using these technologies will have to fully exploit the processing capabilities of modern massively parallel architectures, since there is a unique mesh to handle in the coupled physical/stochastic space.

3.4. Robust multi-fidelity modelling for optimization and certification

Due to the computational cost, it is of prominent importance to consider multi-fidelity approaches gathering high-fidelity and low-fidelity computations. Note that low-fidelity solutions can be given by both the use of surrogate models in the stochastic space, and/or eventually some simplified choices of physical models of some element of the system. Procedures which deal with optimization considering uncertainties for complex problems may require the evaluation of costly objective and constraint functions hundreds or even thousands of times. The associated costs are usually prohibitive. For these reason, the robustness of the optimal solution should be assessed, thus requiring the formulation of efficient methods for coupling optimization and stochastic spaces. Different approaches will be explored. Work will be developed along three axes:

1. a robust strategy using the statistics evaluation will be applied separately, *i.e.* using only low or high-fidelity evaluations. Some classical optimization algorithms will be used in this case. Influence of high-order statistics and model reduction in the robust design optimization will be explored, also by further developing some low-cost methods for robust design optimization working on the so-called Simplex^2 method [45] ;
2. a multi-fidelity strategy by using in an efficient way low fidelity and high-fidelity estimators both in physical and stochastic space will be conceived, by using a Bayesian framework for taking into account model discrepancy and a PC expansion model for building a surrogate model ;
3. develop advanced methods for robust optimization. In particular, the Simplex^2 method will be modified for introducing a hierarchical refinement with the aim to reduce the number of stochastic samples according to a given design in an adaptive way.

This work is related to the activities foreseen in the EU contract MIDWEST, in the ANR LabCom project VIPER (currently under evaluation), in a joint project with DGA and VKI, in two projects under way with AIRBUS and SAFRAN-HERAKLES.

4. Application Domains

4.1. De-anti icing systems

Impact of large ice debris on downstream aerodynamic surfaces and ingestion by aft mounted engines must be considered during the aircraft certification process. It is typically the result of ice accumulation on unprotected surfaces, ice accretions downstream of ice protected areas, or ice growth on surfaces due to delayed activation of ice protection systems (IPS) or IPS failure. This raises the need for accurate ice trajectory simulation tools to support pre-design, design and certification phases while improving cost efficiency. Present ice trajectory simulation tools have limited capabilities due to the lack of appropriate experimental aerodynamic force and moment data for ice fragments and the large number of variables that can affect the trajectories of ice particles in the aircraft flow field like the shape, size, mass, initial velocity, shedding location, etc... There are generally two types of model used to track shed ice pieces. The first type of model makes the assumption that ice pieces do not significantly affect the flow. The second type of model intends to take into account ice pieces interacting with the flow. We are concerned with the second type of models, involving fully coupled time-accurate aerodynamic and flight mechanics simulations, and thus requiring the use of high efficiency adaptive tools, and possibly tools allowing to easily track moving objects in the flow. We will in particular pursue and enhance our initial work based on adaptive immerse boundary capturing of moving ice debris, whose movements are computed using basic mechanical laws.

In [31] it has been proposed to model ice shedding trajectories by an innovative paradigm that is based on CArtesian grids, PEnalization and LEvel Sets (LESCAPE code). Our objective is to use the potential of high order unstructured mesh adaptation and immersed boundary techniques to provide a geometrically flexible extension of this idea. These activities will be linked to the development of efficient mesh adaptation and time stepping techniques for time dependent flows, and their coupling with the immersed boundary methods we started developing in the FP7 EU project STORM [24], [76]. In these methods we compensate for the error at solid walls introduced by the penalization by using anisotropic mesh adaptation [50], [68], [69]. From the numerical point of view one of the major challenges is to guarantee efficiency and accuracy of the time stepping in presence of highly stretched adaptive and moving meshes. Semi-implicit, locally implicit, multi-level, and split discretizations will be explored to this end.

Besides the numerical aspects, we will deal with modelling challenges. One source of complexity is the initial conditions which are essential to compute ice shedding trajectories. It is thus extremely important to understand the mechanisms of ice release. With the development of next generations of engines and aircraft, there is a crucial need to better assess and predict icing aspects early in design phases and identify breakthrough technologies for ice protection systems compatible with future architectures. When a thermal ice protection system is activated, it melts a part of the ice in contact with the surface, creating a liquid water film and therefore lowering ability of the ice block to adhere to the surface. The aerodynamic forces are then able to detach the ice block from the surface [33]. In order to assess the performance of such a system, it is essential to understand the mechanisms by which the aerodynamic forces manage to detach the ice. The current state of the art in icing codes is an empirical criterion. However such an empirical criterion is unsatisfactory. Following the early work of [34], [30] we will develop appropriate asymptotic PDE approximations allowing to describe the ice formation and detachment, trying to embed in this description elements from damage/fracture mechanics. These models will constitute closures for aerodynamics/RANS and URANS simulations in the form of PDE wall models, or modified boundary conditions.

In addition to this, several sources of uncertainties are associated to the ice geometry, size, orientation and the shedding location. In very few papers [78], some sensitivity analysis based on Monte Carlo method have been conducted to take into account the uncertainties of the initial conditions and the chaotic nature of the ice particle motion. We aim to propose some systematic approach to handle every source of uncertainty in an efficient way relying on some state-of-art techniques developed in the Team. In particular, we will perform an uncertainty propagation of some uncertainties on the initial conditions (position, orientation, velocity,...) through a low-fidelity model in order to get statistics of a multitude of particle tracks. This study will be done in collaboration with ETS (Ecole de Technologies Supérieure, Canada). The longterm objective is to produce footprint maps and to analyse the sensitivity of the models developed.

4.2. Energy

We will develop modelling and design tools, as well as dedicated platforms, for Rankine cycles using complex fluids (organic compounds), and for wave energy extraction systems.

Organic Rankine Cycles (ORCs) use heavy organic compounds as working fluids. This results in superior efficiency over steam Rankine cycles for source temperatures below 900 K. ORCs typically require only a single-stage rotating component making them much simpler than typical multi-stage steam turbines. The strong pressure reduction in the turbine may lead to supersonic flows in the rotor, and thus to the appearance of shocks, which reduces the efficiency due to the associated losses. To avoid this, either a larger multi stage installation is used, in which smaller pressure drops are obtained in each stage, or centripetal turbines are used, at very high rotation speeds (of the order of 25,000 rpm). The second solution allows to keep the simplicity of the expander, but leads to poor turbine efficiencies (60-80%) - w.r.t. modern, highly optimized, steam and gas turbines - and to higher mechanical constraints. The use of *dense-gas working fluids*, *i.e.* operating close to the saturation curve, in properly chosen conditions could increase the turbine critical Mach number avoiding the formation of shocks, and increasing the efficiency. Specific shape optimization may enhance these effects, possibly allowing the reduction of rotation speeds. However, dense gases may have significantly different properties with respect to dilute ones. Their dynamics is governed by a thermodynamic parameter known as the fundamental derivative of gas dynamics

$$\Gamma = 1 + \frac{\rho}{c}\left(\frac{\partial c}{\partial \rho}\right)_s, \tag{1}$$

where ρ is the density, c is the speed of sound and s is the entropy. For ideal gas $\Gamma = (\gamma+1)/2 > 1$. For some complex fluids and some particular conditions of pressure and temperature, Γ may be lower that one, implying that $(\partial c/\partial \rho)_s < 0$. This means that the acceleration of pressure perturbations through a variable density fluids may be reversed and become a deceleration. It has been shown that, for $\Gamma << 1$, compression shocks are strongly reduced, thus alleviating the shock intensity. This has great potential in increasing the efficiency. This is why so much interest is put on dense gas ORCs.

The simulation of these gases requires accurate thermodynamic models, such as Span-Wagner or Peng-Robinson (see [43]). The data to build these models is scarce due to the difficulty of performing reliable experiments. The related uncertainty is thus very high. Our work will go in the following directions:

1. develop deterministic models for the turbine and the other elements of the cycle. These will involve multi-dimensional high fidelity, as well as intermediate and low fidelity (one- and zero-dimensional), models for the turbine, and some 0D/1D models for other element of the cycle (pump, condenser, etc) ;
2. validation of the coupling between the various elements. The following aspects will be considered: characterization of the uncertainties on the cycle components (e.g. empirical coefficients modelling the pump or the condenser), calibration of the thermodynamic parameters, model the uncertainty of each element, and the influence of the unsteady experimental data ;
3. demonstrate the interest of a specific optimization of geometry, operating conditions, and the choice of the fluid, according to the geographical location by including local solar radiation data. Multi-objective optimization will be considered to maximize performance indexes (e.g. Carnot efficiency, mechanical work and energy production), and to reduce the variability of the output.

This work will provide modern tools for the robust design of ORCs systems. It benefits from the direct collaboration with the SME EXOES (ANR LAbCom VIPER), and from a collaboration with LEMMA.

Wave energy conversion is an emerging sector in energy engineering. The design of new and efficient Wave Energy Converters (WECs) is thus a crucial activity. As pointed out by Weber [93], it is more economical to raise the technology performance level (TPL) of a wave energy converter concept at low technology readiness level (TRL). Such a development path puts a greater demand on the numerical methods used. The findings of Weber also tell us that important design decisions as well as optimization should be performed as early in the development process as possible. However, as already mentioned, today the wave energy sector relies heavily on the use of tools based on simplified linear hydrodynamic models for the prediction of motions, loads, and power production. Our objective is to provide this sector, and especially SMEs, with robust design tools to minimize the uncertainties in predicted power production, loads, and costs of wave energy.

Following our initial work [53], we will develop, analyse, compare, and use for multi-fidelity optimization,non-linear models of different scales (fidelity) ranging from simple linear hydrodynamics over asymptotic discrete nonlinear wave models, to non-hydrostatic anisoptropic Euler free surface solvers. We will not work on the development of small scale models (VOF-RANS or LES) but may use such models, developed by our collaborators, for validation purposes. These developments will benefit from all our methodological work on asymptotic modelling and high order discretizations. As shown in [53], asymptotic models foe WECs involve an equation for the pressure on the body inducing a PDE structure similar to that of incompressible flow equations. The study of appropriate stable and efficient high order approximations (coupling velocity-pressure, efficient time stepping) will be an important part of this activity. Moreover, the flow-floating body interaction formulation introduces time stepping issues similar to those encountered in fluid structure interaction problems, and require a clever handling of complex floater geometries based on adaptive and ALE techniques. For this application, the derivation of fully discrete asymptotics may actually simplify our task.

Once available, we will use this hierarchy of models to investigate and identify the modelling errors, and provide a more certain estimate of the cost of wave energy. Subsequently we will look into optimization cycles by comparing time-to-decision in a multi-fidelity optimization context. In particular, this task will include the development and implementation of appropriate surrogate models to reduce the computational cost of expensive high fidelity models. Here especially artificial neural networks (ANN) and Kriging response surfaces (KRS) will be investigated. This activity on asymptotic non-linear modelling for WECs, which has had very little attention in the past, will provide entirely new tools for this application. Multi-fidelity robust optimization is also an approach which has never been applied to WECs.

This work is the core of the EU OCEANEranet MIDWEST project, which we coordinate. It will be performed in collaboration with our European partners, and with a close supervision of European SMEs in the sector, which are part of the steering board of MIDWEST (WaveDragon, Waves4Power, Tecnalia).

4.3. Materials engineering

Because of their high strength and low weight, ceramic-matrix composite materials (CMCs) are the focus of active research for aerospace and energy applications involving high temperatures, either military or civil. Though based on brittle ceramic components, these composites are not brittle due to the use of a fibre/matrix interphase that preserves the fibres from cracks appearing in the matrix. Recent developments aim at implementing also in civil aero engines a specific class of Ceramic Matrix Composite materials (CMCs) that show a self-healing behaviour. Self-healing consists in filling cracks appearing in the material with a dense fluid formed in-situ by oxidation of part of the matrix components. Self-healing (SH) CMCs are composed of a complex three-dimensional topology of woven fabrics containing fibre bundles immersed in a matrix coating of different phases. The oxide seal protects the fibres which are sensitive to oxidation, thus delaying failure. The obtained lifetimes reach hundreds of thousands of hours [81].

The behaviour of a fibre bundle is actually extremely variable, as the oxidation reactions generating the self-healing mechanism have kinetics strongly dependent on temperature and composition. In particular, the lifetime of SH-CMCs depends on: (i) temperature and composition of the surrounding atmosphere; (ii) composition and topology of the matrix layers; (iii) the competition of the multidimensional diffusion/oxidation/volatilization processes; (iv) the multidimensional flow of the oxide in the crack; (v) the inner topology of fibre bundles; (vi) the distribution of critical defects in the fibres. Unfortunately, experimental investigations on the full materials are too long (they can last years) and their output too qualitative (the coupled effects can only be observed a-posteriori on a broken sample). Modelling is thus essential to study and to design SH-CMCs.

In collaboration wit the LCTS laboratory (a joint CNRS-CEA-SAFRAN-Bordeaux University lab devoted to the study of thermo-structural materials in Bordeaux), we are developing a multi-scale model in which a structural mechanics solver is coupled with a closure model for the crack physico chemistry. This model is obtained as a multi-dimensional asymptotic crack averaged approximation fo the transport equations (Fick's laws) with chemical reactions sources, plus a potential model for the flow of oxide [46], [51], [79]. We have demonstrated the potential of this model in showing the importance of taking into account the multi-dimensional topology of a fibre bundle (distribution of fibres) in the rupture mechanism. This means that the 0-dimensional model used in most of the studies (se e.g. [41]) will underestimate appreciably the lifetime of the material. Based on these recent advances, we will further pursue the development of multi-scale multi-dimensional asymptotic closure models for the parametric design of self healing CMCs. Our objectives are to provide: (i) new, non-linear multi-dimensional mathematical model of CMCs, in which the physico-chemistry of the self-healing process is more strongly coupled to the two-phase (liquid gas) hydro-dynamics of the healing oxide ; (ii) a model to represent and couple crack networks ; (iii) a robust and efficient coupling with the structural mechanics code ; (iv) validate this platform with experimental data obtained at the LCTS laboratory. The final objective is to set up a multi-scale platform for the robust prediction of lifetime of SH-CMCs, which will be a helpful tool for the tailoring of the next generation of these materials.

4.4. Coastal and civil engineering

Our objective is to bridge the gap between the development of high order adaptive methods, which has mainly been performed in the industrial context and environmental applications, with particular attention to coastal and hydraulic engineering. We want to provide tools for adaptive non-linear modelling at large and intermediate scales (near shore, estuarine and river hydrodynamics). We will develop multi-scale adaptive models for free surface hydrodynamics. Beside the models and codes themselves, based on the most advanced numerics we will develop during this project, we want to provide sufficient know how to control, adapt and optimize these tools.

We will focus our effort in the understanding of the interactions between asymptotic approximations and numerical approximations. This is extremely important in at least two aspects. The first is the capability of a numerical model to handle highly dispersive wave propagation. This is usually done by high accuracy asymptotic PDE expansions. Here we plan to make heavily use of our results concerning the relations between vertical asymptotic expansions and standard finite element approximations. In particular, we will invest some effort in the development of $xy+z$ adaptive finite element approximations of the incompressible Euler equations. Local $p-$adaptation of the vertical approximation may provide a "variable depth" approximation exploiting numerics instead of analytical asymptotics to control the physical behaviour of the model.

Another important aspect which is not understood well enough at the moment is the role of dissipation in wave breaking regions. There are several examples of breaking closure, going from algebraic and PDE-based eddy viscosity methods [64], [83], [77], [48], to hybrid methods coupling dispersive PDEs with hyperbolic ones, and trying to mimic wave breaking with travelling bores [87], [88], [86], [62], [54]. In both cases, numerical dissipation plays an important role and the activation or not of the breaking closure, as the quantitative contribution of numerical dissipation to the flow has not been properly investigated. These elements must be clarified to allow full control of adaptive techniques for the models used in this type of applications.

Another point we want to clarify is how to optimize the discretization of asymptotic PDE models. In particular, when adding mesh size(s) and time step, we are in presence of at least 3 (or even more) small parameters. The relations between physical ones have been more or less investigates, as have been the ones between purely numerical ones. We plan to study the impact of numerics on asymptotic PDE modelling by reverting the usual process and studying asymptotic limits of finite element discretizations of the Euler equations. Preliminary results show that this does allow to provide some understanding of this interaction and to possibly propose considerably improved numerical methods [32].

5. Highlights of the Year

5.1. Highlights of the Year

- In September 2019 Martin Parisot, previously CR in the ANGE team, has joined CARDAMOM;
- In September 2019 Nicolas Barral, previously post-doc in the Computational Geoscience and Energy division of the Department of Earth Science and Engineering at Imperial College London, has joined CARDAMOM
- H. Beaugendre has contributed to the organization of Inria's Autumn school, November 4-8 2019, Inria Bordeaux Sud-Ouest.
  School's objective: The school will aim at simulating a physical problem, from its modeling to its implementation in a high performance computing (HPC) framework. The school will offer both plenary courses and hands-on sessions. The physical problem considered will be the harmonic wave propagation.
  The first day will be dedicated to the modeling of the problem and its discretization using a Discontinuous Galerkin scheme. The following two days will be dedicated to linear algebra for solving large sparse systems. Background on direct, iterative and hybrid methods for sparse linear systems will be discussed. Hands-on on related parallel solvers will then be proposed. Will follow a session dedicated to advanced parallel schemes using task-based paradigms, including a hands-on with the starpu runtime system. The ultimate hands-on session will be devoted to the use of parallel profiling tools. The school will be closed with plenary talks illustrating the usage of such a workflow in an industrial context.
  38 participants, mostly PhD students and Post-docs.
  This school received support form cea, Inria, prace and sysnum.

5.1.1. Awards

In November 2019 M. Ricchiuto has been granted the honorary appointment of Adjunct Professor at the Civil and Environmental Engineering department of Duke University in North Carolina (USA).

6. New Software and Platforms

6.1. AeroSol

KEYWORD: Finite element modelling

FUNCTIONAL DESCRIPTION: The AeroSol software is a high order finite element library written in C++. The code has been designed so as to allow for efficient computations, with continuous and discontinuous finite elements methods on hybrid and possibly curvilinear meshes. The work of the team CARDAMOM (previously Bacchus) is focused on continuous finite elements methods, while the team Cagire is focused on discontinuous Galerkin methods. However, everything is done for sharing the largest part of code we can. More precisely, classes concerning IO, finite elements, quadrature, geometry, time iteration, linear solver, models and interface with PaMPA are used by both of the teams. This modularity is achieved by mean of template abstraction for keeping good performances. The distribution of the unknowns is made with the software PaMPA , developed within the team TADAAM (and previously in Bacchus) and the team Castor.

NEWS OF THE YEAR: In 2019, the following points were addressed in AeroSol

*Update, documentation, and wiki for the test case *exact solution of Riemann problem and exact Godunov solver

*Development of Droplet model, and of a Baer and Nunziato diphasic model.

*Beginning of implementation of eddy viscosity models (k-epsilon, Spalart-Almarras) turbulence models.

*Add the possibility of mesh dependent data (for example, a flow computed by AeroSol with the Euler system) for being used as input for another model (e.g. advection of droplets within this flow). This feature is used also for wall distance for turbulent models.

*Penalization problems, with single core mesh adaptation was merged in the master branch.

*Improvements of PETSc usage: possibility of solving linear problems that are not of size nvar, usage of MUMPS LU solver through PETSc.

*Interfacing with SLEPc for solving eigenvalues and eigenvectors problems.

*High order visualization based on GMSH.

*Beginning of interfacing with PARMMG for parallel mesh adaptation.

*Clean of warning, error messages, etc...

- Participants: Benjamin Lux, Damien Genet, Mario Ricchiuto, Vincent Perrier, Héloïse Beaugendre, Subodh Madhav Joshi, Christopher Poette, Marco Lorini, Jonathan Jung and Enrique Gutierrez Alvarez
- Partner: BRGM
- Contact: Vincent Perrier
- URL: https://team.inria.fr/cardamom/aerosol/

6.2. Mmg

Mmg Platform

KEYWORDS: Mesh adaptation - Anisotropic - Mesh generation - Mesh - Isovalue discretization

SCIENTIFIC DESCRIPTION: The Mmg plateform gathers open source software for two-dimensional, surface and volume remeshing. The platform software perform local mesh modifications. The mesh is iteratively modified until the user prescriptions satisfaction.

The 3 softwares can be used by command line or using the library version (C, C++ and Fortran API) : - Mmg2d performs mesh generation and isotropic and anisotropic mesh adaptation. - Mmgs allows isotropic and anisotropic mesh adaptation for 3D surface meshes. - Mmg3d is a new version af the MMG3D4 software. It remesh both the volume and surface mesh of a tetrahedral mesh. It performs isotropic and anisotropic mesh adaptation and isovalue discretization of a level-set function.

The platform software allow to control the boundaries approximation: The "ideal" geometry is reconstruct from the piecewise linear mesh using cubic Bezier triangular partches. The surface mesh is modified to respect a maximal Hausdorff distance between the ideal geometry and the mesh.

Inside the volume, the software perform local mesh modifications (such as edge swap, pattern split, isotropic and anisotropic Delaunay insertion...).

FUNCTIONAL DESCRIPTION: The Mmg plateform gathers open source software for two-dimensional, surface and volume remeshing. It provides three applications : 1) mmg2d: generation of a triangular mesh , adaptation and optimization of a triangular mesh 2) mmgs: adaptation and optimization of a surface triangulation representing a piecewise linear approximation of an underlying surface geometry 3) mmg3d: adaptation and optimization of a tetrahedral mesh and isovalue discretization

The platform software perform local mesh modifications. The mesh is iteratively modified until the user prescription satisfaction.

NEWS OF THE YEAR: Release 5.3.0 improves: - the mmg3d algorithm for mesh adaptation (better convergency and edge lengths closest to 1) - the software behaviour in case of failure (warnings/error messages are printed only 1 time and there is no more exits in the code) - the mmg2d software that now uses the same structure than mmgs and mmg3d

It adds: - the -hsiz option for mmg2d/s/3d (that allows to generate a uniform mesh of size) - the -nosurf option for mmg2d (that allows to not modify the mesh boundaries) - the -opnbdy option for mmg3d (that allow to preserve an open boundary inside a volume mesh) - the possibility to provide meshes containing prisms to mmg3d (the prisms entities are preserved while the tetra ones are modified)

- Participants: Algiane Froehly, Charles Dapogny, Pascal Frey and Luca Cirrottola
- Partners: Université de Bordeaux - CNRS - IPB - UPMC
- Contact: Algiane Froehly
- URL: http://www.mmgtools.org

6.3. MMG3D

Mmg3d

KEYWORDS: Mesh - Anisotropic - Mesh adaptation

SCIENTIFIC DESCRIPTION: Mmg3d is an open source software for tetrahedral remeshing. It performs local mesh modifications. The mesh is iteratively modified until the user prescriptions satisfaction.

Mmg3d can be used by command line or using the library version (C, C++ and Fortran API) : - It is a new version af the MMG3D4 software. It remesh both the volume and surface mesh of a tetrahedral mesh. It performs isotropic and anisotropic mesh adaptation and isovalue discretization of a level-set function.

Mmg3d allows to control the boundaries approximation: The "ideal" geometry is reconstruct from the piecewise linear mesh using cubic Bezier triangular partches. The surface mesh is modified to respect a maximal Hausdorff distance between the ideal geometry and the mesh.

Inside the volume, the software perform local mesh modifications (such as edge swap, pattern split, isotropic and anisotropic Delaunay insertion...).

FUNCTIONAL DESCRIPTION: Mmg3d is one of the software of the Mmg platform. Is is dedicated to the modification of 3D volume meshes. It perform the adaptation and the optimization of a tetrahedral mesh and allow to discretize an isovalue.

Mmg3d perform local mesh modifications. The mesh is iteratively modified until the user prescription satisfaction.

- Participants: Algiane Froehly, Charles Dapogny, Pascal Frey and Luca Cirrottola
- Partners: Université de Bordeaux - CNRS - IPB - UPMC
- Contact: Algiane Froehly
- URL: http://www.mmgtools.org

6.4. SH-COMP

KEYWORDS: Finite element modelling - Multi-physics simulation - Chemistry - Incompressible flows - 2D

FUNCTIONAL DESCRIPTION: Numerical modelling of the healing process in ceramic matrix composites

- Participants: Gérard Vignoles, Gregory Perrot, Guillaume Couegnat, Mario Ricchiuto and Giulia Bellezza
- Partner: LCTS (UMR 5801)
- Contact: Mario Ricchiuto

6.5. SLOWS

Shallow-water fLOWS

KEYWORDS: Simulation - Free surface flows - Unstructured meshes

SCIENTIFIC DESCRIPTION: Three different approaches are available, based on conditionally depth-positivity preserving implicit schemes, or on conditionally depth-positivity preserving genuinely explicit discretizations, or on an unconditionally depth-positivity preserving space-time approach. Newton and frozen Newton loops are used to solve the implicit nonlinear equations. The linear algebraic systems arising in the discretization are solved with the MUMPS library. This year implicit and explicit (extrapolated) multistep higher order time integration methods have been implemented, and a mesh adaptation technique based on simple mesh deformation has been also included.

FUNCTIONAL DESCRIPTION: SLOWS is a C-platform allowing the simulation of free surface shallow water flows with friction. It can be used to simulate near shore hydrodynamics, wave transformations processes, etc.

- Participants: Maria Kazolea and Mario Ricchiuto
- Contact: Mario Ricchiuto
- URL: https://team.inria.fr/cardamom/slows-shallow-water-flows/

6.6. TUCWave

KEYWORD: Physical simulation

SCIENTIFIC DESCRIPTION: A novel work that advances a step ahead the methodology of the solution of dispersive models. TUCWave uses a high-order well-balanced unstructured finite volume (FV) scheme on triangular meshes for modeling weakly nonlinear and weakly dispersive water waves over varying bathymetries, as described by the 2D depth-integrated extended Boussinesq equations of Nwogu (1993), rewritten in conservation law form. The FV scheme numerically solves the conservative form of the equations following the median dual node-centered approach, for both the advective and dispersive part of the equations. The code developed follows an efficient edge based structured technique. For the advective fluxes, the scheme utilizes an approximate Riemann solver along with a well-balanced topography source term up-winding. Higher order accuracy in space and time is achieved through a MUSCL-type reconstruction technique and through a strong stability preserving explicit Runge-Kutta time stepping. Special attention is given to the accurate numerical treatment of moving wet/dry fronts and boundary conditions. Furthermore, the model is applied to several examples of wave propagation over variable topographies and the computed solutions are compared to experimental data.

FUNCTIONAL DESCRIPTION: Fortran Planform which accounts for the study of near shore processes

- Participants: Argiris Delis, Ioannis Nikolos and Maria Kazolea
- Partner: Technical University of Crete
- Contact: Maria Kazolea

6.7. Fmg

KEYWORD: Mesh adaptation

FUNCTIONAL DESCRIPTION: FMG is a library deforming an input/reference simplicial mesh w.r.t. a given smoothness error monitor (function gradient or Hessian), metric field, or given mesh size distribution. Displacements are computed by solving an elliptic Laplacian type equation with a continuous finite element method. The library returns an adapted mesh with a corresponding projected solution, obtained by either a second order projection, or by an ALE finite element remap. The addiction of a new mass conservative approach developed ad-hoc for shallow water flows is under way.

NEWS OF THE YEAR: - Development of the Elasticity model to compute the nodes displacement. - Development of a new model to compute the nodes displacement. This mixed model takes the advantages of the Laplacian model and the Elasticity model: a refined mesh where the solution varies a lot and a smooth gradation of the edges size elsewhere. - Extension in three dimension

- Participants: Leo Nouveau, Luca Arpaia, Mario Ricchiuto and Luca Cirrottola
- Contact: Algiane Froehly

6.8. ParMmg

KEYWORDS: 3D - Mesh adaptation - Anisotropic - Isotropic - Isovalue discretization - Distributed Applications - MPI communication

FUNCTIONAL DESCRIPTION: The ParMmg software build parallel (MPI based) mesh adaptation capabilities on top of the sequential open-source remesher Mmg, iteratively called over sub-meshes of the initial mesh.

ParMmg is available: - through command line , - in library mode using the dedicated API.

RELEASE FUNCTIONAL DESCRIPTION: The version 1.2 of ParMmg provide 3D volume mesh adaptation with constrained surface.

It adds to the previous release: - Mesh repartitioning through parallel interface displacement , - Support for Scotch renumeration.

- Participants: Algiane Froehly and Luca Cirrottola
- Partners: FUI Icarus - ExaQUte
- Contact: Algiane Froehly
- URL: https://mmgtools.org

7. New Results

7.1. Modelling of free surface flows

- Participants: Umberto Bosi, Mathieu Colin, Maria Kazolea, Mario Ricchiuto
- Corresponding member: Maria Kazolea
  This year we continued our work on free surface flow modelling. We can dived our work on four main axis. First, we presented a depth-integrated Boussinesq model for the efficient simulation of nonlinear wave-body interaction [4]. The model exploits a ÂÂunifiedÂÂ Boussinesq framework, i.e. the fluid under the body is also treated with the depth-integrated approach. The unified Boussinesq approach was initially proposed by Jiang [60] and recently analysed by Lannes [67]. The choice of Boussinesq-type equations removes the vertical dimension of the problem, resulting in a wave-body model with adequate precision for weakly nonlinear and dispersive waves expressed in horizontal dimensions only. The framework involves the coupling of two different domains with different flow characteristics. Inside each domain, the continuous spectral/hp element method is used to solve the appropriate flow model since it allows to achieve high-order, possibly exponential, convergence for non-breaking waves. Flux-based conditions for the domain coupling are used, following the recipes provided by the discontinuous Galerkin framework. The main contribution of this work is the inclusion of floating surface-piercing bodies in the conventional depth-integrated Boussinesq framework and the use of a spectral/hp element method for high-order accurate numerical discretization in space. The model is verified using manufactured solutions and validated against published results for wave-body interaction. The model is shown to have excellent accuracy and is relevant for applications of waves interacting with wave energy devices. The outcome of this work is the phd thesis of Uberto Bosi.[1].

Second, a detailed analysis of undular bore dynamics in channels of variable cross-section is performed and presented in [5] . Two undular bore regimes, low Froude number (LFN) and high Froude number (HFN), are simulated with a Serre Green Naghdi model, and the results are compared with the experiments by Treske (1994). We show that contrary to Favre waves and HFN bores, which are controlled by dispersive non-hydrostatic mechanisms, LFN bores correspond to a hydrostatic phenomenon. The dispersive-like properties of the LFN bores is related to wave refraction on the banks in a way similar to that of edge waves in the near shore. A fully hydrostatic asymptotic model for these dispersive-like bores is derived and compared to the observations, confirming our claim.

An other part of our last year's work was focused on wave breaking for Boussineq-type equations [3]. The aim of this work was to develop a model able to represent the propagation and transformation of waves in nearshore areas. The focus is on the phenomena of wave breaking, shoaling and run-up. These different phenomena are represented through a hybrid approach obtained by the coupling of non-linear Shallow Water equations with the extended Boussinesq equations of Madsen and Sorensen. The novelty is the switch tool between the two modelling equations: a critical free surface Froude criterion. This is based on a physically meaningful new approach to detect wave breaking, which corresponds to the steepening of the wave's crest which turns into a roller. To allow for an appropriate discretization of both types of equations, we consider a finite element Upwind Petrov Galerkin method with a novel limiting strategy, that guarantees the preservation of smooth waves as well as the monotonicity of the results in presence of discontinuities.We provide a detailed discussion of the implementation of the newly proposed detection method, as well as of two other well known criteria which are used for comparison. An extensive benchmarking on several problems involving different wave phenomena and breaking conditions allows to show the robustness of the numerical method proposed, as well as to assess the advantages and limitations of the different detection methods.

We also continue to work on the modelling of free surface flows by investigating a new family of models, derived from the so-called Isobe-Kakinuma models. The Isobe–Kakinuma model is a system of Euler–Lagrange equations for a Lagrangian approximating Luke's Lagrangian for water waves. In [23], We consider the Isobe–Kakinuma model for two-dimensional water waves in the case of the flat bottom. We show theoretically the existence of a family of small amplitude solitary wave solutions to the Isobe–Kakinuma model in the long wave regime. We have also performed numerical computations for a toy system included large amplitude solitary wave solutions. Our computations suggest the existence of a solitary wave of extreme form with a sharp crest. This models seems very promising for future research.

7.2. Modelling of icing and de-icing of aircrafts

- Participants: Héloïse Beaugendre, Mathieu Colin and Francois Morency
- Corresponding member: Héloïse Beaugendre

  In-flight icing on an aircrafts surface can be a major hazard in aeronautics's safety. Numerical simulations of ice accretion on aircraft is a common procedure to anticipate ice formation when flying in a supercooled water droplets cloud. Numerical simulations bring a better understanding of ice accretion phenomena, performance degradations and lead to even more efficient thermal de-icing systems designs. Such simulations imply modelling the phase change of water and the mass and energy transfers. The Messinger model developed in the 1950 is still used today as a reliable basis for new models development. This model estimates the ice growth rate using mass and energy balances coupled to a runback water flow. The main parameter introduced with this approach is the freezing fraction, denoting the fraction of incoming water that effectively freezes on the airfoil.

  In-flight ice accretion code predictions depend on heat loss over rough surfaces. The equivalent sand grain roughness models the friction coefficient, but an additional model is needed for heat transfer prediction. The turbulent Prandtl number correction and the sublayer Stanton-based models are commonly used. This year, both models have been used with the Spalart-Allmaras turbulence model to predict heat transfer over rough surfaces typical of ice accretion. The objective here is to compare the results of the two models. First, the sublayer Stanton-based model is rewritten in the context of a turbulent Prandtl number correction formulation. Then, the two models are implemented in the open source software, SU2, and then verified and validated for flow over rough flat plates, airfoils, and wings. The two models' predictions evolve differently with the local Reynolds number, but are always within the experimental 20% error margin. The paper related to those developments are under revision.

In the work [17], the objective is to model an ice accretion on an airfoil using a Messinger-based approach and to make a sensitivity analysis of roughness models on the ice shape. The test case is performed on a 2D NACA0012 airfoil. A typical test case on a NACA0012 airfoil under icing conditions is run and confronted with the literature for verification prior to further investigations. Ice blocks profiles comparisons will highlight the differences implied by the choice of the roughness correction, which impact the heat transfer coefficient.

Numerical simulation of separated flow around an iced airfoil is still a challenge. Predictions of post-stall aerodynamic performance by RANS models are unsatisfactory. Recent hybrid RANS/LES methods, based on modified DDES models, have shown promising results for separated flow. However, questions still arise about the best compromise between computation time and accuracy for the unsteady 3D simulations. The span width of the domain and the best grid practice to obtain accurate results still has to be investigated, especially taking into account the recent method improvements. A recent method such as shear-layer adapted DDES should give acceptable flow prediction with a relatively coarse mesh. In the paper [18], we further study the effects of span width length on predicted aerodynamic coefficients and on the pressure coefficient. The study is done using the open-source software SU2. The backward facing step and a stalled NACA0012 is used to validate the numerical results. Then, the numerical flow around an iced Model 5-6 is studied, especially the flow within the separation bubble behind the ice. The accuracy of the CFD results is discussed and a recommendation is made about the span width of the computation domain and the grid size.

In order to spare time and resources while increasing the results' accuracy of the stalled wing configuration's aerodynamic coefficients, the following study [16] offers a parametric grid study for the DDES model. For three different grid refinements, characteristics of lift and eddy phenomena are presented and compared to determine, for an infinite wing, the best compromise between time and resources' consumption, and results's accuracy. Using the open software SU2 6.1 (Stanford University Unstructured), we generate three different types of grid refinements around an airfoil, developed spanwise to obtain a straight wing. On the same stalled configuration for each mesh, CFD solutions are ran with the DDES model, and the raw data are post processed with the open software ParaView 5.6. We then compare the aerodynamic coefficients' distributions obtained by the three mesh. The general modelling of vortex shedding's topology and turbulence viscosity are compared with the literature to ensure the right rendering of vortex structures. Chordwise pressure and friction coefficients' distributions as well as the spanwiselift coefficient are also compared. We conclude with the optimum mesh in term of results and resources' consumption.

7.3. High order embedded and immersed boundary methods

- Participants: Héloïse Beaugendre, Mirco Ciallella, Benjamin Constant and Mario Ricchiuto
- Corresponding member: Héloïse Beaugendre
  In the last years the team has invested some effort in developing the high order embedded method known as "shifted boundary method". In this method, geometrical boundaries are not meshed exactly but embedded in the mesh. Boundary conditions are imposed on a surrogate boundary, toughly defined by the collection of mesh faces "closest" to the true boundary. To recover high order of accuracy, the boundary condition imposed on this surrogate boundary is modified to account for the distance from the true boundary.

This year's work has focused on two aspects. First, we proposed an efficient extension of the method to elliptic diffusion equations in mixed form (e.g., Darcy flow, heat diffusion problems with rough coefficients, etc.) [10] Our aim is to obtain an improved formulation that, for linear finite elements, is at least second-order accurate for both flux and primary variable, when either Dirichlet or Neumann boundary conditions are applied. Following previous work of Nishikawa and Mazaheri in the context of residual distribution methods, we consider the mixed form of the diffusion equation (i.e., with Darcy-type operators), and introduce an enrichment of the primary variable. This enrichment is obtained exploiting the relation between the primary variable and the flux variable, which is explicitly available at nodes in the mixed formulation. The proposed enrichment mimics a formally quadratic pressure approximation, although only nodal unknowns are stored, similar to a linear finite element approximation. We consider both continuous and discontinuous finite element approximations and present two approaches: a non-symmetric enrichment, which, as in the original references, only improves the consistency of the overall method; and a symmetric enrichment, which enables a full error analysis in the classical finite element context. Combined with the shifted boundary method, these two approaches are extended to high-order embedded computations, and enable the approximation of both primary and flux (gradient) variables with second-order accuracy, independently on the type of boundary conditions applied. We also show that the the primary variable is third-order accurate, when pure Dirichlet boundary conditions are embedded.

Second, using the same ideas underlying the shifted boundary method, a novel approach to handle shock waves has been proposed. In this method shocks are seen as embedded boundaries on which appropriately shifted jump conditions are imposed, allowing to connect the upstream and downstream domains. This new technique, named "shifted shock-fitting", has been implemented on two-dimensional unstructured grids to deal with shocks by treating them as they were immersed boundary. The new algorithm is aimed at coupling a floating shock-fitting technique with the shifted boundary method, so far introduced only to simulate flows with embedded boundaries (see [15], full length paper in revision on *J.Comput.Phys.*).
A new PhD in collaboration with ONERA has started (Benjamin Constant 's thesis) involving the numerical simulation of unsteady flows around complex geometries in aeronautics. In the CFD simulation process, mesh generation is the main bottleneck when one wishes to study realistic configurations, such as an aircraft landing gear. A mesh can represent a month to several months of engineer time for a specialist, which is prohibitive in the pre-design phase where several geometries are evaluated in a very short time frame. For this reason, Inria and Onera have been interested for several years in the development of an immersed boundary method, which does not require representing obstacles by mesh conforming to the wall, thus simplifying the generation of mesh. The consideration of the wall is carried out by the introduction of a forcing term at certain points in the vicinity of obstacles. In our approach, this technique is combined with a method of generating adaptive octree cartesian mesh. This allows us to exploit the advantages of Cartesian mesh (generation and rapid adaptation, performance gains of a dedicated Cartesian solver). In order to model the boundary layer, a wall model is used to avoid an extra cost. This method has been implemented for the simulation of steady turbulent flows around geometries studied in compressible aerodynamics (winged fuselage, engine air intake, helicopter fuselage...), providing a very good compromise between the quality of the aerodynamic solution and the time it takes to return the solution from the definition of geometry. However, the quality of the solution obtained by steady simulations is not sufficient to predict the acoustics satisfactorily. Indeed, oscillations appear for certain sizes of interest (such as turbulent viscosity or pressure fluctuations) in the vicinity of the wall. In addition, the passage of grids of different levels causes reflections, which can greatly degrade the prediction of the acoustic solution. The objective of this thesis is to solve these two problems in order to be able to perform unsteady simulations around complex geometries, such as a landing gear. On the one hand, we will study an algorithm to regularize the solution at the points of interest of the IBM method located near the wall. Together, we will also be interested in improving the wall model, in collaboration with modeling specialists from the department. We will do a study by error

estimators to analyze the impact of these improvements on the solution. Validations on academic test cases will be carried out. A second step is to improve the transfer of the solution between grids of different levels (for which the mesh size double). We will propose an algorithm to regularize this passage, by geometrically modifying the mesh and by modifying the transfer formula of the solution at the passage of the fitting. A validation will be carried out on an unsteady case of LEISA profile. Finally, a demonstrative application that is both geometrically complex and of acoustic interest will be performed, typically a LAGOON or Gulfstream landing gear.

7.4. Composites Materials

- Participants: Giulia Bellezza, Mathieu Colin and Mario Ricchiuto
- Corresponding member: Mario Ricchiuto
  Self-healing is an important phenomenon in new-generation refractory ceramic-matrix composites, obtained by the oxidation of a glass-forming phase in the composite. The dynamics of oxygen diffusion, glass formation and flow are the basic ingredients of a self-healing model that has been developed here in 2D in a trans-verse crack of a mini composite [11]. The presented model can work on a realistic image of the material section and is able to simulate healing and quantify the exposure of the material to oxygen, a prerequisite for its lifetime prediction. Crack reopening events are handled satisfactorily, and secondary healing can be simulated. This papers describes and discusses a typical case in order to show the model potentialities.

  Additional work involve two main topics. The first one is dedicated to the modeling of the propagation of a self-healing oxyde in a crack. The aim here is to introduce new models which describe both the self-healing behavior and oxygen diffusion towards fibers. In general, the evolution of an incompressible fluid can be described by the Navier-Stokes equations. However, we observe that a direct numerical method applied to these equations will induce a significant computational cost, especially in our case, due to the long lifespan of the material. Thus, alternatively, we derive several asymptotic models obtained by performing a dimensional analysis on the Navier-Stokes equations : we focus here on shallow water models and thin film models. The second aspect under study is more theoretical. We propose in the full generality a link between the BD entropy introduced by D. Bresch and B. Desjardins for the viscous shallow-water equations and the Bernis-Friedman (called BF) dissipative entropy introduced to study the lubrications equations. Different dissipative entropies are obtained playing with the drag terms on the viscous shallow water equations. It helps for instance to prove global existence of nonnegative weak solutions for the lubrication equations starting from the global existence of nonnegative weak solutions for appropriate viscous shallow-water equations.

7.5. Adaptation techniques

- Participants: Nicolas Barral, Héloïse Beaugendre, Luca Cirrottola, Algiane Froehly, Mario Ricchiuto.
- Corresponding member: Nicolas Barral
  In [14] we presented an algorithm to perform PDE-based r-adaptation in three-dimensional numerical simulations of unsteady compressible flows on unstructured meshes. A Laplacian-based model for the moving mesh is used to follow the evolving shock-wave patterns in the fluid flow, while the finite volume ALE formulation of the flow solver is employed to implicitly perform a conservative re-mapping of the solution from the previous to the current mesh, at each time step of the simulation.We show the application of this method to compressible flows on three-dimensional geometries. To this aim, an improved relaxation scheme has been developed in order to preserve the validity of the mesh throughout the time simulation in three dimensions, where the geometrical constraints typically restrict the allowable mesh motion.

  Similar adaptive strategies have been investigate for shallow water flows in the context of space-time residual distribution methods [7]. In the scalar case, these schemes can be designed to be unconditionally (w.r.t. the time step) positive, even on the distorted space-time prisms which arise from moving the nodes of an unstructured triangular mesh. Consequently, a local increase in mesh resolution does not impose a more restrictive stability constraint on the time-step, which can instead be chosen according to accuracy or physical requirements. Moreover, schemes of this type are analogous to conservative ALE formulations and automatically satisfy a discrete geometric conservation law. For shallow water flows over variable bed topography, the so-called C-property (retention of hydrostatic balance between flux and source terms, required to maintain the steady state of still, flat, water) can also be satisfied by considering the mass balance equation in terms of free surface level instead of water depth, even when the mesh is moved. Combined with a simple implementation of Laplacian based r-adaptation, this technique has been shown to allow up to 60% CPU time savings for a given error.

We also extended these methods to curvilinear coordinates to do shallow water simulations on the sphere for oceanographic applications [2]. To provide enhanced resolution of moving fronts present in the flow we consider adaptive discrete approximations on moving triangulations of the sphere. To this end, we re- state all Arbitrary Lagrangian Eulerian (ALE) transport formulas, as well as the volume transformation laws, for a 2D manifold. Using these results, we write the set of ALE-SWEs on the sphere. We then propose a Residual Distribution discrete approximation of the governing equations. Classical properties as the DGCL and the C-property (well balancedness) are reformulated in this more general context. An adaptive mesh movement strategy is proposed. The discrete framework obtained is thoroughly tested on standard benchmarks in large scale oceanography to prove their potential as well as the advantage brought by the adaptive mesh movement.

8. Partnerships and Cooperations

8.1. Regional Initiatives

Title: ETRURIA: Robust simulation tools for non-hydrostatic free surface flows

Type: Apple à Projets Recherche Région Nouvelle Aquitaine

Coordinator: M. Ricchiuto

Other partners: BRGM, UMR EPOC (P. Bonneton)

Abstract: The objective of this project is to combine high order continuous finite elements, with embedded methods and mesh adaptation in the simulation of coastal and urban inundation. Realistic validation cases will be provided by BRGM. This project co-funds (50%) the PhD of S. Michel.

8.2. National Initiatives

8.2.1. ANR VISCAP

Title: VIrtual Self-healing Composites for Aeronautic Propulsion

Type: ANR

Duration: 48 months

Starting date : 1st Jan 2018

Coordinator: Vignoles Gerard (Université de Bordeaux and LCTS - UMR 5801)

Abstract: Self-healing Ceramic-Matrix Composites (SH-CMCs) have extremely long lifetimes even under severe thermal, mechanical and chemical solicitations. They are made of ceramic fibres embedded in a brittle ceramic matrix subject to multi-cracking, yielding a damageable-elastic mechanical behaviour. These materials have the particularity of protecting themselves against corrosion by the formation of a sealing oxide that fills the matrix cracks, delaying considerably the fibres degradation. Applications encompass civil aeronautic propulsion engine hot parts and they represent a considerable market; however this is only possible if the lifetime duration of the materials is fully certified. The ambition of this innovative project is to provide reliable, experimentally validated numerical models able to reproduce the behaviour of SH-CMCs. The starting point is an existing image-based coupled model of progressive oxidative degradation under tensile stress of a mini-composite (i.e. a unidirectional bundle of fibres embedded in multi-layered matrix). Important improvements will be brought to this model in order to better describe several physic-chemical phenomena leading to a non-linear behaviour: this will require an important effort in mathematical analysis and numerical model building. A systematic benchmarking will allow creating a large database suited for the statistical analysis of the impact of material and environmental parameter variations on lifetime. Experimental verifications of this model with respect to tests carried out on model materials using in-situ X-ray tomography ? in a specially adapted high-temperature environmental & mechanical testing cell ? and other characterizations are proposed. The extension of the modelling procedure to Discrete Crack Networks for the large-scale description of the material life will be the next action; it will require important developments on mesh manipulations and on mathematical model analysis. Finally, experimental validation will be carried out by comparing the results of the newly created software to tests run on 3D composite material samples provided by the industrial partner of the project. The project originality lies in a multidisciplinary character, mixing competences in physico-chemistry, mechanics, numerical and mathematical modelling, software engineering and high-performance computing. It aims creating a true computational platform describing the multi-scale, multidimensional and multi-physics character of the phenomena that determine the material lifetime. Important outcomes in the domain of civil aircraft jet propulsion are expected, that could relate to other materials than those considered in this study.

8.2.2. FUI ICARUS

Title: Intensive Calculation for AeRo and automotive engines Unsteady Simulations.

Type: FUI

Duration: January 2017 - December 2019

Coordinator: Turbomeca, Safran group

Abstract: Large Eddy Simulation is an accurate simulation tool for turbulent flows which is becoming more and more attractive as the parallel computing techniques and platforms become more and more efficient. This project aims at improving the performances of some existing simulation tools (such as AVBP, Yales and ARGO), at developing meshing/re-meshing tools tailored to LES simulations, at improving the ergonomy of these tools to the industrial world (improved interfaces, data handling, code coupling, etc), and validate the progress made on case studies representative of typical design simulations in the automotive and aeronautic industry

8.2.3. APP University of Bordeaux

Title : Modélisation d’un système de dégivrage thermique

Type : Project University of Bordeaux

Duration : 36 months

Starting : October 2016

Coordinator : H. Beaugendre and M. Colin

Abstract : From the beginning of aeronautics, icing has been classified as a serious issue : ice accretion on airplanes is due to the presence of supercooled droplets inside clouds and can lead to major risks such as aircrash for example. As a consequence, each airplane has its own protection system : the most important one is an anti-icing system which runs permanently. In order to reduce gas consumption, de-icing systems are developed by manufacturers. One alternative to real experiment consists in developing robust and reliable numerical models : this is the aim of this project. These new models have to take into account multi-physics and multi-scale environnement : phase change, thermal transfer, aerodynamics flows, etc. We aim to use thin films equations coupled to level-set methods in order to describe the phase change of water. The overall objective is to provide a simulation plateform, able to provide a complete design of these systems.

8.3. European Initiatives

8.3.1. FP7 & H2020 Projects

Program: FETHPC-02

Project acronym: ExaQute

Project title: Exascale quantification of uncertainties for technology and science simulation

Duration: June 2018 - April 2019

Coordinator: CIMNE (Spain)

Other partners: BSC (Spain), TUM (Germany), IT4 (Czech Republic), EPFL (Switzerland), UPC (Spain), Structure (Germany).

Abstract: The ExaQUte project aims at constructing a framework to enable Uncertainty Quantification and Optimization Under Uncertainties in complex engineering problems, using computational simulations on Exascale systems. The description of complex geometries will be possible by employing embedded methods, which guarantee a high robustness in the mesh generation and adaptation steps, while allowing preserving the exact geometry representation. The efficient exploitation of the Exascale system will be addressed by combining State-of-the-Art dynamic task-scheduling technologies with space-time accelerated solution methods, where parallelism is harvested both in space and time. The methods and tools developed in ExaQUte will be applicable to many fields of science and technology. The chosen application focuses on wind engineering, a field of notable industrial interest for which currently no reliable solution exist.

8.3.2. Collaborations in European Programs, Except FP7 & H2020

Program: OCEANEraNET

Project acronym: MIDWEST

Project title: Multi-fIdelity Decision making tools for Wave Energy SysTems

Duration: December 2015 - April 2019

Coordinator: Mario Ricchiuto

Other partners: Chalmers University (Sweden), DTU Compute (Denmark), IST Lisbon (Portugal)

Abstract: Wave energy converters (WECs) design currently relies on low-fidelity linear hydrodynamic models. While these models disregard fundamental nonlinear and viscous effects - which might lead provide sub-optimal designs - high-fidelity fully nonlinear Navier-Stokes models are prohibitively computational expensive for optimization. The MIDWEST project will provide an efficient asymptotic nonlinear finite element model of intermediate fidelity, investigate the required fidelity level to resolve a given engineering output, construct a multi-fidelity optimization platform using surrogate models blending different fidelity models. Combining know how in wave energy technology, finite element modelling, high performance computing, and robust optimization, the MIDWEST project will provide a new efficient decision making framework for the design of the next generation WECs which will benefit all industrial actors of the European wave energy sector.

8.4. International Initiatives

8.4.1. Inria Associate Teams Not Involved in an Inria International Labs

8.4.1.1. HAMster

Title: High order Adaptive moving MeSh finiTE elements in immeRsed computational mechanics

International Partner (Institution - Laboratory - Researcher):

Duke (United States) - Civil and Environmental Engineering and Mechanical Engineering and Material Science - Guglielmo Scovazzi

Inria Bordeaux -SO (France) - CARDAMOM team - Mario Ricchiuto

Start year: 2017

See also: https://team.inria.fr/athamster/

This project focuses on adaptive unstructured mesh finite element-type methods for fluid flows with moving fronts. These fronts may be interfaces between different fluids, or fluid/solid, and modelling or physical fronts (e.g. shock waves) present in the flow. The two teams involved in the project have developed over the years complementary strategies, one focusing more on an Eulerian description aiming at capturing fronts on adaptive unstructured grids, the other is working more on Lagrangian approaches aiming at following exactly some of these features. Unfortunately, classical Lagrangian methods are at a disadvantage in the presence of complex deformation patterns, especially for fronts undergoing large deformations, since the onset of vorticity quickly leads to mesh rotation and eventually tangling. On the other end, capturing approaches, as well as Immersed Boundary/Embedded (IB/EB) methods, while providing enormous flexibility when considering complex cases, require a careful use of mesh adaptivity to guarantee an accurate capturing of interface physics. The objective of this team is to study advanced hybrid methods combining high order, adaptive, monotone capturing techniques developed in an Eulerian or ALE setting, with fitting techniques and fully Lagrangian approaches.

8.4.2. Inria International Partners

8.4.2.1. Inria International Chairs

IIC ABGRALL Rémi

Title: Numerical approximation of complex PDEs & Interaction between modes, schemes, data and ROMs

International Partner (Institution - Laboratory - Researcher):

ETH Zurich (Switzerland) - Institut fur Mathematik & Computational Science - Rémi Abgrall

Duration: 2019 - 2023

Start year: 2019

8.5. International Research Visitors

8.5.1. Visits of International Scientists

- Claes Eskilsson, associated professor at Aalborg University, visited Mario Ricchiuto in Jul 2019.
- Francois Morency, Professeur at Ecole de Technologie Supérieure de Montréal has visited Héloïse Beaugendre to work on aircraft icing, roughness modeling and performance degradation, in January 2019 and July 2019.
- Masahito Ohta, Professor at Tokyo University of Science visited Mathieu Colin in Dec 2019.
- Nicolas Perinet, Postocdoral fellow at University of Chile has visited Mario Ricchiuto to work on the benchmarking of the SLOWS CODE in October 2019.

- Guglielmo Scovazzi, Prof. at Duke University, has visited M. Ricchiuto in the summer to work on the shifted boundary method;
- Davide Torlo, PhD candidate at U. Zurich, visited M. Ricchiuto in June 2019 to work on relaxation finite element approximations of the shallow water equations

8.5.1.1. Internships

- Mirco Ciallella (Inria, M. Sc. Student). Until Jan 2019.
- Simon Le Berre (Inria, M. Sc. Student). From Apr 2019 until Sep 2019.

9. Dissemination

9.1. Promoting Scientific Activities

9.1.1. Scientific Events: Organisation

9.1.1.1. Member of the Organizing Committees

- M. Ricchiuto co-organized the workshop Hywec2 on the hydrodynamics of wave energy converters. The workshop has been organized in the framework of the work packages 3 and 5 of the Excellence Cluster Sysnum as one of two twin events devoted to marine renewable energies organized in Bilbao (the VI Marine Energy Conference, June 25th) and Bordeaux. The event is also supported by the Oceanera-net Midwest and the Fondation Del Duca. Its main goals have been to focus on PDE and numerical modelling techniques, with attention on advanced and recent approaches, and to give an overview of examples of industrial techniques and applications with several European industrial actors. For more info refer to the web https://hywec2.sciencesconf.org.

9.1.2. Scientific Events: Selection

9.1.2.1. Chair of Conference Program Committees

Mathieu Colin is a member of the scientific committee of the JEF day's.

9.1.2.2. Member of the Conference Program Committees

M. Ricchiuto has co-organized the mini-symposium “Some modern questions in the simulation of advection dominated problems”, MS FT-1-10 at the ICIAM conference in Valencia

9.1.2.3. Member of the Editorial Boards

- Mathieu Colin is a member of the board of the journal Applications and Applied Mathematics: An International Journal (AAM)
- M. Ricchiuto is a member of the editorial boards of Computers & Fluids (Elsevier) and of Water Waves (Springer)

9.1.2.4. Reviewer - Reviewing Activities

We reviewed papers for top international journals in the main scientific themes of the team : Nonlinearity, Water Waves, Analysis and PDE, Comm. Cont. Math., Journal of Scientific Computing, Open Physics, Computational and applied mathematics, Journal of Fluid Mechanics.

9.2. Teaching - Supervision - Juries

9.2.1. Teaching

- License: Nicolas Barral, TD d'Analyse Numérique, 24h, L3, ENSEIRB-MATMÉCA, France
- Master : Nicolas Barral, TD C++, 48h, M1, ENSEIRB-MATMÉCA, France
- Master : Nicolas Barral, Techniques de maillage, 36h, M2, ENSEIRB-MATMÉCA et Université de Bordeaux, France
- License: Héloïse Beaugendre, Encadrement de projets sur la modélisation de la portance, 20h, L3, ENSEIRB-MATMÉCA, France
- Master : Héloïse Beaugendre, TD C++, 48h, M1, ENSEIRB-MATMÉCA, France
- Master : Héloïse Beaugendre, Calcul Haute Performance (OpenMP-MPI), 40h, M1, ENSEIRB-MATMÉCA et Université de Bordeaux, France
- Master : Héloïse Beaugendre, Responsable de filière de 3ème année, 15h, M2, ENSEIRB-MATMÉCA, France
- Master : Héloïse Beaugendre, Calcul parallèle (MPI), 39h, M2, ENSEIRB-MATMÉCA, France
- Master : Héloïse Beaugendre, Encadrement de projets de la filière Calcul Haute Performance, 6h, M2, ENSEIRB-MATMÉCA, France
- Master : Héloïse Beaugendre, Encadrement de projets sur la modélisation de la pyrolyse, 20h, M1, ENSEIRB-MATMÉCA, France
- Master : Héloïse Beaugendre , Projet fin d'études, 4h, M2, ENSEIRB-MATMÉCA, FRANCE
- Master : Mathieu Colin : Integration, M1, 54h, ENSEIRB-MATMÉCA, FRANCE
- Master : Mathieu Colin : Fortran 90, M1, 44h, ENSEIRB-MATMÉCA, FRANCE
- Master : Mathieu Colin : PDE, M1, 30h, University of Bordeaux, FRANCE
- Master : Mathieu Colin : Analysis, L1, 47h, ENSEIRB-MATMÉCA, FRANCE
- Master : Mathieu Colin : projet professionnel and internship responsibility : 15 h, ENSEIRB-MATMÉCA, FRANCE
- Master : Mathieu Colin : Encadrement de projets TER, 20h, ENSEIRB-MATMÉCA, FRANCE
- Master : Mathieu Colin : responsable relation entreprise formation en alternance ENSEIRB-MATMECA (30h)
- Master : Mathieu Colin : suivi d'apprenti en entreprise (28h)
- Master : Mario Ricchiuto, Multiphysics Course, 21h cours magistrale, M2, ENSEIRB-MATMÉCA, FRANCE

9.2.2. Supervision

PhD : Umberto Bosi, A unified spectral/hp element depth-integrated Boussinesq model for nonlinear wave-floating body interaction, U. Bordeaux, defended in June 2019, supervised by M. Ricchiuto (see [1])

PhD in progress : E. Solai, Multi-fidelity modeling of an immersive battery cooling system for electric vehicles, started in November 2018, co-supervised by H. Beaugendre and P.M. Congedo

PhD in progres: B. Constant, high order immersed methods for turbulent flows, started in September 2019, supervised by H. Beaugendre

PhD in progress : S. Michel, shallow water simulations with immersed higher order residual methods on adaptive meshes, started in November 2018, supervised by M. Ricchiuto

PhD in progress : G. Bellezza, multi scale modelling for self-healing composite materials, started in February 2019, supervised by M. Ricchiuto and G. Vignoles (LCTS)

PhD in progress : M. Ciallella, bridging shock fitting and embedded methods to handle shock waves in hyperbolic systems, started in October 2019, supervised by M. Ricchiuto and R. Paciorri (U. Roma La Sapienza)

PhD in progress : A. Cauquis, high order shock capturing methods for tsunami simulations, started in November 2019, supervised by M. Ricchiuto and P. Heinrich (CEA)

9.2.3. Juries

Héloïse Beaugendre has contributed to the following theses defense:

- Iñigo Bidaguren, BCAM, Bilboa, Spain in June 2019 (as examiner)
- Pierre Trontin HDR, Toulouse University in September 2019 (as examiner)
- Quentin Carmouze, Côte D'Azur University in November 2019 (as reviewer)

Maria Kazolea has contributed to the following theses defense:

- Umberto Bosi PhD, University of Bordeaux, April 2019 (as examiner)

Mario Ricchiuto has participated to the following juries:

- A. Menasria, PhD ENSAM Paritech, in March 2019 (as president)
- Julien Carlier, PhD U. Paris-Saclay, in December 2019 (as reviewer)

10. Bibliography

Publications of the year

Doctoral Dissertations and Habilitation Theses

[1] U. BOSI.*A unified spectral/hp element depth-integrated Boussinesq model for nonlinear wave-floating body interaction*, Université de Bordeaux, June 2019, https://tel.archives-ouvertes.fr/tel-02297587

Articles in International Peer-Reviewed Journal

[2] L. ARPAIA, M. RICCHIUTO.*Well balanced residual distribution for the ALE spherical shallow water equations on moving adaptive meshes*, in "Journal of Computational Physics", 2020, vol. 405, 109173 [*DOI :* 10.1016/J.JCP.2019.109173], https://hal.inria.fr/hal-02422335

[3] P. BACIGALUPPI, M. RICCHIUTO, P. BONNETON.*Implementation and Evaluation of Breaking Detection Criteria for a Hybrid Boussinesq Model*, in "Water Waves", 2019, forthcoming, https://hal.archives-ouvertes.fr/hal-02383888

[4] U. BOSI, A. P. ENGSIG-KARUP, C. ESKILSSON, M. RICCHIUTO.*A spectral/hp element depth-integrated model for nonlinear wave-body interaction*, in "Computer Methods in Applied Mechanics and Engineering", 2019, vol. 348, p. 222-249 [*DOI :* 10.1016/J.CMA.2019.01.020], https://hal.inria.fr/hal-02001091

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Invited Conferences

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International Conferences with Proceedings

[15] M. CIALLELLA, M. RICCHIUTO, R. PACIORRI, A. BONFIGLIOLI.*Shifted shock-fitting: a new paradigm to handle shock waves for Euler equations*, in "AIDAA 2019 - XXV International congress of the Italian association of aeronautics and astronautics", Rome, Italy, September 2019, https://hal.inria.fr/hal-02292439

[16] V. HUCK, F. MORENCY, H. BEAUGENDRE.*Grid study for Delayed Detached Eddy-Simulation's grid of a pre-stalled wing*, in "CASI Aero 2019 - Canadian Aeronautics and Space Institute's AERO 2019 Conference", Laval, Canada, June 2019, https://hal.inria.fr/hal-02408993

[17] K. IGNATOWICZ, F. MORENCY, H. BEAUGENDRE.*Numerical simulation of ice accretion using Messinger-based approach: effects of surface roughness*, in "CASI Aero 2019 - Canadian Aeronautics and Space Institute's AERO 2019 Conference", Laval, Canada, May 2019, https://hal.inria.fr/hal-02409011

[18] G. TAGAWA, V. HUCK, F. MORENCY, H. BEAUGENDRE.*Shear-Layer Adapted DDES Analysis of 3D Stalled Flow Over an Iced Airfoil*, in "AIAA Aviation 2019 Forum", Dallas, United States, American Institute of Aeronautics and Astronautics, June 2019 [*DOI :* 10.2514/6.2019-3308], https://hal.inria.fr/hal-02408946

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[19] M. LORINI, M. RICCHIUTO.*Adaptive discontinuous Galerkin immersed boundary method for compressible Navier–Stokes simulations*, in "FEF2019 - 20th International Conference on Fluid Flow Problems", Chicago, United States, March 2019, https://hal.inria.fr/hal-02294951

[20] V. MOUREAU, P. BE´NARD, G. LARTIGUE, R. MERCIER, M. CAILLER, A. FROEHLY, C. DOBRZYNSKI.*Dynamic mesh adaptation for moving fronts and interfaces: application to the modeling of premixed flames and primary atomization*, in "APS-DFD meeting", Seattle, WA, United States, November 2019, https://hal.archives-ouvertes.fr/hal-02388149

[21] V. MOUREAU, P. BE´NARD, G. LARTIGUE, R. MERCIER, M. CAILLER, A. FROEHLY, C. DOBRZYNSKI.*Dynamic mesh adaptation for moving fronts and interfaces: application to the modeling of premixed flames and primary atomization*, in "Tetrahedron Workshop VI", Inria, Saclay, France, October 2019, https://hal.archives-ouvertes.fr/hal-02388150

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Project-Team CARMEN

Modélisation et calculs pour l'électrophysiologie cardiaque

IN PARTNERSHIP WITH:
Université de Bordeaux

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Modeling and Control for Life Sciences

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Project-Team CARMEN

Creation of the Team: 2011 October 01, updated into Project-Team: 2016 June 01

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1. Team, Visitors, External Collaborators

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Abir Amri [Tunis El Manar University, from May 2019 until Jun 2019]
Veronica Anaya [Universidad Nacional Autonoma de Mexico, from Jun 2019 until Jul 2019]
Yves Bourgault [University of Ottawa, Jun 2019]
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Administrative Assistant

Nathalie Robin [Inria, Administrative Assistant]

2. Overall Objectives

2.1. Overall Objectives

The Carmen team develops and uses models and numerical methods to simulate the electrophysiology of the heart from the molecular to the whole-organ scale, and its relation to measurable signals inside the heart and on the body surface. It aims at

- improving understanding of normal and pathological cardiac electrophysiology,
- improving the efficiency and accuracy of numerical models, and
- exploitation of all available electrical signals for diagnosis, in particular for prediction of life-threatening cardiac arrhythmias.

The numerical models used and developed by the team incorporate the gating dynamics of the ion channels in the cardiac cell membranes and the heterogeneities and coupling processes on the cellular scale into macroscopic reaction-diffusion models. At the same time we use reduced models to solve the inverse problems related to non-invasive electrical imaging of the heart.

The fields involved in our research are: ordinary and partial differential equations (PDE), inverse problems, numerical analysis, high-performance computing, image segmentation, and mesh construction.

A main goal of the team is to contribute to the work packages defined in the IHU LIRYC (http://ihu-liryc.fr), an institute founded in 2011 that focuses on cardiac arrhythmia.

We cooperate with physiologists and cardiologists on several projects. The team is building new models and powerful simulation tools that will help to understand the mechanisms behind cardiac arrhythmias and to establish personalized and optimized treatments. A particular challenge consists in making the simulations reliable and accessible to the medical community.

3. Research Program

3.1. Complex models for the propagation of cardiac action potentials

The contraction of the heart is coordinated by a complex electrical activation process which relies on about a million ion channels, pumps, and exchangers of various kinds in the membrane of each cardiac cell. Their interaction results in a periodic change in transmembrane potential called an action potential. Action potentials in the cardiac muscle propagate rapidly from cell to cell, synchronizing the contraction of the entire muscle to achieve an efficient pump function. The spatio-temporal pattern of this propagation is related both to the function of the cellular membrane and to the structural organization of the cells into tissues. Cardiac arrythmias originate from malfunctions in this process. The field of cardiac electrophysiology studies the multiscale organization of the cardiac activation process from the subcellular scale up to the scale of the body. It relates the molecular processes in the cell membranes to the propagation process and to measurable signals in the heart and to the electrocardiogram, an electrical signal on the torso surface.

Several improvements of current models of the propagation of the action potential are being developed in the Carmen team, based on previous work [56] and on the data available at IHU LIRYC:

- Enrichment of the current monodomain and bidomain models [56], [67] by accounting for structural heterogeneities of the tissue at an intermediate scale. Here we focus on multiscale analysis techniques applied to the various high-resolution structural data available at the LIRYC.
- Coupling of the tissues from the different cardiac compartments and conduction systems. Here, we develop models that couple 1D, 2D and 3D phenomena described by reaction-diffusion PDEs.

These models are essential to improve our in-depth understanding of cardiac electrical dysfunction. To this aim, we use high-performance computing techniques in order to numerically explore the complexity of these models.

We use these model codes for applied studies in two important areas of cardiac electrophysiology: atrial fibrillation [60] and sudden-cardiac-death (SCD) syndromes [7], [6] [64]. This work is performed in collaboration with several physiologists and clinicians both at IHU Liryc and abroad.

3.2. Simplified models and inverse problems

The medical and clinical exploration of the cardiac electric signals is based on accurate reconstruction of the patterns of propagation of the action potential. The correct detection of these complex patterns by non-invasive electrical imaging techniques has to be developed. This problem involves solving inverse problems that cannot be addressed with the more compex models. We want both to develop simple and fast models of the propagation of cardiac action potentials and improve the solutions to the inverse problems found in cardiac electrical imaging techniques.

The cardiac inverse problem consists in finding the cardiac activation maps or, more generally, the whole cardiac electrical activity, from high-density body surface electrocardiograms. It is a new and a powerful diagnosis technique, which success would be considered as a breakthrough. Although widely studied recently, it remains a challenge for the scientific community. In many cases the quality of reconstructed electrical potential is not adequate. The methods used consist in solving the Laplace equation on the volume delimited by the body surface and the epicardial surface. Our aim is to

- study in depth the dependance of this inverse problem on inhomogeneities in the torso, conductivity values, the geometry, electrode positions, etc., and
- improve the solution to the inverse problem by using new regularization strategies, factorization of boundary value problems, and the theory of optimal control.

Of course we will use our models as a basis to regularize these inverse problems. We will consider the following strategies:

- using complete propagation models in the inverse problem, like the bidomain equations, for instance in order to localize electrical sources;
- constructing families of reduced-order models using e.g. statistical learning techniques, which would accurately represent some families of well-identified pathologies; and
- constructing simple models of the propagation of the activation front, based on eikonal or level-set equations, but which would incorporate the representation of complex activation patterns.

Additionaly, we will need to develop numerical techniques dedicated to our simplified eikonal/level-set equations.

3.3. Numerical techniques

We want our numerical simulations to be efficient, accurate, and reliable with respect to the needs of the medical community. Based on previous work on solving the monodomain and bidomain equations [4], [5], [8], [1], we will focus on

- High-order numerical techniques with respect to the variables with physiological meaning, like velocity, AP duration and restitution properties.
- Efficient, dedicated preconditioning techniques coupled with parallel computing.

Existing simulation tools used in our team rely, among others, on mixtures of explicit and implicit integration methods for ODEs, hybrid MPI-OpenMP parallellization, algebraic multigrid preconditioning, and Krylov solvers. New developments include high-order explicit integration methods and task-based dynamic parallelism.

3.4. Cardiac Electrophysiology at the Microscopic Scale

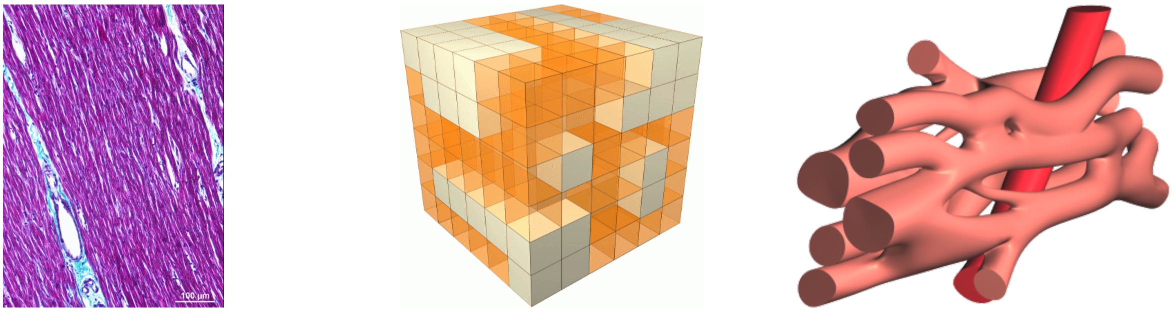
Numerical models of whole-heart physiology are based on the approximation of a perfect muscle using homogenisation methods. However, due to aging and cardiomyopathies, the cellular structure of the tissue changes. These modifications can give rise to life-threatening arrhythmias. For our research on this subject and with cardiologists of the IHU LIRYC Bordeaux, we aim to design and implement models that describe the strong heterogeneity of the tissue at the cellular level and to numerically explore the mechanisms of these diseases.

The literature on this type of model is still very limited [74]. Existing models are two-dimensional [65] or limited to idealized geometries, and use a linear (purely resistive) behaviour of the gap-juction channels that connect the cells. We propose a three-dimensional approach using realistic cellular geometry (figure 1), nonlinear gap-junction behaviour, and a numerical approach that can scale to hundreds of cells while maintaining a sub-micrometer spatial resolution (10 to 100 times smaller than the size of a cardiomyocyte) [52], [51], [49]. P-E. Bécue defended his PhD thesis on this topic in December 2018.

4. Application Domains

4.1. Scientific context: the LIRYC

The University Hospital of Bordeaux (*CHU de Bordeaux*) is equipped with a specialized cardiology hospital, the *Hôpital Cardiologique du Haut-Lévêque*, where the group of Professor Michel Haïssaguerre has established itself as a global leader in the field of cardiac electrophysiology [63], [61], [48]. Their discoveries in the area of atrial fibrillation and sudden cardiac death syndromes are widely acclaimed, and the group is a national and international referral center for treatment of cardiac arrhythmia. Thus the group also sees large numbers of patients with rare cardiac diseases.



A *B* *C*

*Figure 1. **A:** The cardiac muscle consists of a branching network of elongated muscle cells, interspersed with other structures. Sheets of connective tissue (blue) can grow between the muscle cells and become pathogenic. **B:** Current models can only represent such alterations in a coarse way by replacing model elements with different types; each cube in this illustration would represent hundreds of cells. **C:** This hand-crafted example illustrates the type of geometric model we are experimenting with. Each cell is here represented by hundreds of elements.*

In 2011 the group has won the competition for a 40 million euro *Investissements d'Avenir* grant for the establishment of IHU Liryc, an institute that combines clinical, experimental, and numerical research in the area of cardiac arrhythmia (http://ihu-liryc.fr). The institute works in all areas of modern cardiac electrophysiology: atrial arrhythmias, sudden death due to ventricular fibrillation, heart failure related to ventricular dyssynchrony, and metabolic disorders. It is recognized as one of the most important centers worldwide in this area.

The Carmen team was founded to partner with IHU Liryc. We bring applied mathematics and scientific computing closer to experimental and clinical cardiac electrophysiology. In collaboration with experimental and clinical researchers at Liry we work to enhance fundamental knowledge of the normal and abnormal cardiac electrical activity and of the patterns of the electrocardiogram, and we develop new simulation tools for training, biological, and clinical applications.

4.2. Basic experimental electrophysiology

Our modeling is carried out in coordination with the experimental teams from IHU Liryc. It help to write new concepts concerning the multiscale organisation of the cardiac action potentials that will serve our understanding in many electrical pathologies. For example, we model the structural heterogeneities at the cellular scale [50], and at an intermediate scale between the cellular and tissue scales.

At the atrial level, we apply our models to understand the mechanisms of complex arrythmias and the relation with the heterogeneities at the insertion of the pulmonary veins. We will model the heterogeneities specific to the atria, like fibrosis or fatty infiltration [69] [60]. These heterogeneities ara thought to play a major role in the development of atrial fibrillation.

At the ventricular level, we focus on (1) modeling the complex coupling between the Purkinje network and the ventricles, which is supposed to play a major role in sudden cardiac death, and (2) modeling the heteogeneities related to the complex organization and disorganization of the myocytes and fibroblasts, which is important in the study of infarct scars for instance.

4.3. Clinical electrophysiology

Treatment of cardiac arrhythmia is possible by pharmacological means, by implantation of pacemakers and defibrillators, and by curative ablation of diseased tissue by local heating or freezing. In particular the ablative therapies create challenges that can be addressed by numerical means. Cardiologists would like to know, preferably by noninvasive means, where an arrhythmia originates and by what mechanism it is sustained.

We address this issue in the first place using inverse models, which attempt to estimate the cardiac activity from a (high-density) electrocardiogram. A new project aims at performing this estimation on-site in the catheterization laboratory and presenting the results, together with the cardiac anatomy, on the screen that the cardiologist uses to monitor the catheter positions [66].

An important prerequisite for this kind of interventions and for inverse modeling is the creation of anatomical models from imaging data. The Carmen team contributes to better and more efficient segmentation and meshing through the IDAM project.

5. Highlights of the Year

5.1. Highlights of the Year

Mark Potse has been recruited on a permanent position researcher at Bordeaux University.

The team has been involved in the organization of the 10th international conference on Functional Imaging and Modeling of the Heart (FIMH), that was held at Bordeaux in July 2019.

The Direction Generale de l'offre de soins (DGOS) has accepted to found the clinical project of phase III Parkeo2 In this project 11 hospitals in France will use the software OptimDBS for the planification of deep cerebral surgery. The project will start in October 2020 and will last three years.

6. New Software and Platforms

6.1. CEPS

Cardiac ElectroPhysiology Simulation

KEYWORDS: Simulation - Health - Mesh - Cardiac - 3D - Cardiac Electrophysiology

SCIENTIFIC DESCRIPTION: As compared to other existing softwares, CEPS aims at providing a more general framework of integration for new methods or models and a better efficiency in parallel. CEPS is designed to run on massively parallel architectures, and to make use of state-of-the-art and well known computing libraries to achieve realistic and complex heart simulations. CEPS also includes software engineering and validation tools.

FUNCTIONAL DESCRIPTION: CEPS is a modular high-performance computing software for performing numerical simulations in cardiac electrophysiology. It is based on modules : - management of geometries represented by meshes in 3D, 2D or 1D (volumes, surfaces, trees), - model simulation of cellular electrophysiology, - calculating the tissue propagation of the action potentials in the cardiac geometries, - calculation of extracardiac potentials, - time approximation methods in order 2, 3 and 4 specific to electrocardiography.

- Participants: Mehdi Juhoor, Nejib Zemzemi, Antoine Gerard, Charlie Douanla Lontsi, Pierre-Elliott Bécue, Marc Fuentes, Yves Coudière, Michael Leguebe, Andjela Davidovic, Pauline Migerditichan and Florian Caro
- Partners: Université de Bordeaux - Fondation Bordeaux Université - CHU de Bordeaux - Inria
- Contact: Michael Leguebe
- URL: https://gforge.inria.fr/projects/ceps/

6.2. OptimDBS

Optimizing the Deep Brain Stimulation

KEYWORDS: Image analysis - Deep brain stimulation - Statistical learning

FUNCTIONAL DESCRIPTION: Targeting software for deep brain stimulation

- Participants: Nejib Zemzemi, Louise-Amelie Schmitt, Emmanuel Cuny and Julien Engelhardt
- Partner: CHU de Bordeaux
- Contact: Nejib Zemzemi
- URL: https://gitlab.inria.fr/optimdbs/optimdbs-medinria/-/wikis/home

6.3. Platforms

6.3.1. CEMPACK

CEMPACK is a new collection of software that was previously archived in different places. It includes the high-performance simulation code Propag and a suite of software for the creation of geometric models, preparing inputs for Propag, and analysing its outputs. In 2017 the code was collected in an archive on Inria's GitLab platform, and a public website was created for documentation (http://cempack.gforge.inria.fr). The main components of CEMPACK are the following.

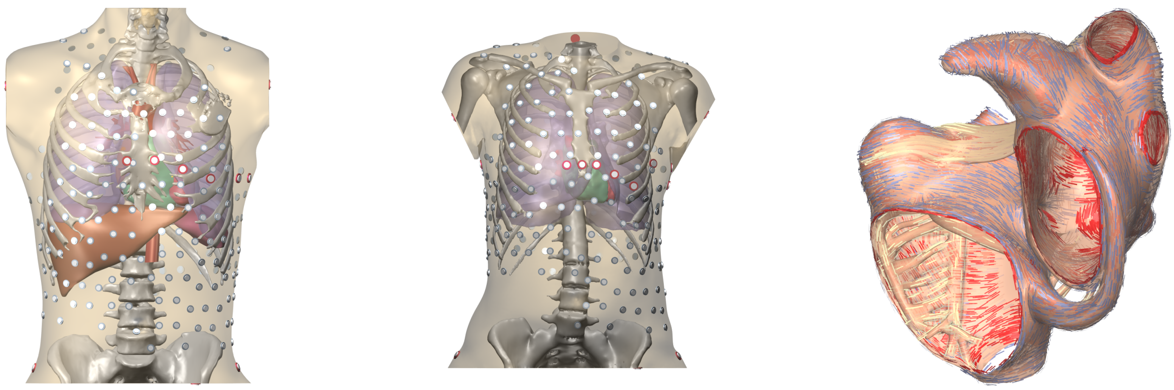
Propag-5.1 Applied modeling studies performed by the Carmen team in collaboration with IHU Liryc and foreign partners [7] [71], [60], [57], [53] rely on high-performance computations on the national supercomputers Irene, Occigen, and Turing. The Propag-5 code is optimized for these systems. It is the result of a decades-long development first at the *Université de Montréal* in Canada, then at Maastricht University in the Netherlands, and finally at the Institute of Computational Science of the *Università della Svizzera italiana* in Lugano, Switzerland. Since 2016 most of the development on Propag has been done by M. Potse at the Carmen team [72]. The code scales excellently to large core counts and, as it is controlled completely with command-line flags and configuration files, it can be used by non-programmers. It also features

- a plugin system for membrane models,
- a completely parallel workflow, including the initial anatomy input and mesh partitioning, which allows it to work with meshes of more than 10^9 nodes,
- a flexible output scheme allowing hundreds of different state variables and transient variables to be output to file, when desired, using any spatial and temporal subsampling,
- a configurable, LUSTRE-aware parallel output system in which groups of processes write HDF5/netCDF files, and
- CWEB documentation of the entire code base.

The code has been stable and reliable for several years. It can be considered the workhorse for our HPC work until CEPS takes over.

Gepetto The Gepetto suite, named after a famous model maker, transforms a surface mesh of the heart into a set of (semi-)structured meshes for use by the Propag software or others. It creates the different fiber orientations in the model, including the transmurally rotating ventricular fibers and the various bundle structures in the atria (figure 2), and creates layers with possibly different electrophysiological properties across the wall. A practically important function is that it automatically builds the matching heart and torso meshes that Propag uses to simulate potentials in the torso (at a resolution of 1 mm) after projecting simulation results from the heart model (at 0.1 to 0.2 mm) on the coarser torso mesh [68]. Like Propag, the Gepetto software results from a long-term development that started in Montreal, Canada, around 2002. The code for atrial fiber structure was developed by our team.

Blender plugins Blender (https://www.blender.org) is a free software package for the production of 3-D models, renderings, and animations, comparable to commercial software such as Cinema4D. CEMPACK includes a set of plugins for Blender that facilitate the production of anatomical models and the visualization of measured and simulated data. It uses the MMG remeshing library, which is developed by the CARDAMOM team at Inria Bordeaux.



A *B* *C*

*Figure 2. **A and B:** Complete heart-torso geometries created with CEMPACK tools. **C:** Bundle structures and different layers of fiber orientation created by the Gepetto software.*

6.3.2. MUSIC

MUSIC is a multimodal platform for cardiac imaging developed by the imaging team at IHU LIRYC in collaboration with the Inria team Asclepios (https://bil.inria.fr/fr/software/view/1885/tab). It is based on the medInria software also developed by the Asclepios team. MUSIC is a cross-platform software for segmentation of medical imaging data, meshing, and ultimately also visualization of functional imaging data and model results.

Several members of the Carmen team use MUSIC for their work, and the team contributes to the software through the IDAM project.

7. New Results

7.1. Modelling, direct simulation and prediction of cardiac phenomena

Using high-performance simulations on a detailed model of the human atria [58] we investigated several aspects of atrial fibrillation (AF). We showed that AF initiation by rapid pacing is sensitive to very small changes in parameter values [70] [32], [38] , and investigated effects of antiarrhythmic drugs and interventions [59] [34] and pathologies [35]. An example movie is available online at https://www.potse.nl/papers/potse/potse-fimh19.html.

High-performance simulations of human ventricular activity have contributed to the testing of new electrocardiographic mapping methods (“inverse models”) [73], [36].

We are also developing new methods to help with the treatment of these patients by rapidly guiding an ablation catheter to the origin (strictly speaking: the exit site) of an arrhythmia. These methods are also being tested with simulated data. [33].

We contributed to work by Prof. Michel Haissaguerre and his team in which it is argued that many patients who are now believed to suffer from abnormalities in the genes for specific cardiac ion channels are in reality affected by structural diseases of the heart muscle [62] [26], [41]. These influential publications represent an important change in thinking about these patients and their treatment.

Simple mitochondrial model based on thermodynamic fluxes (PhD work of B. Tarraf): Mitochondria are involved in the regulation of calcium which plays a crucial role in the propagation of cardiac action potentials. However, they are not taken into account in the ionic models that are used to perform simulations at the tissue level. In the framework of the ANR MITOCARD project, we wrote a simple model of mitochondrial calcium regulation based on an extensive review of models of the litterature, which are not suited for further calibration due to their excessive complexity [39]. Now that the equations are written down, we are performing a parameter analysis on the whole model before including other key biological mechanisms.

In a collaboration with Jeremy Darde (IMT Toulouse), we have developed a numerical method on a cartesian grid to solve the direct problem of Electrical Impedance Tomography (EIT) in complex geometries, with first-order convergence. The objective is to solve then the inverse problem of EIT to identify heterogeneities of conductivities on the torso volume.

7.2. Inverse problems: parameter estimation, data assimilation and ECGi

- Data assimilation: In A. Gérard PhD thesis, it is showed that accounting for the anisotropy in the atria is crucial to reconstruct correctly activation maps compatible with a mono-domain model from sparse punctuals activation times. To this purpose, we have developed a new data assimilation method for the mono-domain model, using a Luenberger filter and a Kalman-type filter (ROUKF), based on the dissimilarity measure introduced in A. Collin PhD thesis.
- Parameter estimation: We have been working on the following theoretical question: What are the condition under which the parameters, in the mathematical codomain and bidomain models, are identifiables. Then we proposed an algorithm capable of estimating different ion-channels conductance parameters. mettre ref?
- ECGI: Several approaches have been investigated to improve the resolution of ECGi.
  - development of a new algorithm to choose the regularization coefficient for the resolution of ECGi with the Method of Fondamental Solutions (MFS).
  - a study using a parametrized model of action potentials, showing that accounting for the endocardium can improve the resolution of ECGi.
  - in joint work with Laura Bear (IHU Liryc), development of a new method for improving the resolution of ECGI by combining several solutions obtained with various numerical methods (FEM and MFS). The method is based on the selection of the smallest residuals on the torso surface.
  - Development of new methods for the ECGI problem, based on machine learning methods. The idea is to learn activation maps from body surface signals.
  - collaborative work on the set up of an experimental platform for the experimental non-invasive validation of the reconstruction of cardiac signals

7.3. Numerical schemes

- Very-high order Finite Volume methods: We have showed the very good behavior of a specifically devised domain decomposition technique: the communications are minimized without impacting the accuracy or the order of convergence of the scheme. The total amount of communications dos not increase significantly between the second and the 6th order. The 6th-order Finite-Volume scheme is thus the most performing scheme.
- Numerical analysis of a cartesian method for elliptic problems with immersed interfaces: We have studied the convergence of a cartesian method for elliptic problems with immersed interfaces previously published [54]. The convergence is proved for the original second-order method in one-dimension and for a first-order version in two dimensions. The proof uses a discrete maximum principle to obtain estimates of the coefficients of the inverse matrix.

7.4. Miscellanous

- Refactoring of the CEPS software. Our CEPS software underwent an important refactoring phase so that future students spend less time getting hands on the code. Also, several features developped by previous PhD students were merged into the version that we intend to distribute : high order numerical schemes suited for ionic models, volume fraction due to tissue heterogeneities. We are currently in the process of licensing with Inria and University of Bordeaux.
- Deep brain stimulation procedure: We have been working on three different learning methods for the prediction of the optimal pacing sites in the Deep brain stimulation procedure. We also compared the found position to the position of the stimulation sites to the anatomical geometries in the Ewert brain atlas. Results show the robustness of the methods in founding the stimulation regions.
- Generation of boundary conditions for the Boussinesq system: In a collaboration with David Lannes (IMB, Bordeaux) we have developed a new method for the numerical implementation of generating boundary conditions for a one dimensional Boussinesq system. The method is based on a reformulation of the equations and a resolution of the dispersive boundary layer that is created at the boundary.
- Simulation of solid suspensions in incompressible fluids: In a collaboration with B. Lambert and M. Bergmann (IMB, Bordeaux) we have extended a previously published local lubrication model to non-Brownian suspensions of ellipsoidal solid particles in incompressible flows. This lubrication model used virtual spheres to evaluate local lubrication corrections instead of the global corrections found in the classical lubrication theory.

8. Partnerships and Cooperations

8.1. Regional Initiatives

The project "Cardiac Arrhythmia Localization Methods," granted by the Région Nouvelle-Aquitaine, with matching from funds held by our clinical collaboraters H. Cochet and P. Jaïs, has started. The purpose of this project is to develop a tool that can predict the exit site of an arrhythmia with moderate accuracy (1 cm) in an absolute sense, with respect to the anatomy of the heart in situ, and with a resolution of about 2 mm in a relative sense, with respect to a nearby pacing site. This tool must fulfill the following criteria:

- it uses only data that are already recorded in the cathlab by other systems: ECG data and electroanatomical mapping data;
- it must work in nearly real-time; catheter displacement advice must be available within 5 seconds after a paced beat;
- it must work automatically, requiring the operator only to indicate which ECG data correspond to the target arrhythmia; and
- it must be safe and easy to operate.

We will in the first place test a number of proposed methods using synthetic data, produced with our realistic models of cardiac electrophysiology and accurate geometric models of different patients. This in-silico testing phase will answer a number of important practical questions. Subsequently we will use offline clinical data, and within 2 years we aim to build a clinical prototype that can be tested (without interfering in the procedure) in the cathlab. In order to work real-time we will initially use very simple methods. However, the clinical prototype and the collectoin of synthetic data that we created will later serve also as a platform to test also more sophisticated inverse methods.

8.2. National Initiatives

8.2.1. ANR EXACARD

We started a collaboration with the STORM team at Inria Bordeaux Sud-Ouest to work on further scaling of the Propag code, to push the limit from about 10^4 to 10^6 parallel processors. A proposal for this project was funded this year by ANR. It allows a postdoc to be employed for 2 years.

8.2.2. ANR MITOCARD

The MITOCARD project (Electrophysiology of Cardiac Mitochondria), coordinated by S. Arbault (Université de Bordeaux, ISM), was granted by the ANR in July 2017. The objective of MITOCARD is to improve understanding of cardiac physiology by integrating the mitochondrial properties of cell signaling in the comprehensive view of cardiac energetics and rhythm pathologies. It was recently demonstrated that in the heart, in striking contrast with skeletal muscle, a parallel activation by calcium of mitochondria and myofibrils occurs during contraction, which indicates that mitochondria actively participate in Ca2+ signaling in the cardiomyocyte. We hypothesize that the mitochondrial permeability transition pore (mPTP), by rhythmically depolarizing inner mitochondrial membrane, plays a crucial role in mitochondrial Ca2+ regulation and, as a result, of cardiomyocyte Ca2+ homeostasis. Moreover, mitochondrial reactive oxygen species (ROS) may play a key role in the regulation of the mPTP by sensing mitochondrial energetics balance. Consequently, a deeper understanding of mitochondrial electrophysiology is mandatory to decipher their exact role in the heart's excitation-contraction coupling processes. However, this is currently prevented by the absence of adequate methodological tools (lack of sensitivity or selectivity, time resolution, averaged responses of numerous biological entities). The MITOCARD project will solve that issue by developing analytical tools and biophysical approaches to monitor kinetically and quantitatively the Ca2+ handling by isolated mitochondria in the cardiomyocyte.

MITOCARD is a multi-disciplinary project involving 4 partners of different scientific fields: the CARMEN team as well as

ISM, the largest chemistry laboratory of the Université de Bordeaux, where the necessary measurement methods will be developed;

Liryc, where mitochondria are studied at all levels of integration from the isolated mitochondrion to the intact heart; and

LAAS, the MiCrosystèmes d'Analyse (MICA) group at the Laboratory of Analysis and Architecture of Systems, which develops the biological microsensors for this project.

The project will

- develop chips integrating 4 different electrochemical microsensors to monitor in real-time key mitochondrial signaling parameters: Ca2+, membrane potential, quinone reduction status, O2 consumption, and ROS production;
- develop microwell arrays integrating ring nanoelectrodes to trap single mitochondria within micrometric chambers and measure locally by combined fluorescence microscopy and electrochemical techniques intra- (by fluorescence) and extra-mitochondrial (electrochemistry) metabolites; and
- develop a mathematical model of mitochondrial Ca2+ and ROS handling built on existing knowledge, new hypotheses, and the measured data.

The model may serve both to assess biological assumptions on the role of mitochondria in Ca2+ signaling and to integrate pathological data and provide clues for their global understanding.

8.2.3. GENCI

GENCI (*grand équipement national de calcul intensif*) is the agency that grants access to all national high-performance resources for scientific purposes in France. GENCI projects have to be renewed yearly. Our project renewal *Interaction between tissue structure and ion-channel function in cardiac arrhythmia*, submitted in September 2018, has been granted 8 million core-hours on the three major systems Irene, Occigen, and Turing. This compute time is primarily destined for our research into the interaction between ionic and structural heart disease in atrial fibrillation, Brugada syndrome, and early repolarisation syndrome [7] [71], and for new HPC developments [72].

8.2.4. PHRCN Multi-centric project

This project has been accepted for funding in December 2019. N Zemzemi is partner of the project and Prof. Emmanuel Cuny (PU-PH CHU de Bordeaux) is the Principal investigator. It is entitled "Deep brain stimulation for Parkinson disease: Probabilistic STN Targeting under general anaesthesia without micro-electrode recordings (MER) vs current surgical procedure." It will start in 2020 and end in 2023.

8.2.5. BOUM project on ECGi

This project is coordinated by 2 PhD students (A. Karoui and O. Bouhamama) and 1 postdoc (M. Diallo), and is funded by the French applied and industrial math society (SMAI). It consists in organizing a national workshop on ECGI.

8.2.6. Inria Ciescard project

This project entitled "Combiner des Information Electriques et Structurelles pour aider les cardiologues à mieux Cibler la thérApie caRDiaque" funds an engineer for 2 years to develop some plugins in the software platform Music. The PI is N. Zemzemi.

8.2.7. Inria project OptimDBS

This project is designed to develop a software for the prediction of the optimal Deep stimulation targets based on machine learning techniques. It is funded by Inria as part of the ATT program. The PI is N. Zemzemi

8.3. Transfert

Together with Prof. Emmanuel Cuny and the help of AST (Aquitaine Science Transfert) and Inria Startup Studio, we are working on the creation of a startup company based on the software OptimDBS, and an associated the submitted patent. We follow the Founders 101 program of Inria to help us with the business, marketing, and management parts. The associated patent entitled Méthode de détermination d'une cible cérébrale stéréotaxique has been submitted to INPI by N. Zemzemi, J. Engelhardt, and E. Cuny under the number 71959FR. Our Software is currently used for the treatment of Essential Trauma in a Phase I clinical study at the CHU de Bordeaux and CHU de Lyon. A new PHRC-National multi-centric project has been accepted in December 2019 (see above, funded projects). This project is led by Emmanuel Cuny and aims at assessing the efficiency of our solution in the treatment of Parkinson Disease. The OptimDBS software will be used by 11 medical centers in France.

8.4. European Initiatives

8.4.1. Collaborations in European Programs, Except FP7 & H2020

Program:MSCA-ITN

Project title: "Personalized Therapies for Atrial Fibrillation. A Translational Approach."

Start Feb 2020 - End 2024

Coordinator: for UB/Liyrc: N. Zemzemi, PI: M. Guillem (University of Valencia, Spain)

8.4.2. Collaborations with Major European Organizations

BCAM (Basque Center for Applied Mathematics), Bilbao, Spain: L. Gerardo-Giorda.

We develop surrogate models of Radiofrequency Catheter Ablation for machine learning purposes, with the ambition to provide real-time estimations of lesion depths to clinicians (M. Leguèbe, Y. Coudière).

8.5. International Initiatives

8.5.1. Inria International Labs

International Laboratory for Research in Computer Science and Applied Mathematics

Associate Team involved in the International Lab:

8.5.1.1. EPICARD

Title: inversE Problems In CARDiac electrophysiology

International Partner (Institution - Laboratory - Researcher):

ENIT (Tunisia) - Department of Intelligence Science and Technology - Mourad Bellassoued

Start year: 2018

See also: https://team.inria.fr/carmen/epicard/

Model personalization is a very challenging question in the numerical modeling community, especially for medical applications like cardiac electrophysiology. Our main idea is to adapt the input data like model parameters and boundary conditions of the electrophysiological measurements. There are two mathematical problems raising from this challenge. The first issue is the identifiability of the parameters and the sensitivity of the identification problem to the measured data. The question is: For given measurements, could we prove that there exist a set of parameters that allows to fit these measurements? The second issue is, how can we estimate parameters, when they are identifiable,? Our idea is to provide a theoretical analysis for the identification of each of the parameters and to construct suitable numerical methods to estimate them.

8.5.1.2. Informal International Partners

Y. Coudière works with the group of Prof. Y. Bourgault from the Department of Mathematics and Statistics of the University of Ottawa (Canada). Some results on the numerical analysis of time-stepping methods from C. Douanla's PhD were carried out together, as well as some theoretical results on parameter identification in the PhD of A. Gérard.

M. Potse works with the group of Prof. U. Schotten at Maastricht University (The Netherlands) and the Center for Computational Medicine in Cardiology at the *Università della Svizzera italiana* (Lugano, Switzerland) on simulation studies of atrial fibrillation [60]. The Maastricht group was partially funded by the FP7 project EUTRAF and our simulations were supported by GENCI (section 8.2.3).

N. Zemzemi works with Cesare Corrado at King's College London on the development of new eikonal models allowing conduction velocity adaptation [55].

Mostafa Bendahmane works with Kenneth H. Karlsen at university of Oslo (Norway) on the stochastic bidomain model in electrocardiology [46].

8.6. International Research Visitors

8.6.1. Visits of International Scientists

- Yassine Abidi, Ecole Nationale d'Ingénieurs de Tunis, Jun 2019,
- Abir Amri, Tunis El Manar University, from May 2019 until Jun 2019,
- Veronica Anaya, Universidad Nacional Autonoma de Mexico, from Jun 2019 until Jul 2019
- Yves Bourgault, University of Ottawa, Jun 2019
- Elmahdi Erraji, Cadi Ayyad University, Jun 2019
- Moncef Mahjoub, Tunis El Manar University, from Oct 2019 until Nov 2019

9. Dissemination

9.1. Promoting Scientific Activities

9.1.1. Member of the Organizing Committees

Several members of the team were involved in the organization of the 10th international conference on Functional Imaging and Modeling of the Heart (FIMH), that was held at Bordeaux in July 2019.

M. Leguèbe co-organizes the seminar of team “Calcul Scientifique et Modélisation” (IMB, Université de Bordeaux).

Lisl Weynans co-organizes with Edward Vigmond (IHU Liryc) the bi-monthly journal club of the modelling group at Liryc, and organizes a monthly workgroup about applied numerical methods, within the Scientific Computing and Modelling team at IMB (Institut de Mathématique de Bordeaux)

9.1.2. Journal

9.1.2.1. Member of the Editorial Boards

Mostafa Bendahmane is member of the editorial board of the "Moroccan Journal of Pure and Applied Mathematics", Mark Potse is an associate editor for "Frontiers in Cardiac Electrophysiology" and an Associate editor for "Journal of Electrocardiology".

9.1.3. Invited Talks

- Lisl Weynans: Mini-symposium on "Numerical methods for interfacial dynamics", ICIAM 2019, Valence, Spain.
- Nejib Zemzemi: Maghrebian Meeting of Young Researchers in Pure and Applied Mathematics, MYRPAM. Hammamet, Tunisia 9-12 December, 2019.
- Mostafa Bendahmane: "Recent progress in inverse problems in electrocardiology", at CAMS, American university of Beirut, Libanon.
- Mark Potse: "Atrial fibrillation dynamics", invited talk at the 2019 International Congress on Electrocardiology, Belgrade, Serbia, 2019.
- Mark Potse: "ECG imaging without imaging", invited talk at the 2019 International Congress on Electrocardiology, Belgrade, Serbia, 2019.
- Lisl Weynans: invited talk on "Hywec 2 : The Hydrodynamics of Wave Energy Convertors", Talence, 2019.
- Lisl Weynans: invited talk at the Seminar of "Institut de Mathematiques de Toulouse", 2019.
- Lisl Weynans: invited talk at the Workshop of ANR RheoSuNN, Ecole Polytechnique, Palaiseau, March 2019.
- Yves Coudière: invited plenary talk at the "9e biennale des mathématiques appliquées et industrielles de la SMAI", Guidel, 2019.
- Nejib Zemzemi: invited talk on "Mathematical Modelling of the electrical activity of the heart from ion-channels to the body surface: Forward and Inverse problems", at Institut de recherche mathématique de Rennes, March 14, 2019.

9.1.4. Research Administration

Yves Coudière is a deputy director of Directeur IMB (Institut de Mathématiques de Bordeaux, UMR 5251 CNRS, Ub, Bdx-INP). Gathering around 160 permanent members, it organizes the research in mathematics and applications of mathematics in Bordeaux.

Michael Leguebe is the secretary of the CLHSCT (Comité Local Hygiène et Sécurité au travail) of the Inria BSO research center.

Lisl Weynans is a member of the "conseil UFR maths et interactions", a member of the "conseil scientifique IMB" and a member of the "BCP" of the Inria BSO research center.

9.2. Teaching - Supervision - Juries

9.2.1. Teaching

The 2 assistant professors and 1 professor of the team teach at several levels of the Bordeaux University programs in Mathematics and Neurosciences (respectively, 192, 192 and 96 h/year on average). The researchers also have a regular teaching activity, contributing to several courses in the Applied Mathematics at the Bachelor and Master levels (usually between 16 and 32 h/year).

The PhD student are used to teach between 32 and 64 h/year, usually courses of general mathematics in L1 or mathematics for biologists in L1 or L2.

Teaching responsibilities at the University of Bordeaux:

- Yves Coudière: Master MAS (Mathématiques Appliquées, Statistiques), parcours MNCHP (Modélisation Numérique Calcul Haute Performance),
- Yves Coudière: Licence Mathématique parcours ingénierie mathématique,
- Lisl Weynans: Mineure Mathématiques du parcours International de la Licence
- Mostafa Bendahmane: Responsable de la mobilité internationale des étudiants de Licence MIASHS.

Courses (L for Bachelor level, M for Master level):

- Numerical analysis (L2)
- Programming for scientific computing with C++ (L3)
- Programming projects with Python (M1)
- Numerical approximation of PDEs: Finite Differences, Finite Elements, Finite Volumes (M1, M2)
- Supervision of programming projects (L3, M1)
- Mathematical modelling in L2 parcours medicine and physics
- Linear Algebra, Optimization under constraints (L2 and Essca school)
- Analysis, L2
- Computational Neurosciences, M2
- Neuropsychology and Psychophysiology, L3
- Graduate program EUR Digital Public Health, Bordeaux University, March 2019. Philosophy of science and the role of numerical models: introductory course in the module Modeling in life science

Courses at doctoral level:

- Liryc summer school, July 2019: Computer modeling of cardiac electrophysiology, 3 hours
- Course of mathematics for medicine students: March 2019, course organized by the Ecole Doctorales EDMI and SVS of Bordeaux University Introductory course of mathematical modelling and parameter estimation techniques in complex models (4h30)

9.2.2. Supervision

PhD : Antoine Gérard, Modèles numériques personnalisés de la fibrillation auriculaire , Univ. Bordeaux, July 12th 2019, encadrant: Yves Coudière

PhD in progress : Andony Arrieula, Oct. 2018, encadrant: Mark Potse

PhD in progress: Oumayma Bouhamama, Oct. 2018 , encadrante: Lisl Weynans

PhD in progress : Syed Hassaan Ahmed Bukhari, Oct. 2018, encadrant: Mark Potse

PhD in progress : Amel Karoui, Oct 2017, encadrants: Mostafa Bendahmane and Nejib Zemzemi

PhD in progress : Bachar Tarraf, Oct. 2018, encadrant: Yves Coudière and Michael Leguebe

9.2.3. Juries

- Lisl Weynans: member of the Jury for the recruitment of CR Inria, BSO research center.
- Lisl Weynans : member of the jury for the PhD of Umberto Bosi in applied mathematics (Univ. Bordeaux)
- Yves Coudière: chairman of the jury for the PhD of J. Engelhardt in neurology (Univ. Bordeaux)
- Yves Coudière: member of the jury for the PhD of A. Gérard in applied mathematics (Univ. Bordeaux)
- Nejib Zemzemi : member of the jury for the PhD of Rabeb Chamekh in applied mathematics
- Mostafa Bendahmane: member of the jury for the PhD of Mohamed Zagour in applied mathematics.

9.3. Popularization

9.3.1. Internal or external Inria responsibilities

Coordination of a workgroup entitled "CultureMATH Bordeaux", working on writing dissemination articles for the website https://culturemath.ens.fr.

9.3.2. Education

Organization of "Moi informaticienne, moi mathématicienne (MIMM)": one week internship at the University for young girls (15-16 year old) interested in maths and informatics.

9.3.3. Interventions

- National events: Fête de la Science, Semaine des maths,
- In educational institutions: several talks in high-schools about scientific computing and applied mathematics
- Presentation stand for "Simric" at the 10 years anniversary of the Inria Bordeaux Sud-Ouest centre.
- Modeling stand at the "Journée portes ouvertes de Liryc", 2019.
- Reception of 5 high-school pupils (élèves de 3e, 15 years old).

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Project-Team CQFD

Quality control and dynamic reliability

IN COLLABORATION WITH: Institut de Mathématiques de Bordeaux (IMB)

IN PARTNERSHIP WITH:
CNRS

Université de Bordeaux

RESEARCH CENTER
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THEME
Stochastic approaches

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Project-Team CQFD

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2. Overall Objectives

2.1. Presentation

The core component of our scientific agenda focuses on the development of statistical and probabilistic methods for the modeling and the optimization of complex systems. These systems require dynamic and stochastic mathematical representations with discrete and/or continuous variables. Their complexity poses genuine scientific challenges that can be addressed through complementary approaches and methodologies:

- *Modeling:* design and analysis of realistic and tractable models for such complex real-life systems taking into account various probabilistic phenomena;
- *Estimation:* developing theoretical and computational methods in order to estimate the parameters of the model and to evaluate the performance of the system;
- *Control:* developing theoretical and numerical control tools to optimize the performance.

These three approaches are strongly connected and the most important feature of the team is to consider these topics as a whole. This enables the team to deal with real industrial problems in several contexts such as biology, production planning, trajectory generation and tracking, performance and reliability.

3. Research Program

3.1. Introduction

The scientific objectives of the team are to provide mathematical tools for modeling and optimization of complex systems. These systems require mathematical representations which are in essence dynamic, multi-model and stochastic. This increasing complexity poses genuine scientific challenges in the domain of modeling and optimization. More precisely, our research activities are focused on stochastic optimization and (parametric, semi-parametric, multidimensional) statistics which are complementary and interlinked topics. It is essential to develop simultaneously statistical methods for the estimation and control methods for the optimization of the models.

3.2. Main research topics

Stochastic modeling: Markov chain, Piecewise Deterministic Markov Processes (PDMP), Markov Decision Processes (MDP).
The mathematical representation of complex systems is a preliminary step to our final goal corresponding to the optimization of its performance. The team CQFD focuses on two complementary types of approaches. The first approach is based on mathematical representations built upon physical models where the dynamic of the real system is described by *stochastic processes*. The second one consists in studying the modeling issue in an abstract framework where the real system is considered as black-box. In this context, the outputs of the system are related to its inputs through a *statistical model*. Regarding stochastic processes, the team studies Piecewise Deterministic Markov Processes (PDMPs) and Markov Decision Processes (MDPs). These two classes of Markov processes form general families of controlled stochastic models suitable for the design of sequential decision-making problems. They appear in many fields such as biology, engineering, computer science, economics, operations research and provide powerful classes of processes for the modeling of complex systems. Our contribution to this topic consists in expressing real-life industrial problems into these mathematical frameworks. Regarding statistical methods, the team works on dimension reduction models. They provide a way to understand and visualize the structure of complex data sets. Furthermore, they are important tools in several different areas such as data analysis and machine learning, and appear in many applications such as biology, genetics, environment and recommendation systems. Our contribution to this topic consists in studying semiparametric modeling which combines the advantages of parametric and nonparametric models.

Estimation methods: estimation for PDMP; estimation in non- and semi- parametric regression modeling.
To the best of our knowledge, there does not exist any general theory for the problems of estimating parameters of PDMPs although there already exist a large number of tools for sub-classes of PDMPs such as point processes and marked point processes. To fill the gap between these specific models and the general class of PDMPs, new theoretical and mathematical developments will be on the agenda of the whole team. In the framework of non-parametric regression or quantile regression, we focus on kernel estimators or kernel local linear estimators for complete data or censored data. New strategies for estimating semi-parametric models via recursive estimation procedures have also received an increasing interest recently. The advantage of the recursive estimation approach is to take into account the successive arrivals of the information and to refine, step after step, the implemented estimation algorithms. These recursive methods do require restarting calculation of parameter estimation from scratch when new data are added to the base. The idea is to use only the previous estimations and the new data to refresh the estimation. The gain in time could be very interesting and there are many applications of such approaches.

Dimension reduction: dimension-reduction via SIR and related methods, dimension-reduction via multidimensional and classification methods.
Most of the dimension reduction approaches seek for lower dimensional subspaces minimizing the loss of some statistical information. This can be achieved in modeling framework or in exploratory data analysis context.

In modeling framework we focus our attention on semi-parametric models in order to conjugate the advantages of parametric and nonparametric modeling. On the one hand, the parametric part of the model allows a suitable interpretation for the user. On the other hand, the functional part of the model offers a lot of flexibility. In this project, we are especially interested in the semi-parametric regression model $Y = f(X'\theta) + \varepsilon$, the unknown parameter θ belongs to $\mathbb{R}^p$ for a single index model, or is such that $\theta = [\theta_1, \cdots, \theta_d]$ (where each θ_k belongs to $\mathbb{R}^p$ and $d \leq p$ for a multiple indices model), the noise ε is a random error with unknown distribution, and the link function f is an unknown real valued function. Another way to see this model is the following: the variables X and Y are independent given $X'\theta$. In our semi-parametric framework, the main objectives are to estimate the parametric part θ as well as the nonparametric part which can be the link function f, the conditional distribution function of Y given X or the conditional quantile q_α. In order to estimate the dimension reduction parameter θ we focus on the Sliced Inverse Regression (SIR) method which has been introduced by Li [37] and Duan and Li [35].
Methods of dimension reduction are also important tools in the field of data analysis, data mining and machine learning.They provide a way to understand and visualize the structure of complex data sets.Traditional methods among others are principal component analysis for quantitative variables or multiple component analysis for qualitative variables. New techniques have also been proposed to address these challenging tasks involving many irrelevant and redundant variables and often comparably few observation units. In this context, we focus on the problem of synthetic variables construction, whose goals include increasing the predictor performance and building more compact variables subsets. Clustering of variables is used for feature construction. The idea is to replace a group of "similar" variables by a cluster centroid, which becomes a feature. The most popular algorithms include K-means and hierarchical clustering. For a review, see, e.g., the textbook of Duda [36].

Stochastic control: optimal stopping, impulse control, continuous control, linear programming.
The main objective is to develop *approximation techniques* to provide quasi-optimal feasible solutions and to derive *optimality results* for control problems related to MDPs and PDMPs:

- *Approximation techniques*. The analysis and the resolution of such decision models mainly rely on the maximum principle and/or the dynamic/linear programming techniques together with their various extensions such as the value iteration (VIA) and the policy iteration (PIA) algorithm. However, it is well known that these approaches are hardly applicable in practice and suffer from the so-called *curse of dimensionality*. Hence, solving numerically a PDMP or an MDP is a difficult and important challenge. Our goal is to obtain results which are both consistent from a theoretical point of view and computationally tractable and accurate from an application standpoint. It is important to emphasize that these research objectives were not planned in our initial 2009 program.

  Our objective is to propose approximation techniques to efficiently compute the optimal value function and to get quasi-optimal controls for different classes of constrained and unconstrained MDPs with general state/action spaces, and possibly unbounded cost function. Our approach is based on combining the linear programming formulation of an MDP with probabilistic approximation techniques related to quantization techniques and the theory of empirical processes. An other aim is to apply our methods to specific industrial applications in collaboration with industrial partners such as Airbus Defence & Space, Naval Group and Thales.

  Asymptotic approximations are also developed in the context of queueing networks, a class of models where the decision policy of the underlying MDP is in some sense fixed a priori, and our main goal is to study the transient or stationary behavior of the induced Markov process. Even though the decision policy is fixed, these models usually remain intractable to solve. Given this complexity, the team has developed analyses in some limiting regime of practical interest, i.e., queueing models in the large-network, heavy-traffic, fluid or mean-field limit. This approach is helpful to obtain a simpler mathematical description of the system under investigation, which is often given in terms of ordinary differential equations or convex optimization problems.

- *Optimality results*. Our aim is to investigate new important classes of optimal stochastic control problems including constraints and combining continuous and impulse actions for MDPs and PDMPs. In this framework, our objective is to obtain different types of optimality results. For example, we intend to provide conditions to guarantee the existence and uniqueness of the optimality equation for the problem under consideration and to ensure existence of an optimal (and ϵ-optimal) control strategy. We also plan to analyze the structural properties of the optimal strategies as well as to study the associated infinite dimensional linear programming problem. These results can be seen as a first step toward the development of numerical approximation techniques in the sense described above.

4. Application Domains

4.1. Dependability and safety

Our abilities in probability and statistics apply naturally to industry, in particular in studies of dependability and safety. An illustrative example is the collaboration that started in September 2014 with with THALES Optronique. The goal of this project is the optimization of the maintenance of an onboard system equipped with a HUMS (Health Unit Monitoring Systems). The physical system under consideration is modeled by a piecewise deterministic Markov process. In the context of impulse control, we propose a dynamic maintenance policy, adapted to the state of the system and taking into account both random failures and those related to the degradation phenomenon.

The spectrum of applications of the topics that the team can address is large and can concern many other fields. Indeed non parametric and semi-parametric regression methods can be used in biometry, econometrics or engineering for instance. Gene selection from microarray data and text categorization are two typical application domains of dimension reduction among others. We had for instance the opportunity via the scientific program PRIMEQUAL to work on air quality data and to use dimension reduction techniques as principal component analysis (PCA) or positive matrix factorization (PMF) for pollution sources identification and quantization.

5. New Software and Platforms

5.1. biips

Bayesian Inference with Interacting Particle Systems

KEYWORD: Bayesian estimation

FUNCTIONAL DESCRIPTION: Biips is a software platform for automatic Bayesian inference with interacting particle systems. Biips allows users to define their statistical model in the probabilistic programming BUGS language, as well as to add custom functions or samplers within this language. Then it runs sequential Monte Carlo based algorithms (particle filters, particle independent Metropolis-Hastings, particle marginal Metropolis-Hastings) in a black-box manner so that to approximate the posterior distribution of interest as well as the marginal likelihood. The software is developed in C++ with interfaces with the softwares R, Matlab and Octave.

- Participants: Adrien Todeschini, François Caron, Pierre Del Moral and Pierrick Legrand
- Contact: Adrien Todeschini
- URL: http://biips.gforge.inria.fr

5.2. PCAmixdata

KEYWORD: Statistic analysis

FUNCTIONAL DESCRIPTION: Mixed data type arise when observations are described by a mixture of numerical and categorical variables. The R package PCAmixdata extends standard multivariate analysis methods to incorporate this type of data. The key techniques included in the package are PCAmix (PCA of a mixture of numerical and categorical variables), PCArot (rotation in PCAmix) and MFAmix (multiple factor analysis with mixed data within a dataset). The MFAmix procedure handles a mixture of numerical and categorical variables within a group - something which was not possible in the standard MFA procedure. We also included techniques to project new observations onto the principal components of the three methods in the new version of the package.

- Contact: Marie Chavent
- URL: https://cran.r-project.org/web/packages/PCAmixdata/index.html

5.3. QuantifQuantile

KEYWORD: Regression

FUNCTIONAL DESCRIPTION: QuantifQuantile is an R package that allows to perform quantization-based quantile regression. The different functions of the package allow the user to construct an optimal grid of N quantizers and to estimate conditional quantiles. This estimation requires a data driven selection of the size N of the grid that is implemented in the functions. Illustration of the selection of N is available, and graphical output of the resulting estimated curves or surfaces (depending on the dimension of the covariate) is directly provided via the plot function.

- Contact: Jérôme Saracco
- URL: https://cran.r-project.org/web/packages/QuantifQuantile/index.html

6. New Results

6.1. Power-of-d-Choices with Memory: Fluid Limit and Optimality

Abstract: In multi-server distributed queueing systems, the access of stochastically arriving jobs to resources is often regulated by a dispatcher, also known as load balancer. A fundamental problem consists indesigning a load balancing algorithm that minimizes the delays experienced by jobs. During the last twodecades, the power-of-d-choice algorithm, based on the idea of dispatching each job to the least loadedserver out ofdservers randomly sampled at the arrival of the job itself, has emerged as a breakthroughin the foundations of this area due to its versatility and appealing asymptotic properties. In this paper,we consider the power-of-d-choice algorithm with the addition of a local memory that keeps track of thelatest observations collected over time on the sampled servers. Then, each job is sent to a server withthe lowest observation. We show that this algorithm is asymptotically optimal in the sense that the load balancer can always assign each job to an idle server in the large-system limit. Our results quantify and highlight the importance of using memory as a means to enhance performance in randomized load balancing.

Authors: J. Anselmi (CQFD); F. Dufour (CQFD).

6.2. Hamilton-Jacobi-Bellman Inequality for the Average Control of Piecewise Deterministic Markov Processes

Abstract : The main goal of this work is to study the infinite-horizon long run average continuous-time optimal control problem of piecewise deterministic Markov processes (PDMPs) with the control acting continuously on the jump intensity λ and on the transition measure Q of the process.

Authors : O.L.V. Costa; F. Dufour (CQFD)

6.3. Approximation of discounted minimax Markov control problems and zero-sum Markov games using Hausdorff and Wasserstein distances

Abstract : This work is concerned with a minimax control problem (also known as a robust Markov Decision Process (MDP) or a game against nature) with general state and action spaces under the discounted cost optimality criterion. We are interested in approximating numerically the value function and an optimal strategy of this general discounted minimax control problem. To this end, we derive structural Lipschitz continuity properties of the solution of this robust MDP by imposing suitable conditions on the model, including Lipschitz continuity of the elements of the model and absolute continuity of the Markov transition kernel with respect to some probability measure μ. Then, we are able to provide an approximating minimax control model with finite state and action spaces, and hence computationally tractable, by combining these structural properties with a suitable discretization procedure of the state space (related to a probabilistic criterion) and the action spaces (associated to a geometric criterion). Finally, it is shown that the corresponding approximation errors for the value function and the optimal strategy can be controlled in terms of the discretization parameters. These results are also extended to a two-player zero-sum Markov game.

Authors : F. Dufour (CQFD); T. Prieto-Rumeau

6.4. Combining clustering of variables and feature selection using random forests: the CoV/VSURF procedure

Abstract : Standard approaches to tackle high-dimensional supervised classification problem often include variable selection and dimension reduction procedures. The novel methodology proposed in this paper combines clustering of variables and feature selection. More precisely, hierarchical clustering of variables procedure allows to build groups of correlated variables in order to reduce the redundancy of information and summarizes each group by a synthetic numerical variable. Originality is that the groups of variables (and the number of groups) are unknown a priori. Moreover the clustering approach used can deal with both numerical and categorical variables (i.e. mixed dataset). Among all the possible partitions resulting from dendrogram cuts, the most relevant synthetic variables (i.e. groups of variables) are selected with a variable selection procedure using random forests. Numerical performances of the proposed approach are compared with direct applications of random forests and variable selection using random forests on the original p variables. Improvements obtained with the proposed methodology are illustrated on two simulated mixed datasets (cases n>p and n<p, where n is the sample size) and on a real proteomic dataset. Via the selection of groups of variables (based on the synthetic variables), interpretability of the results becomes easier.

Authors : Marie Chavent (CQFD), Robin Genuer (SISTM), Jerome Saracco (CQFD)

6.5. Statistical model choice including variable selection based on variable importance: A relevant way for biomarkers selection to predict meat tenderness

Abstract : In this work, we describe a new computational methodology to select the best regression model to predict a numerical variable of interest Y and to select simultaneously the most interesting numerical explanatory variables strongly linked to Y. Three regression models (parametric, semi-parametric and non-parametric) are considered and estimated by multiple linear regression, sliced inverse regression and random forests. Both the variables selection and the model choice are computational. A measure of importance based on random perturbations is calculated for each covariate. The variables above a threshold are selected. Then a learning/test samples approach is used to estimate the Mean Square Error and to determine which model (including variable selection) is the most accurate. The R package modvarsel (MODel and VARiable SELection) implements this computational approach and applies to any regression datasets. After checking the good behavior of the methodology on simulated data, the R package is used to select the proteins predictive of meat tenderness among a pool of 21 candidate proteins assayed in semitendinosus muscle from 71 young bulls. The biomarkers were selected by linear regression (the best regression model) to predict meat tenderness. These biomarkers, we confirm the predominant role of heat shock proteins and metabolic ones.

Authors : Marie-Pierre Ellies-Oury, Marie Chavent, Alexandre Conanec, Jérôme Saracco

6.6. Genome sequencing for rightward hemispheric language dominance

Abstract : Most people have left-hemisphere dominance for various aspects of language processing, but only roughly 1 % of the adult population has atypically reversed, rightward hemispheric language dominance (RHLD). The genetic-developmental program that underlies leftward language laterality is unknown, as are the causes of atypical variation. We performed an exploratory whole-genome-sequencing study, with the hypothesis that strongly penetrant, rare genetic mutations might sometimes be involved in RHLD. This was by analogy with situs inversus of the visceral organs (left-right mirror reversal of the heart, lungs etc.), which is sometimes due to monogenic mutations. The genomes of 33 subjects with RHLD were sequenced, and analysed with reference to large population-genetic datasets, as well as thirty-four subjects (14 left-handed) with typical language laterality. The sample was powered to detect rare, highly penetrant, monogenic effects if they would be present in at least 10 of the 33 RHLD cases and no controls, but no individual genes had mutations in more than 5 RHLD cases while being un-mutated in controls. A hypothesis derived from invertebrate mechanisms of left-right axis formation led to the detection of an increased mutation load, in RHLD subjects, within genes involved with the actin cytoskeleton. The latter finding offers a first, tentative insight into molecular genetic influences on hemispheric language dominance.

Authors : Amaia Carrion-castillo, Lise van der Haegen, Nathalie Tzourio-mazoyer, Tulya Kavaklioglu, Solveig Badillo, Marie Chavent, Jérôme Saracco, Marc Brysbaert, Simon Fisher, Bernard Mazoyer, Clyde Francks

6.7. An Original Methodology for the Selection of Biomarkers of Tenderness in Five Different Muscles

Abstract : For several years, studies conducted for discovering tenderness biomarkers have proposed a list of 20 candidates. The aim of the present work was to develop an innovative methodology to select the most predictive among this list. The relative abundance of the proteins was evaluated on five muscles of 10 Holstein cows: gluteobiceps, semimembranosus, semitendinosus, Triceps brachii and Vastus lateralis. To select the most predictive biomarkers, a multi-block model was used: The Data-Driven Sparse Partial Least Square. Semimembranosus and Vastus lateralis muscles tenderness could be well predicted (R^2= 0.95 and 0.94 respectively) with a total of 7 out of the 5 times 20 biomarkers analyzed. An original result is that the predictive proteins were the same for these two muscles: μ-calpain, m-calpain, h2afx and Hsp40 measured in m. gluteobiceps and μ-calpain, m-calpain and Hsp70-8 measured in m. Triceps brachii. Thus, this method is well adapted to this set of data, making it possible to propose robust candidate biomarkers of tenderness that need to be validated on a larger population.

Authors : Ellies-Oury, M.-P., Lorenzo, H., Denoyelle, C., Conanec, A., Saracco, J., Picard B.

6.8. New Approach Studying Interactions Regarding Trade-Off between Beef Performances and Meat Qualities

Abstract : The beef cattle industry is facing multiple problems, from the unequal distribution of added value to the poor matching of its product with fast-changing demand. Therefore, the aim of this study was to examine the interactions between the main variables, evaluating the nutritional and organoleptic properties of meat and cattle performances, including carcass properties, to assess a new method of managing the trade-off between these four performance goals. For this purpose, each variable evaluating the parameters of interest has been statistically modeled and based on data collected on 30 Blonde d'Aquitaine heifers. The variables were obtained after a statistical pre-treatment (clustering of variables) to reduce the redundancy of the 62 initial variables. The sensitivity analysis evaluated the importance of each independent variable in the models, and a graphical approach completed the analysis of the relationships between the variables. Then, the models were used to generate virtual animals and study the relationships between the nutritional and organoleptic quality. No apparent link between the nutritional and organoleptic properties of meat (r = -0.17) was established, indicating that no important trade-off between these two qualities was needed. The 30 best and worst profiles were selected based on nutritional and organoleptic expectations set by a group of experts from the INRA (French National Institute for Agricultural Research) and Institut de l'Elevage (French Livestock Institute). The comparison between the two extreme profiles showed that heavier and fatter carcasses led to low nutritional and organoleptic quality.

Authors : Conanec ,A., Picard, B., Cantalapiedra-Hijar, G., Chavent, M., Denoyelle, C., Gruffat, D., Normand, J., Saracco, J., Ellies-Oury M.P.

6.9. Impact of Speller Size on a Visual P300 Brain-Computer Interface (BCI) System under Two Conditions of Constraint for Eye Movement

Abstract : The vast majority of P300-based brain-computer interface (BCI) systems are based on the well-known P300 speller presented by Farwell and Donchin for communication purposes and an alternative to people with neuromuscular disabilities, such as impaired eye movement. The purpose of the present work is to study the effect of speller size on P300-based BCI usability, measured in terms of effectiveness, efficiency, and satisfaction under overt and covert attention conditions. To this end, twelve participants used three speller sizes under both attentional conditions to spell 12 symbols. The results indicated that the speller size had, in both attentional conditions, a significant influence on performance. In both conditions (covert and overt), the best performances were obtained with the small and medium speller sizes, both being the most effective. The speller size did not significantly affect workload on the three speller sizes. In contrast, covert attention condition produced very high workload due to the increased resources expended to complete the task. Regarding users' preferences, significant differences were obtained between speller sizes. The small speller size was considered as the most complex, the most stressful, the less comfortable, and the most tiring. The medium speller size was always considered in the medium rank, which is the speller size that was evaluated less frequently and, for each dimension, the worst one. In this sense, the medium and the large speller sizes were considered as the most satisfactory. Finally, the medium speller size was the one to which the three standard dimensions were collected: high effectiveness, high efficiency, and high satisfaction. This work demonstrates that the speller size is an important parameter to consider in improving the usability of P300 BCI for communication purposes. The obtained results showed that using the proposed medium speller size, performance and satisfaction could be improved.

Authors :Ron-Angevin, R., Garcia, L., Fernandez-Rodriguez, A., Saracco, J., André, J.-M., Lespinet-Najib, V.

6.10. High-Dimensional Multi-Block Analysis of Factors Associated with Thrombin Generation Potential

Abstract : The identification of novel biological factors associated with thrombin generation, a key biomarker of the coagulation process, remains a relevant strategy to disentangle pathophysiological mechanisms underlying the risk of venous thrombosis (VT). As part of the MARseille THrombosis Association Study (MARTHA), we measured whole blood DNA methylation levels, plasma levels of 300 proteins, 3 thrombin generation biomarkers (endogeneous thrombin potential, peak and lagtime), clinical and genetic data in 700 patients with VT. The application of a novel high-dimensional multi-levels statistical methodology we recently developed, the data driven sparse Partial Least Square method (ddsPLS), on the MARTHA datasets enabled us 1/ to confirm the role of a known mutation of the variability of endogenous thrombin potential and peak, 2/ to identify a new signature of 7 proteins strongly associated with lagtime.

Authors : Lorenzo, H., Razzaq, M., Odeberg, J., Saracco, J., Tregouet, D.-A., Thiébaut, R.

6.11. Multiple-output quantile regression through optimal quantization

Abstract : A new nonparametric quantile regression method based on the concept of optimal quantization was developed recently and was showed to provide estimators that often dominate their classical, kernel-type, competitors. In the present work, we extend this method to multiple-output regression problems. We show

how quantization allows approximating population multiple-output regression quantiles based on halfspace depth. We prove that this approximation becomes arbitrarily accurate as the size of the quantization grid goes to infinity. We also derive a weak consistency result for a sample version of the proposed regression quantiles. Through simulations, we compare the performances of our estimators with (local constant and local bilinear) kernel competitors. The results reveal that the proposed quantization-based estimators, which are local constant in nature, outperform their kernel counterparts and even often dominate their local bilinear kernel competitors. The various approaches are also compared on artificial and real data.

Authors : Charlier, I., Paindaveine, D., Saracco, J.

6.12. Artificial evolution, fractal analysis and applications

Abstract :

This document contains a selection of research works to which I have contributed. It is structured around two themes, artificial evolution and signal regularity analysis and consists of three main parts: Part I: Artificial evolution, Part II: Estimation of signal regularity and Part III: Applications, combination of signal processing, fractal analysis and artificial evolution. In order to set the context and explain the coherence of the rest of the document, this manuscript begins with an introduction, Chapter 1, providing a list of collaborators and of the research projects carried out. Theoretical contributions focus on two areas: evolutionary algorithms and the measurement of signal regularity and are presented in Part I and Part II respectively. These two themes are then exploited and applied to real problems in Part III. Part I, Artificial Evolution, consists of 8 chapters. Chapter 2 contains a brief presentation of various types of evolutionary algorithms (genetic algorithms, evolutionary strategies and genetic programming) and presents some contributions in this area, which will be detailed later in the document. Chapter 3, entitled Prediction of Expected Performance for a Genetic Programming Classifier proposes a method to predict the expected performance for a genetic programming (GP) classifier without having to run the program or sample potential solutions in the research space. For a given classification problem, a pre-processing step to simplify the feature extraction process is proposed. Then the step of extracting the characteristics of the problem is performed. Finally, a PEP (prediction of expected performance) model is used, which takes the characteristics of the problem as input and produces the predicted classification error on the test set as output. To build the PEP model, a supervised learning method with a GP is used. Then, to refine this work, an approach using several PEP models is developed, each now becoming a specialized predictors of expected performance (SPEP) specialized for a particular group of problems. It appears that the PEP and SPEP models were able to accurately predict the performance of a GP-classifier and that the SPEP approach gave the best results. Chapter 4, entitled A comparison of fitness-case sampling methods for genetic programming presents an extensive comparative study of four fitness-case sampling methods, namely: Interleaved Sampling, Random Interleaved Sampling, Lexicase Selection and the proposed Keep-Worst Interleaved Sampling. The algorithms are compared on 11 symbolic regression problems and 11 supervised classification problems, using 10 synthetic benchmarks and 12 real-world datasets. They are evaluated based on test performance, overfitting and average program size, comparing them with a standard GP search. The experimental results suggest that fitness-case sampling methods are particularly useful for difficult real-world symbolic regression problems, improving performance, reducing overfitting and limiting code growth. On the other hand, it seems that fitness-case sampling cannot improve upon GP performance when considering supervised binary classification. Chapter 5, entitled Evolving Genetic Programming Classifiers with Novelty Search, deals with a new and unique approach towards search and optimization, the Novelty Search (NS), where an explicit objective function is replaced by a measure of solution novelty. This chapter proposes a NS-based GP algorithm for supervised classification. Results show that NS can solve real-world classification tasks, the algorithm is validated on real-world benchmarks for binary and multiclass problems. Moreover, two new versions of the NS algorithm are proposed, Probabilistic NS (PNS) and a variant of Minimal Criteria NS (MCNS). The former models the behavior of each solution as a random vector and eliminates all of the original NS parameters while reducing the computational overhead of the NS algorithm. The latter uses a standard objective function to constrain and bias the search towards high performance solutions. This chapter also discusses the effects of NS on GP search dynamics and code growth.

The results show that NS can be used as a realistic alternative for supervised classification, and specifically for binary problems the NS algorithm exhibits an implicit bloat control ability. In Chapter 6, entitled Evaluating the Effects of Local Search in Genetic Programming, a memetic GP that incorporates a local search (LS) strategy to refine GP individuals expressed as syntax trees is studied in the context of symbolic regression. A simple parametrization for GP trees is proposed, by weighting each function with a parameter (unique for each function used in the construction of a tree). These parameters are then optimized using a trust region optimization algorithm which is therefore used here as a local search method. Then different heuristic methods are tested over several benchmark and real-world problems to determine which individuals from the tree population should be subjected to a LS. The results show that the best performances (in term of both quality of the solution and bloat control) was achieved when LS is applied to all of the solutions or to random individuals chosen from the top percentile (with respect to fitness) of the population. Chapter 7, entitled A Local Search Approach to Genetic Programming for Binary Classification, proposes a memetic GP, tailored for binary classification problems, extending the work on symbolic regression presented in the previous chapter. In particular, a small linear subtree is added on the top of the root node of the original tree and each node in a tree is weighted by a real-valued parameter, which is then numerically optimized using the trust-region algorithm used as a local search method. Experimental results show that potential classifiers produced by GP are improved by the local searcher, and hence the overall search is improved achieving substantial performance gains. Application on well-known benchmarks provided results competitive with state-of-the-art. Chapter 8, entitled RANSAC-GP: Dealing with Outliers in Symbolic Regression with Genetic Programming, presents a hybrid methodology based on the RAndom SAmpling Consensus (RANSAC) algorithm and GP, called RANSAC-GP. RANSAC is an approach to deal with outliers in parameter estimation problems, widely used in computer vision and related fields. This work presents the first application of RANSAC to symbolic regression with GP. The proposed algorithm is able to deal with extreme amounts of contamination in the training set, evolving highly accurate models even when the amount of outliers reaches 90Part II, Estimation of signal regularity consists of 3 chapters. Chapter 9, entitled Hölderian Regularity, provides some reminders and some theoretical contributions on the estimation of Hölderian regularity. Some details are given on the estimation of the Hölder exponent using oscillation method or a wavelet transform. These approaches and improved versions are compared on synthetic signals. The FracLab software, were all the above methods have been integrated, is also presented at the end of this chapter. The work proposed in Chapter 10, entitled Theoretical comparison of the DFA and variants for the estimation of the Hurst exponent, involves a theoretical and numerical comparison between the Detrended Fluctuation Analysis (DFA) and its variants, namely DMA, AFA, RDFA and the proposed Continuous DFA method, in which the trend is constrained to be continuous. The DFA is a well-established method to detect long-range correlations in time series. It has been used in a wide range of applications, from biomedical applications to signal denoising. It allows the Hurst exponent of a pure mono-fractal time series to be estimated. It operates as follows: after integration, the signal is split into segments. Using a least-squares criterion, local trends are deduced. The resulting piecewise linear trend is then subtracted to the whole signal. The power of the residual is computed for different segment lengths and its log-log representation allows the Hurst exponent to be deduced. The comparison performed in this chapter is based on a new common matrix writing formalism of the square of the fluctuation function from the instantaneous correlation function of the process for all these methods. In the case where the process under study is stationary in the broad sense, the statistical mean of the square of the fluctuation function is thus expressed as a weighted sum of the terms of the autocorrelation function, and this without any approximation. More precisely, the mathematical expectation of the square of the fluctuation function can be seen for each method as the autocorrelation function of the output of a filter dependent on this method and calculated for a lag equal to zero, i.e. the power of the filter output. In the general case, this analytical framework provides a means of comparing the DFA and its variants that is different from a traditional synthetic signal performance study, and explains the different behaviours of these regularity estimation methods, using the proposed filter analysis. Chapter 11 contains two patents with THALES AVS related to the work presented in the previous chapter. Part III of this manuscript, Applications, combination of signal processing, fractal analysis and artificial evolution, contains contributions combining the tools previously mentioned in order to develop new tools such as in the Chapters 12 and 13 or contributions on the resolution of real problems in the biomedical field, such as in the Chapters 14, 15 and 16. Chapter 12, entitled "The Estimation of Hölderian Regularity using Genetic

Programming", presents a GP approach to synthesize estimators for the pointwise Hölder exponent in 2D signals. The optimization problem to solve is to minimize the error between a prescribed regularity and the estimated regularity given by an image operator. The search for optimal estimators is then carried out using a GP algorithm. Experiments confirm that the GPoperators produce a good estimation of the Hölder exponent in images of multifractional Brownian motions. In fact, the evolved estimators significantly outperform a traditional method by as much as one order of magnitude. These results provide further empirical evidence that GP can solve difficult problems of applied mathematics. In Chapter 13, entitled "Optimization of the Hölder Image Descriptor using a Genetic Algorithm", a local descriptor based on the Hölder exponent is studied. The proposal is to find an optimal number of dimensions for the descriptor using a genetic algorithm (GA). To guide the GA search, fitness is computed based on the performance of the descriptor when applied to standard region matching problems. This criterion is quantified using the F-Measure, derived from recall and precision analysis. Results show that it is possible to reduce the size of the canonical Hölder descriptor without degrading the quality of its performance. In fact, the best descriptor found through the GA search is nearly 70performance on standard tests. Chapter 14, entitled "Interactive evolution for cochlear implants fitting", presents a study that intends to make cochlear implants more adaptable to environment and to simplify the process of fitting, by designing and using a specific interactive evolutionary algorithm combined with signal processing. Real experiments on volunteer implanted patients are presented, that show the efficiency of interactive evolution for this purpose. In Chapter 15, entitled "Feature extraction and classification of EEG signals. The use of a genetic algorithm for an application on alertness prediction", the development of computer systems for the automatic analysis and classification of mental states of vigilance; i.e., a person's state of alertness is studied. Such a task is relevant to diverse domains, where a person is expected or required to be in a particular state. For instance, pilots, security personnel or medical staffs are expected to be in a highly alert state, and a brain computer interface could help confirm this or detect possible problems. In this chapter, a combination of an evolutionary algorithm and signal processing is used. The purpose of this algorithm was to select an electrode and a frequency range to use in order to discriminate between the two states of vigilance. This approach determined the most useful electrode for the classification task. Using the recording of this electrode, the prediction obtained has a reliability rate of 89.33

In Chapter 16, entitled "Regularity and Matching Pursuit Feature Extraction for the Detection of Epileptic Seizures", a novel methodology for feature extraction on EEG signals that allows to perform a highly accurate classification of epileptic states is presented. Specifically, Hölderian regularity and the Matching Pursuit algorithm are used as the main feature extraction techniques, and are combined with basic statistical features to construct the final feature sets. These sets are then delivered to a Random Forests classification algorithm to differentiate between epileptic and non-epileptic readings. Several versions of the basic problem are tested and statistically validated producing perfect accuracy in most problems and 97.6a well known database, reveals that the proposal achieves state-of-the-art performance.The experimental results suggest that using a feature extraction methodology composed of regularity analysis, a Matching Pursuit algorithm and time-domain statistic measures together with a classifier produces a system that can predict epileptic states with competitive performance that matches or even surpass other novel methods. Finally the last chapter concludes this manuscript and provides perspectives for future work.

Authors : Pierrick Legrand

6.13. Self-affinity of an Aircraft Pilot's Gaze Direction as a Marker of Visual Tunneling

Abstract : For the last few years, a great deal of interest has been paid to crew monitoring systems in order to tackle potential safety problems during a flight. They aim at detecting any degraded physiological and/or cognitive state of an aircraft pilot, such as attentional tunneling or excessive focalization. Indeed, they might have a negative impact on his performance to pursue his mission with adequate flight safety levels. One of the usual approaches consists in using sensors to collect physiological signals which are analyzed in real-time. Two main families exist to process the signals. The first one combines feature extraction and machine learning whereas the second is based on deep-learning approaches but may require a large amount

of labelled data. Here, we focused on the first family. In this case, various features can be deduced from the data by different approaches: spectrum analysis, a priori modelling and nonlinear dynamical system analysis techniques including the estimation of the self-affinity of the signals. In this paper, our purpose was to analyze whether the self-affinity of the pilot gaze direction can be related to his cognitive state. To this end, an experiment was carried out on 18 subjects in a representative aircraft environment based on a modified version of the software MATB-II. The scenarii were designed to elicit different levels of mental workload eventually associated to attentional tunneling. A database to train the machine learning step was first created by recording the directions of gaze of the subjects with an eye-tracker. The self-affinities of these signals were extracted with the Detrended Fluctuation Analysis method. They constituted the inputs of the classifier based on a Support Vector Machine. Then, new signals were analyzed and classified. Preliminary results showed promising abilities to detect attentional tunnelling episodes for different levels of mental workload.

Authors : Bastien Berthelot, Patrick Mazoyer, Sarah Egea, Jean-Marc André, Eric Grivel

6.14. Filtering-based Analysis Comparing the DFA with the CDFA for Wide Sense Stationary Processes

Abstract : The detrended fluctuation analysis (DFA) is widely used to estimate the Hurst exponent. Although it can be outperformed by wavelet based approaches, it remains popular because it does not require a strong expertise in signal processing. Recently, some studies were dedicated to its theoretical analysis and its limits. More particularly, some authors focused on the so-called fluctuation function by searching a relation with an estimation of the normalized covariance function under some assumptions. This paper is complementary to these works. We first show that the square of the fluctuation function can be expressed in a similar matrix form for the DFA and the variant we propose, called Continuous-DFA (CDFA), where the global trend is constrained to be continuous. Then, using the above representation for wide-sense-stationary processes, the statistical mean of the square of the fluctuation function can be expressed from the correlation function of the signal and consequently from its power spectral density, without any approximation. The differences between both methods can be highlighted. It also confirms that they can be seen as ad hoc wavelet based techniques.

Authors : Bastien Berthelot, Eric Grivel, Pierrick Legrand, Jean-Marc André, Patrick Mazoyer, et al

6.15. 2D Fourier Transform Based Analysis Comparing the DFA with the DMA

Abstract : Even if they can be outperformed by other methods, the detrended fluctuation analysis (DFA) and the detrended moving average (DMA) are widely used to estimate the Hurst exponent because they are based on basic notions of signal processing. For the last years, a great deal of interest has been paid to compare them and to better understand their behaviors from a mathematical point of view. In this paper, our contribution is the following: we first propose to express the square of the socalled fluctuation function as a 2D Fourier transform (2D-FT) of the product of two matrices. The first one is defined from the instantaneous correlations of the signal while the second, called the weighting matrix, is representative of each method. Therefore, the 2D-FT of the weighting matrix is analyzed in each case. In this study, differences between the DFA and the DMA are pointed out when the approaches are applied on non-stationary processes

Authors : Bastien Berthelot, Eric Grivel, Pierrick Legrand, Marc Donias, Jean-Marc André, et al.

6.16. Interpréter les Fonctions de Fluctuation du DFA et du DMA comme le Résultat d'un Filtrage

Abstract : The detrended uctuation analysis (DFA) and the detrending moving average (DMA) are often used to estimate the regularity of the signal, since they do not require a strong expertise in the eld of signal processing while providing good results. In this paper, our contribution is twofold. We propose a framework that allows these approaches to be compared. It is based on a matrix form of the square of the uctuation function. Using the above representation for wide-sense-stationary processes, we show that the statistical mean of the square of the uctuation function can be expressed from the correlation function of the signal and consequently from its power spectral density, without any approximation. The dierences between both methods can be highlighted. It also conrms that they can be seen as ad hoc wavelet based techniques to estimate the Hurst exponent.

Authors : Bastien Berthelot, Eric Grivel, Pierrick Legrand, Jean-Marc Andre, Patrick Mazoyer, et al.

6.17. A perturbation analysis of stochastic matrix Riccati diffusions

Abstract : Matrix differential Riccati equations are central in filtering and optimal control theory. The purpose of this article is to develop a perturbation theory for a class of stochastic matrix Riccati diffusions. Diffusions of this type arise, for example, in the analysis of ensemble Kalman-Bucy filters since they describe the flow of certain sample covariance estimates. In this context, the random perturbations come from the fluctuations of a mean field particle interpretation of a class of nonlinear diffusions equipped with an interacting sample covariance matrix functional. The main purpose of this article is to derive non-asymptotic Taylor-type expansions of stochastic matrix Riccati flows with respect to some perturbation parameter. These expansions rely on an original combination of stochastic differential analysis and nonlinear semigroup techniques on matrix spaces. The results here quantify the fluctuation of the stochastic flow around the limiting deterministic Riccati equation, at any order. The convergence of the interacting sample covariance matrices to the deterministic Riccati flow is proven as the number of particles tends to infinity. Also presented are refined moment estimates and sharp bias and variance estimates. These expansions are also used to deduce a functional central limit theorem at the level of the diffusion process in matrix spaces.

Authors : Adrian N. Bishop, Pierre Del Moral, Angele Niclas

6.18. On the stability of matrix-valued Riccati diffusions

Abstract : The stability properties of matrix-valued Riccati diffusions are investigated. The matrix-valued Riccati diffusion processes considered in this work are of interest in their own right, as a rather prototypical model of a matrix-valued quadratic stochastic process. Under rather natural observability and controllability conditions, we derive time-uniform moment and fluctuation estimates and exponential contraction inequalities. Our approach combines spectral theory with nonlinear semigroup methods and stochastic matrix calculus. This analysis seem to be the first of its kind for this class of matrix-valued stochastic differential equation. This class of stochastic models arise in signal processing and data assimilation, and more particularly in ensemble Kalman-Bucy filtering theory. In this context, the Riccati diffusion represents the flow of the sample covariance matrices associated with McKean-Vlasov-type interacting Kalman-Bucy filters. The analysis developed here applies to filtering problems with unstable signals.

Authors : Adrian N. Bishop, Pierre Del Moral

6.19. A variational approach to nonlinear and interacting diffusions

Abstract : The article presents a novel variational calculus to analyze the stability and the propagation of chaos properties of nonlinear and interacting diffusions. This differential methodology combines gradient flow estimates with backward stochastic interpolations, Lyapunov linearization techniques as well as spectral theory. This framework applies to a large class of stochastic models including non homogeneous diffusions, as well as stochastic processes evolving on differentiable manifolds, such as constraint-type embedded manifolds on Euclidian spaces and manifolds equipped with some Riemannian metric. We derive uniform as well as almost sure exponential contraction inequalities at the level of the nonlinear diffusion flow, yielding what seems to be the first result of this type for this class of models. Uniform propagation of chaos properties w.r.t. the time parameter are also provided. Illustrations are provided in the context of a class of gradient flow diffusions arising in fluid mechanics and granular media literature. The extended versions of these nonlinear Langevin-type diffusions on Riemannian manifolds are also discussed.

Authors : Marc Arnaudon (IMB), Pierre Del Moral (CMAP, CQFD)

6.20. An explicit Floquet-type representation of Riccati aperiodic exponential semigroups

Abstract : The article presents a rather surprising Floquet-type representation of time-varying transition matrices associated with a class of nonlinear matrix differential Riccati equations. The main difference with conventional Floquet theory comes from the fact that the underlying flow of the solution matrix is aperiodic. The monodromy matrix associated with this Floquet representation coincides with the exponential (fundamental) matrix associated with the stabilizing fixed point of the Riccati equation. The second part of this article is dedicated to the application of this representation to the stability of matrix differential Riccati equations. We provide refined global and local contraction inequalities for the Riccati exponential semigroup that depend linearly on the spectral norm of the initial condition. These refinements improve upon existing results and are a direct consequence of the Floquet-type representation, yielding what seems to be the first results of this type for this class of models.

Authors : Adrian N. Bishop, Pierre Del Moral

6.21. Uniform propagation of chaos and creation of chaos for a class of nonlinear diffusions

Abstract : We are interested in nonlinear diffusions in which the own law intervenes in the drift. This kind of diffusions corresponds to the hydrodynamical limit of some particle system. One also talks about propagation of chaos. It is well-known, for McKean-Vlasov diffusions, that such a propagation of chaos holds on finite-time interval. We here aim to establish a uniform propagation of chaos even if the external force is not convex, with a diffusion coefficient sufficiently large. The idea consists in combining the propagation of chaos on a finite-time interval with a functional inequality, already used by Bolley, Gentil and Guillin, see [BGG12a, BGG12b]. Here, we also deal with a case in which the system at time t = 0 is not chaotic and we show under easily checked assumptions that the system becomes chaotic as the number of particles goes to infinity together with the time. This yields the first result of this type for mean field particle diffusion models as far as we know.

Authors : Pierre Del Moral and Julian Tugaut

6.22. Stability Properties of Systems of Linear Stochastic Differential Equations with Random Coefficients

Abstract : This work is concerned with the stability properties of linear stochastic differential equations with random (drift and diffusion) coefficient matrices, and the stability of a corresponding random transition matrix (or exponential semigroup). We consider a class of random matrix drift coefficients that involves random perturbations of an exponentially stable flow of deterministic (time-varying) drift matrices. In contrast with more conventional studies, our analysis is not based on the existence of Lyapunov functions, and it does not rely on any ergodic properties. These approaches are often difficult to apply in practice when the drift/diffusion coefficients are random. We present rather weak and easily checked perturbation-type conditions for the asymptotic stability of time-varying and random linear stochastic differential equations. We provide new log-Lyapunov estimates and exponential contraction inequalities on any time horizon as soon as the fluctuation parameter is sufficiently small. These seem to be the first results of this type for this class of linear stochastic differential equations with random coefficient matrices.

Authors : Adrian N. Bishop, Pierre Del Moral

6.23. On One-Dimensional Riccati Diffusions

Abstract : This article is concerned with the fluctuation analysis and the stability properties of a class of one-dimensional Riccati diffusions. These one-dimensional stochastic differential equations exhibit a quadratic drift function and a non-Lipschitz continuous diffusion function. We present a novel approach, combining tangent process techniques, Feynman-Kac path integration, and exponential change of measures, to derive

sharp exponential decays to equilibrium. We also provide uniform estimates with respect to the time horizon, quantifying with some precision the fluctuations of these diffusions around a limiting deterministic Riccati differential equation. These results provide a stronger and almost sure version of the conventional central limit theorem. We illustrate these results in the context of ensemble Kalman-Bucy filtering. To the best of our knowledge, the exponential stability and the fluctuation analysis developed in this work are the first results of this kind for this class of nonlinear diffusions.

Authors: Adrian N. Bishop, Pierre Del Moral, Kengo Kamatani, Bruno Remillard

6.24. Adaptive Approximate Bayesian Computational Particle Filters for Underwater Terrain-Aided Navigation.

Authors : C. Palmier, K. Dahia, N. Merlinge, P. Del Moral, D. Laneuville & C. Musso

6.25. Inference for conditioned Galton-Watson trees from their Harris path

Tree-structured data naturally appear in various fields, particularly in biology where plants and blood vessels may be described by trees, but also in computer science because XML documents form a tree structure. This paper is devoted to the estimation of the relative scale parameter of conditioned GaltonWatson trees. New estimators are introduced and their consistency is stated. A comparison is made with an existing approach of the literature. A simulation study shows the good behavior of our procedure on finite-sample sizes and from missing or noisy data. An application to the analysis of revisions of Wikipedia articles is also considered through real data.

Authors: Romain Azaïs, Alexandre Genadot and Benoit Henry

7. Bilateral Contracts and Grants with Industry

7.1. Bilateral Contracts with Industry

7.1.1. Naval Group

Participants: Huilong Zhang, François Dufour, Dann Laneuville, Alexandre Genadot.
The increasing complexity of warfare submarine missions has led Naval Group to study new tactical help functions for underwater combat management systems. In this context, the objective is to find optimal trajectories according to the current mission type by taking into account sensors, environment and surrounding targets. This problem has been modeled as a discrete-time Markov decision process with finite horizon. A quantization technique has been applied to discretize the problem in order to get a finite MDP for which standard methods such as the dynamic and/or the linear programming approaches can be applied. Different kind of scenarios have been considered and studied.

7.1.2. Thales Optronique

Participants: Benoîte de Saporta, François Dufour, Tiffany Cerchi.
Maintenance, optimization, fleet of industrial equipements The topic of this collaboration with Université de Montpellier and Thales Optronique is the application of Markov decision processes to the maintenance optimization of a fleet of industrial equipments.

7.1.3. Case Law Analytics

Pierrick Legrand is a consultant for the startup Case Law Analytics. Thje object of the consulting is confidential.

8. Partnerships and Cooperations

8.1. National Initiatives

8.1.1. QuAMProcs of the program Project Blanc of the ANR

The mathematical analysis of metastable processes started 75 years ago with the seminal works of Kramers on Fokker-Planck equation. Although the original motivation of Kramers was to « elucidate some points in the theory of the velocity of chemical reactions », it turns out that Kramers' law is observed to hold in many scientific fields: molecular biology (molecular dynamics), economics (modelization of financial bubbles), climate modeling, etc. Moreover, several widely used efficient numerical methods are justified by the mathematical description of this phenomenon.
Recently, the theory has witnessed some spectacular progress thanks to the insight of new tools coming from Spectral and Partial Differential Equations theory.
Semiclassical methods together with spectral analysis of Witten Laplacian gave very precise results on reversible processes. From a theoretical point of view, the semiclassical approach allowed to prove a complete asymptotic expansion of the small eigenvalues of Witten Laplacian in various situations (global problems, boundary problems, degenerate diffusions, etc.). The interest in the analysis of boundary problems was rejuvenated by recent works establishing links between the Dirichlet problem on a bounded domain and the analysis of exit event of the domain. These results open numerous perspectives of applications. Recent progress also occurred on the analysis of irreversible processes (e.g. on overdamped Langevin equation in irreversible context or full (inertial) Langevin equation).
The above progresses pave the way for several research tracks motivating our project: overdamped Langevin equations in degenerate situations, general boundary problems in reversible and irreversible case, non-local problems, etc.

8.1.2. Chaire Stress Test of the Ecole Polytechnique

The Chaire “Stress Testing” is a specific research program between Ecole Polytechnique, BNP Paribas, Fondation de l'Ecole Polytechnique, and is hosted at Polytechnique by the Center of Applied Mathematics. This research project is part of an in-depth reflection on the increasingly sophisticated issues surrounding stress tests (under the impulse of the upcoming European Banking regulation). Simulation of extreme adverse scenarios is an important topic to better understand which critical configurations can lead to financial and systemic crises. These scenarios may depend on complex phenomena, for which we partially lack information, making the modeling incomplete and uncertain. Last, the data are multivariate and reflect the dependency between driving variables. From the above observations, different lines of research are considered:
1. the generation of stress test and meta-modeling scenarios using machine learning;
2. the quantification of uncertainties in risk metrics;
3. modeling and estimation of multidimensional dependencies.

8.1.3. ANR StocMC (2014-2018) of the program Project Blanc of the ANR

The involved research groups are Inria Rennes/IRISA Team SUMO; Inria Rocquencourt Team Lifeware; LIAFA University Paris 7; Bordeaux University.
The aim of this research project is to develop scalable model checking techniques that can handle large stochastic systems. Large stochastic systems arise naturally in many different contexts, from network systems to system biology. A key stochastic model we will consider is from the biological pathway of apoptosis, the programmed cell death.

8.1.4. ANR BNPSI: Bayesian Non Parametric methods for Signal and Image Processing

Statistical methods have become more and more popular in signal and image processing over the past decades. These methods have been able to tackle various applications such as speech recognition, object tracking, image segmentation or restoration, classification, clustering, etc. We propose here to investigate the use of Bayesian nonparametric methods in statistical signal and image processing. Similarly to Bayesian parametric methods, this set of methods is concerned with the elicitation of prior and computation of posterior distributions, but now on infinite-dimensional parameter spaces. Although these methods have become very popular in statistics and machine learning over the last 15 years, their potential is largely underexploited in signal and image processing. The aim of the overall project, which gathers researchers in applied probabilities, statistics, machine learning and signal and image processing, is to develop a new framework for the statistical signal and image processing communities. Based on results from statistics and machine learning we aim at defining new models, methods and algorithms for statistical signal and image processing. Applications to hyperspectral image analysis, image segmentation, GPS localization, image restoration or space-time tomographic reconstruction will allow various concrete illustrations of the theoretical advances and validation on real data coming from realistic contexts.

8.1.5. Gaspard Monge Program for Optimisation and Operational Research (2017-2019)

The involved research groups are Inria Bordeaux Sud-Ouest Team CQFD and Thales Optronique. This new collaboration with Thales Optronique that started in October 2017 is funded by the Fondation Mathématique Jacques Hadamard. This is the continuation of the PhD Thesis of A. Geeraert. The objective of this project is to optimize the maintenance of a multi-component equipment that can break down randomly. The underlying problem is to choose the best dates to repair or replace components in order to minimize a cost criterion that takes into account costs of maintenance but also the cost associated to the unavailability of the system for the customer. In the PhD thesis of A. Geeraert, the model under consideration was rather simple and only a numerical approximation of the value function was provided. Here, our objective is more ambitious. A more realistic model will be considered and our aim is to provide a tractable quasi-optimal control strategy that can be applied in practice to optimize the maintenance of such equipments.

8.1.6. Mission pour les initiatives transverses et interdisciplinaires, Défi Modélisation du Vivant, projet MISGIVING

The aim of MISGIVING (MathematIcal Secrets penGuins dIVING) is to use mathematical models to understand the complexity of the multiscale decision process conditioning not only the optimal duration of a dive but also the diving behaviour of a penguin inside a bout. A bout is a sequence of succesive dives where the penguin is chasing prey. The interplay between the chasing period (dives) and the resting period due to the physiological cost of a dive (the time spent at the surface) requires some kind of optimization.

8.2. European Initiatives

8.2.1. Collaborations in European Programs, Except FP7 & H2020

Program: Direcion General de Investigacion Cientifica y Tecnica, Gobierno de Espana

Project acronym: GAMECONAPX

Project title: Numerical approximations for Markov decision processes and Markov games

Duration: 01/2017 - 12/2019

Coordinator: Tomas Prieto-Rumeau, Department of Statistics and Operations Research, UNED (Spain)

Abstract:
This project is funded by the Gobierno de Espana, Direcion General de Investigacion Cientifica y Tecnica (reference number: MTM2016-75497-P) for three years to support the scientific collaboration between Tomas Prieto-Rumeau, Jonatha Anselmi and Francois Dufour. This research project is concerned with numerical approximations for Markov decision processes and Markov games. Our goal is to propose techniques allowing to approximate numerically the optimal value function and

the optimal strategies of such problems. Although such decision models have been widely studied theoretically and, in general, it is well known how to characterize their optimal value function and their optimal strategies, the explicit calculation of these optimal solutions is not possible except for a few particular cases. This shows the need for numerical procedures to estimate or to approximate the optimal solutions of Markov decision processes and Markov games, so that the decision maker can really have at hand some approximation of his optimal strategies and his optimal value function. This project will explore areas of research that have been, so far, very little investigated. In this sense, we expect our techniques to be a breakthrough in the field of numerical methods for continuous-time Markov decision processes, but particularly in the area of numerical methods for Markov game models. Our techniques herein will cover a wide range of models, including discrete- and continuous-time models, problems with unbounded cost and transition rates, even allowing for discontinuities of these rate functions. Our research results will combine, on one hand, mathematical rigor (with the application of advanced tools from probability and measure theory) and, on the other hand, computational efficiency (providing accurate and ?applicable? numerical methods). In this sense, particular attention will be paid to models of practical interest, including population dynamics, queueing systems, or birth-and-death processes, among others. So, we expect to develop a generic and robust methodology in which, by suitably specifying the data of the decision problem, an algorithm will provide the approximations of the value function and the optimal strategies. Therefore, the results that we intend to obtain in this research project will be of interest for researchers in the fields of Markov decision processes and Markov games, both for the theoretical and the applied or practitioners communities

8.3. International Initiatives

8.3.1. Declared Inria International Partners

Tree-Lab, ITT. TREE-LAB is part of the Cybernetics research line within the Engineering Science graduate program offered by the Department of Electric and Electronic Engineering at Tijuana's Institute of Technology (ITT), in Tijuana Mexico. TREE-LAB is mainly focused on scientific and engineering research within the intersection of broad scientific fields, particularly Computer Science, Heuristic Optimization and Pattern Analysis. In particular, specific domains studied at TREE-LAB include Genetic Programming, Classification, Feature Based Recognition, Bio-Medical signal analysis and Behavior-Based Robotics. Currently, TREE-LAB incorporates the collaboration of several top researchers, as well as the participation of graduate (doctoral and masters) and undergraduate students, from ITT. Moreover, TREE-LAB is actively collaborating with top researchers from around the world, including Mexico, France, Spain, Portugal and USA.

8.4. International Research Visitors

8.4.1. Visits of International Scientists

Oswaldo Costa (Escola Politécnica da Universidade de São Paulo, Brazil) collaborate with the team on the theoretical aspects of continuous control of piecewise-deterministic Markov processes. He visited the team during two weeks in december 2019.

Tomas Prieto-Rumeau (Department of Statistics and Operations Research, UNED, Madrid, Spain) visited the team during one week in 2019. The main subject of the collaboration is the approximation of Markov Decision Processes

Anna Jaskiewicz (Politechnika Wrocławska) visited the team during one week in 2019. The main subject of the collaboration is the approximation of Markov Decision Processes

8.4.2. Visits to International Teams

Pierrick Legrand visited the Instituto Tecnológico de Tijuana from 08/12/2019 to 17/12/2019.

9. Dissemination

9.1. Promoting Scientific Activities

9.1.1. Member of the Organizing Committees

Pierrick Legrand is co-organisor of the international conference EA 2019 in Mulhouse https://ea2019.inria.fr/.

9.1.2. Chair of Conference Program Committees

F. Dufour is the chair of the Program Committee of the SIAM Conference on Control and Its Applications (CT19) in Pittsburgh, USA, 2019.

9.1.3. Journal

9.1.3.1. Member of the Editorial Boards

P. Del Moral is an associate editor for the journal Stochastic Analysis and Applications since 2001.

P. Del Moral is an associate editor for the journal Annals of Applied Probability since 2018.

F. Dufour is corresponding editor of the SIAM Journal of Control and Optimization since 2018.

F. Dufour is associate editor of the journal Applied Mathematics & Optimization (AMO) since 2018.

F. Dufour is associate editor of the journal Stochastics: An International Journal of Probability and Stochastic Processes since 2018.

F. Dufour is the representative of the SIAM activity group in control and system theory for the journal SIAM News since 2014.

J. Saracco is an associate editor of the journal Case Studies in Business, Industry and Government Statistics (CSBIGS) since 2006.

9.1.3.2. Reviewer - Reviewing Activities

All the members of CQFD are regular reviewers for several international journals and conferences in applied probability, statistics and operations research.

9.1.4. Scientific Expertise

J. Saracco is elected member of the council of the Société Française de Statistique (SFdS, French Statistical Society). A. Genadot is member of the scientific council of the mathematical institute of Bordeaux.

P. Del Moral is a member of the Data Science Foundation of the American Institute of Mathematical Sciences.

9.1.5. Research Administration

J. Saracco is deputy director of IMB (Institut de Mathématiques de Bordeaux, UMR CNRS 5251) since 2015.

M. Chavent is member of the national evaluation committee of Inria.

M. Chavent and Pierrick Legrand are members of the council of the Institut de Mathématique de Bordeaux.

F. Dufour has been the coordinator for the Inria evaluation of the theme "Stochastic Approaches"

9.2. Teaching - Supervision - Juries

9.2.1. Teaching

Licence : P. Legrand, Algèbre, 129h, L1, Université de Bordeaux, France.

Licence : P. Legrand, Espaces Euclidiens, 46,5h, L2, Université de Bordeaux, France.

Licence : P. Legrand, Informatique pour les mathématiques, 30h, L2, Université de Bordeaux, France.

DU : P. Legrand, Evolution Artificielle, Big data, 8h, DU, Bordeaux INP, France.

Licence : A. Genadot, Bases en Probabilités, 18h, L1, Université de Bordeaux, France.

Licence : A. Genadot, Projet Professionnel de l'étudiant, 8h, L1, Université de Bordeaux, France.

Licence : A. Genadot, Probabilité, 30h, L2, Université de Bordeaux, France.

Licence : A. Genadot, Techniques d'Enquêtes, 10h, L2, Université de Bordeaux, France.

Licence : A. Genadot, Modélisation Statistiques, 16.5h, L3, Université de Bordeaux, France.

Licence : A. Genadot, Préparation Stage, 15h, L3, Université de Bordeaux, France.

Licence : A. Genadot, TER, 5h, L3, Université de Bordeaux, France.

Licence : A. Genadot, Processus, 16.5h, L3, Université de Bordeaux, France.

Licence : A. Genadot, Statistiques, 20h, L3, Bordeaux INP, France.

Master : A. Genadot, Savoirs Mathématiques, 81h, M1, Université de Bordeaux et ESPE, France.

Master : A. Genadot, Martingales, 29h, M1, Université de Bordeaux, France.

Licence : F. Dufour, Probabilités et statistiques, 70h, first year of école ENSEIRB-MATMECA, Institut Polytechnique de Bordeaux, France.

Master : F. Dufour, Approche probabiliste et methode de Monte Carlo, 24h, third year of école ENSEIRB-MATMECA, Institut Polytechnique de Bordeaux, France.

9.2.2. Supervision

PhD: Hadrien Lorenzo, "Supervised analysis of high dimensional multi block data", supervised by Jérôme Saracco (CQFD) and Rodolphe Thebaut (Inserm), thesis defense: 27/11/19 in Bordeaux.

PhD in progress: Alex Mourer, "Variables importance in clustering", CIFRE Safran Aircraft Engines, supervised by Jérôme Lacaille (Safran), Madalina Olteanou (SAMM, Paris1), Alex Mourer (doctorant), Marie Chavent (CQFD).

PhD in progress: de Nathanaël Randriamihamison, "Contiguity Constrained Hierarchical Agglomerative Clustering for Hi-C data analysis", supervised by Nathalie Vialaneix (MIAT, INRA Toulouse), Pierre Neuvial (IMT, CNRS), Marie Chavent (CQFD) .

PhD in progress: Alexandre Conanec, "Modulation et optimisation statistique de données multi-tableaux : modélisation des facteurs de variations dans la gestion des compromis entre différents jeux de données", supervised by Marie Chavent(CQFD), Jérôme Saracco (CQFD), Marie-Pierre Ellies (INRA).

PhD in progress: Loic Labache , "Création d'un atlas cérébral évolutif de régions fonctionnelles définies à partir d'une cohorte de 297 sujets ayant effectués 20 tâches cognitives en IRMf ", supervised by Jérôme Saracco (CQFD), Marc Joliot (CEA).

PhD in progress: Tiffany Cherchi, "Automated optimal fleet management policy for airborne equipment", Montpellier University, since 2017, supervised by B. De Saporta and F. Dufour.

PhD in progress: Bastien Berthelot, "Algorithmes de traitement du signal pour l'extraction de signatures robustes sur des bio-signaux", CIFRE THALES, supervised by P. Legrand.

PhD in progress: Jimmy Bondu, "Classication de trajectoires d'objets par apprentissage.", CIFRE THALES, supervised by P. Legrand.

PhD in progress: Camille Palmier , “Nouvelles approches de fusion multi-capteurs par filtrage particulaire pour le recalage de navigation inertielle par corrélation de cartes”, CIFRE, supervised by P. Del Moral, Dann Laneuville (NavalGroup) and Karim Dahia (ONERA)

9.3. Popularization

9.3.1. Internal or external Inria responsibilities

Alexandre Genadot is a member of the Commission des emplois de recherche Inria BSO. Pierrick Legrand is a member of the commission consultative section 26 of the IMB.

10. Bibliography

Publications of the year

Doctoral Dissertations and Habilitation Theses

[1] P. LEGRAND.*Artificial evolution, fractal analysis and applications*, Université de Bordeaux, November 2019, Habilitation à diriger des recherches, https://hal.inria.fr/tel-02429815

Articles in International Peer-Reviewed Journal

[2] J. ANSELMI.*Combining Size-Based Load Balancing with Round-Robin for Scalable Low Latency*, in "IEEE Transactions on Parallel and Distributed Systems", 2019, p. 1-3, forthcoming [*DOI :* 10.1109/TPDS.2019.2950621], https://hal.archives-ouvertes.fr/hal-02276789

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Project-Team FLOWERS

Flowing Epigenetic Robots and Systems

IN PARTNERSHIP WITH:
Ecole nationale supérieure des techniques avancées

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Robotics and Smart environments

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Project-Team FLOWERS

Creation of the Team: 2008 April 01, updated into Project-Team: 2011 January 01

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A5.1.2. - Evaluation of interactive systems
A5.1.4. - Brain-computer interfaces, physiological computing
A5.1.5. - Body-based interfaces
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2. Overall Objectives

2.1. Overall Objectives

Can a machine learn like a child? Can it learn new skills and new knowledge in an unknown and changing environment? How can an embodied agent, e.g. a robot, discover its body and its relationships with the physical and social environment? How can its cognitive capacities continuously develop without the intervention of an engineer? What can it learn through natural social interactions with humans?

These are the questions that are being investigated in the FLOWERS research team at Inria Bordeaux Sud-Ouest and Ensta ParisTech. Rather than trying to imitate the intelligence of adult humans like in the field of Artificial Intelligence, we believe that trying to reconstruct the processes of development of the child's mind will allow for more adaptive, more robust and more versatile machines. This fundamental approach to the challenge of **autonomous learning** is called developmental robotics, or epigenetic robotics, and integrates concepts and theories from artificial intelligence, machine learning, neuroscience and developmental psychology. As many theories in neuroscience and developmental psychology are not formalized, this implies a crucial computational modeling activity, which in return provides means to assess the internal coherence of theories and sketch new hypothesis about the development of the human child's sensorimotor and cognitive abilities. Such computational modelling is also used as a foundational conceptual basis to build flexible lifelong autonomous machine learning systems.

Our team focuses in particular on the study of developmental constraints that allow for efficient open-ended learning of novel sensorimotor and interaction skills in embodied systems. In particular, we study constraints that guide exploration in large sensorimotor spaces:

- Mechanisms of intrinsically motivated exploration and active learning, including artificial curiosity, allowing to learn diverse skills in the absence of any external rewards, and in particular to self-organize developmental trajectories (also called automated curriculum learning) and collect efficiently learning data;
- Mechanisms of adequately constrained optimization and statistical inference for sample efficient sensorimotor skill acquisition (e.g. for optimizing motor policies in real robots through few interactions with the real world);
- Mechanisms for social learning, e.g. learning by imitation or demonstration, which implies both issues related to machine learning and human-robot interaction;
- Constraints related to embodiment, in particular through the concept of morphological computation, as well as the structure of motor primitives/muscle synergies that can leverage the properties of morphology and physics for simplifying motor control and perception;
- Maturational constraints which, coupled with the other constraints, can allow the progressive release of novel sensorimotor degrees of freedom to be explored;

We also study how these constraints on exploration can allow a machine to bootstrap multimodal perceptual abstractions associated to motor skills, in particular in the context of modelling language acquisition as a developmental process grounded in action.

Among the developmental principles that characterize human infants and can be used in developmental machines, FLOWERS focuses on the following three principles:

- **Exploration is progressive.** The space of skills that can be learnt in real world sensorimotor spaces is so large and complicated that not everything can be learnt at the same time. Simple skills are learnt first, and only when they are mastered, new skills of progressively increasing difficulty become the behavioural focus;
- **Internal representations are (partially) not innate but learnt and adaptive.** For example, the body map, the distinction self/non-self and the concept of "object" are discovered through experience with initially uninterpreted sensors and actuators, guided by experience, the overall pre-determined connection structure of the brain, as well as a small set of simple innate values or preferences.
- **Exploration can be self-guided and/or socially guided.** On the one hand, internal and intrinsic motivation systems regulate and organize spontaneous exploration; on the other hand, exploration can be guided through social learning and interaction with caretakers.

2.1.1. Research axis

The work of FLOWERS is organized around the following axis:

- **Curiosity-driven exploration and sensorimotor learning:** intrinsic motivation are mechanisms that have been identified by developmental psychologists to explain important forms of spontaneous exploration and curiosity. In FLOWERS, we try to develop computational intrinsic motivation systems, and test them on embodied machines, allowing to regulate the growth of complexity in exploratory behaviours. These mechanisms are studied as active learning mechanisms, allowing to learn efficiently in large inhomogeneous sensorimotor spaces and environments;
- **Cumulative learning of sensorimotor skills:** FLOWERS develops machine learning algorithms that can allow embodied machines to acquire cumulatively sensorimotor skills. In particular, we develop optimization and reinforcement learning systems which allow robots to discover and learn dictionaries of motor primitives, and then combine them to form higher-level sensorimotor skills.
- **Natural and intuitive social learning:** FLOWERS develops interaction frameworks and learning mechanisms allowing non-engineer humans to teach a robot naturally. This involves two sub-themes: 1) techniques allowing for natural and intuitive human-robot interaction, including simple ergonomic interfaces for establishing joint attention; 2) learning mechanisms that allow the robot to use the guidance hints provided by the human to teach new skills;
- **Discovering and abstracting the structure of sets of uninterpreted sensors and motors:** FLOWERS studies mechanisms that allow a robot to infer structural information out of sets of sensorimotor channels whose semantics is unknown, for example the topology of the body and the sensorimotor contingencies (propriocetive, visual and acoustic). This process is meant to be open-ended, progressing in continuous operation from initially simple representations to abstract concepts and categories similar to those used by humans.
- **Body design and role of the body in sensorimotor and social development:** We study how the physical properties of the body (geometry, materials, distribution of mass, growth, ...) can impact the acquisition of sensorimotor and interaction skills. This requires to consider the body as an experimental variable, and for this we develop special methodologies for designing and evaluating rapidly new morphologies, especially using rapid prototyping techniques like 3D printing.
- **Intelligent Tutoring Systems:**FLOWERS develops methods for online personalization of teaching sequences for educational software and MOOCs. This work builds on top of online optimization methods and motivational research previously developed.

3. Research Program

3.1. Research Program

Research in artificial intelligence, machine learning and pattern recognition has produced a tremendous amount of results and concepts in the last decades. A blooming number of learning paradigms - supervised, unsupervised, reinforcement, active, associative, symbolic, connectionist, situated, hybrid, distributed learning... - nourished the elaboration of highly sophisticated algorithms for tasks such as visual object recognition, speech recognition, robot walking, grasping or navigation, the prediction of stock prices, the evaluation of risk for insurances, adaptive data routing on the internet, etc... Yet, we are still very far from being able to build machines capable of adapting to the physical and social environment with the flexibility, robustness, and versatility of a one-year-old human child.

Indeed, one striking characteristic of human children is the nearly open-ended diversity of the skills they learn. They not only can improve existing skills, but also continuously learn new ones. If evolution certainly provided them with specific pre-wiring for certain activities such as feeding or visual object tracking, evidence shows that there are also numerous skills that they learn smoothly but could not be “anticipated” by biological evolution, for example learning to drive a tricycle, using an electronic piano toy or using a video game joystick. On the contrary, existing learning machines, and robots in particular, are typically only able to learn a single pre-specified task or a single kind of skill. Once this task is learnt, for example walking with two legs, learning is over. If one wants the robot to learn a second task, for example grasping objects in its visual field, then an engineer needs to re-program manually its learning structures: traditional approaches to task-specific machine/robot learning typically include engineer choices of the relevant sensorimotor channels, specific design of the reward function, choices about when learning begins and ends, and what learning algorithms and associated parameters shall be optimized.

As can be seen, this requires a lot of important choices from the engineer, and one could hardly use the term "autonomous" learning. On the contrary, human children do not learn following anything looking like that process, at least during their very first years. Babies develop and explore the world by themselves, focusing their interest on various activities driven both by internal motives and social guidance from adults who only have a folk understanding of their brains. Adults provide learning opportunities and scaffolding, but eventually young babies always decide for themselves what activity to practice or not. Specific tasks are rarely imposed to them. Yet, they steadily discover and learn how to use their body as well as its relationships with the physical and social environment. Also, the spectrum of skills that they learn continuously expands in an organized manner: they undergo a developmental trajectory in which simple skills are learnt first, and skills of progressively increasing complexity are subsequently learnt.

A link can be made to educational systems where research in several domains have tried to study how to provide a good learning experience to learners. This includes the experiences that allow better learning, and in which sequence they must be experienced. This problem is complementary to that of the learner that tries to learn efficiently, and the teacher here has to use as efficiently the limited time and motivational resources of the learner. Several results from psychology [59] and neuroscience [85] have argued that the human brain feels intrinsic pleasure in practicing activities of optimal difficulty or challenge. A teacher must exploit such activities to create positive psychological states of flow [73].

A grand challenge is thus to be able to build machines that possess this capability to discover, adapt and develop continuously new know-how and new knowledge in unknown and changing environments, like human children. In 1950, Turing wrote that the child's brain would show us the way to intelligence: "Instead of trying to produce a program to simulate the adult mind, why not rather try to produce one which simulates the child's" [154]. Maybe, in opposition to work in the field of Artificial Intelligence who has focused on mechanisms trying to match the capabilities of "intelligent" human adults such as chess playing or natural language dialogue [91], it is time to take the advice of Turing seriously. This is what a new field, called developmental (or epigenetic) robotics, is trying to achieve [109] [158]. The approach of developmental robotics consists in importing and implementing concepts and mechanisms from developmental psychology [117], cognitive linguistics [72], and developmental cognitive neuroscience [96] where there has been a considerable amount of research and theories to understand and explain how children learn and develop. A number of general principles are underlying this research agenda: embodiment [63] [131], grounding [89], situatedness [49], self-organization [150] [132], enaction [156], and incremental learning [67].

Among the many issues and challenges of developmental robotics, two of them are of paramount importance: exploration mechanisms and mechanisms for abstracting and making sense of initially unknown sensorimotor channels. Indeed, the typical space of sensorimotor skills that can be encountered and learnt by a developmental robot, as those encountered by human infants, is immensely vast and inhomogeneous. With a sufficiently rich environment and multimodal set of sensors and effectors, the space of possible sensorimotor activities is simply too large to be explored exhaustively in any robot's life time: it is impossible to learn all possible skills and represent all conceivable sensory percepts. Moreover, some skills are very basic to learn, some other very complicated, and many of them require the mastery of others in order to be learnt. For example, learning to manipulate a piano toy requires first to know how to move one's hand to reach the piano and how to touch specific parts of the toy with the fingers. And knowing how to move the hand might require to know how to track it visually.

Exploring such a space of skills randomly is bound to fail or result at best on very inefficient learning [128]. Thus, exploration needs to be organized and guided. The approach of epigenetic robotics is to take inspiration from the mechanisms that allow human infants to be progressively guided, i.e. to develop. There are two broad classes of guiding mechanisms which control exploration:

1. **internal guiding mechanisms,** and in particular intrinsic motivation, responsible of spontaneous exploration and curiosity in humans, which is one of the central mechanisms investigated in FLOWERS, and technically amounts to achieve online active self-regulation of the growth of complexity in learning situations;
2. **social learning and guidance,** a learning mechanisms that exploits the knowledge of other agents in the environment and/or that is guided by those same agents. These mechanisms exist in many different forms like emotional reinforcement, stimulus enhancement, social motivation, guidance, feedback or imitation, some of which being also investigated in FLOWERS;

3.1.1. Internal guiding mechanisms

In infant development, one observes a progressive increase of the complexity of activities with an associated progressive increase of capabilities [117], children do not learn everything at one time: for example, they first learn to roll over, then to crawl and sit, and only when these skills are operational, they begin to learn how to stand. The perceptual system also gradually develops, increasing children perceptual capabilities other time while they engage in activities like throwing or manipulating objects. This make it possible to learn to identify objects in more and more complex situations and to learn more and more of their physical characteristics.

Development is therefore progressive and incremental, and this might be a crucial feature explaining the efficiency with which children explore and learn so fast. Taking inspiration from these observations, some roboticists and researchers in machine learning have argued that learning a given task could be made much easier for a robot if it followed a developmental sequence and “started simple” [53] [79]. However, in these experiments, the developmental sequence was crafted by hand: roboticists manually build simpler versions of a complex task and put the robot successively in versions of the task of increasing complexity. And when they wanted the robot to learn a new task, they had to design a novel reward function.

Thus, there is a need for mechanisms that allow the autonomous control and generation of the developmental trajectory. Psychologists have proposed that intrinsic motivations play a crucial role. Intrinsic motivations are mechanisms that push humans to explore activities or situations that have intermediate/optimal levels of novelty, cognitive dissonance, or challenge [59] [73] [75]. The role and structure of intrinsic motivation in humans have been made more precise thanks to recent discoveries in neuroscience showing the implication of dopaminergic circuits and in exploration behaviours and curiosity [74] [93] [147]. Based on this, a number of researchers have began in the past few years to build computational implementation of intrinsic motivation [128] [129] [145] [57] [94] [112] [146]. While initial models were developed for simple simulated worlds, a current challenge is to manage to build intrinsic motivation systems that can efficiently drive exploratory behaviour in high-dimensional unprepared real world robotic sensorimotor spaces [129], [128], [130], [143]. Specific and complex problems are posed by real sensorimotor spaces, in particular due to the fact that they are both high-dimensional as well as (usually) deeply inhomogeneous. As an example for the latter issue, some regions of real sensorimotor spaces are often unlearnable due to inherent stochasticity or difficulty, in which case heuristics based on the incentive to explore zones of maximal unpredictability or uncertainty, which are often used in the field of active learning [70] [90] typically lead to catastrophic results. The issue of high dimensionality does not only concern motor spaces, but also sensory spaces, leading to the problem of correctly identifying, among typically thousands of quantities, those latent variables that have links to behavioral choices. In FLOWERS, we aim at developing intrinsically motivated exploration mechanisms that scale in those spaces, by studying suitable abstraction processes in conjunction with exploration strategies.

3.1.2. Socially Guided and Interactive Learning

Social guidance is as important as intrinsic motivation in the cognitive development of human babies [117]. There is a vast literature on learning by demonstration in robots where the actions of humans in the environment are recognized and transferred to robots [52]. Most such approaches are completely passive: the human executes actions and the robot learns from the acquired data. Recently, the notion of interactive learning has been introduced in [151], [60], motivated by the various mechanisms that allow humans to socially guide a robot [139]. In an interactive context the steps of self-exploration and social guidance are not separated and a robot learns by self exploration and by receiving extra feedback from the social context [151], [99], [113].

Social guidance is also particularly important for learning to segment and categorize the perceptual space. Indeed, parents interact a lot with infants, for example teaching them to recognize and name objects or characteristics of these objects. Their role is particularly important in directing the infant attention towards objects of interest that will make it possible to simplify at first the perceptual space by pointing out a segment of the environment that can be isolated, named and acted upon. These interactions will then be complemented by the children own experiments on the objects chosen according to intrinsic motivation in order to improve the knowledge of the object, its physical properties and the actions that could be performed with it.

In FLOWERS, we are aiming at including intrinsic motivation system in the self-exploration part thus combining efficient self-learning with social guidance [122], [123]. We also work on developing perceptual capabilities by gradually segmenting the perceptual space and identifying objects and their characteristics through interaction with the user [110] and robots experiments [95]. Another challenge is to allow for more flexible interaction protocols with the user in terms of what type of feedback is provided and how it is provided [107].

Exploration mechanisms are combined with research in the following directions:

3.1.3. Cumulative learning, reinforcement learning and optimization of autonomous skill learning

FLOWERS develops machine learning algorithms that can allow embodied machines to acquire cumulatively sensorimotor skills. In particular, we develop optimization and reinforcement learning systems which allow robots to discover and learn dictionaries of motor primitives, and then combine them to form higher-level sensorimotor skills.

3.1.4. Autonomous perceptual and representation learning

In order to harness the complexity of perceptual and motor spaces, as well as to pave the way to higher-level cognitive skills, developmental learning requires abstraction mechanisms that can infer structural information out of sets of sensorimotor channels whose semantics is unknown, discovering for example the topology of the body or the sensorimotor contingencies (proprioceptive, visual and acoustic). This process is meant to be open- ended, progressing in continuous operation from initially simple representations towards abstract concepts and categories similar to those used by humans. Our work focuses on the study of various techniques for:

- autonomous multimodal dimensionality reduction and concept discovery;
- incremental discovery and learning of objects using vision and active exploration, as well as of auditory speech invariants;
- learning of dictionaries of motion primitives with combinatorial structures, in combination with linguistic description;
- active learning of visual descriptors useful for action (e.g. grasping);

3.1.5. Embodiment and maturational constraints

FLOWERS studies how adequate morphologies and materials (i.e. morphological computation), associated to relevant dynamical motor primitives, can importantly simplify the acquisition of apparently very complex skills such as full-body dynamic walking in biped. FLOWERS also studies maturational constraints, which are mechanisms that allow for the progressive and controlled release of new degrees of freedoms in the sensorimotor space of robots.

3.1.6. Discovering and abstracting the structure of sets of uninterpreted sensors and motors

FLOWERS studies mechanisms that allow a robot to infer structural information out of sets of sensorimotor channels whose semantics is unknown, for example the topology of the body and the sensorimotor contingencies (proprioceptive, visual and acoustic). This process is meant to be open-ended, progressing in continuous operation from initially simple representations to abstract concepts and categories similar to those used by humans.

4. Application Domains

4.1. Application Domains

Neuroscience, Developmental Psychology and Cognitive Sciences The computational modelling of life-long learning and development mechanisms achieved in the team centrally targets to contribute to our understanding of the processes of sensorimotor, cognitive and social development in humans. In particular, it provides a methodological basis to analyze the dynamics of the interaction across learning and inference processes, embodiment and the social environment, allowing to formalize precise hypotheses and later on test them in experimental paradigms with animals and humans. A paradigmatic example of this activity is the Neurocuriosity project achieved in collaboration with the cognitive neuroscience lab of Jacqueline Gottlieb, where theoretical models of the mechanisms of information seeking, active learning and spontaneous exploration have been developed in coordination with experimental evidence and investigation, see https://flowers.inria.fr/neurocuriosityproject/.

Personal and lifelong learning robotics Many indicators show that the arrival of personal robots in homes and everyday life will be a major fact of the 21st century. These robots will range from purely entertainment or educative applications to social companions that many argue will be of crucial help in our society. Yet, to realize this vision, important obstacles need to be overcome: these robots will have to evolve in unpredictable homes and learn new skills in a lifelong manner while interacting with non-engineer humans after they left factories, which is out of reach of current technology. In this context, the refoundation of intelligent systems that developmental robotics is exploring opens potentially novel horizons to solve these problems. In particular, this application domain requires advances in artificial intelligence that go beyond the current state-of-the-art in fields like deep learning. Currently these techniques require tremendous amounts of data in order to function properly, and they are severely limited in terms of incremental and transfer learning. One of our goals is to drastically reduce the amount of data required in order for this very potent field to work. We try to achieve this by making neural networks aware of their knowledge, i.e. we introduce the concept of uncertainty, and use it as part of intrinsically motivated multitask learning architectures, and combined with techniques of learning by imitation.

Human-Robot Collaboration. Robots play a vital role for industry and ensure the efficient and competitive production of a wide range of goods. They replace humans in many tasks which otherwise would be too difficult, too dangerous, or too expensive to perform. However, the new needs and desires of the society call for manufacturing system centered around personalized products and small series productions. Human-robot collaboration could widen the use of robot in this new situations if robots become cheaper, easier to program and safe to interact with. The most relevant systems for such applications would follow an expert worker and works with (some) autonomy, but being always under supervision of the human and acts based on its task models.

Environment perception in intelligent vehicles. When working in simulated traffic environments, elements of FLOWERS research can be applied to the autonomous acquisition of increasingly abstract representations of both traffic objects and traffic scenes. In particular, the object classes of vehicles and pedestrians are if interest when considering detection tasks in safety systems, as well as scene categories ("scene context") that have a strong impact on the occurrence of these object classes. As already indicated by several investigations in the field, results from present-day simulation technology can be transferred to the real world with little impact on performance. Therefore, applications of FLOWERS research that is suitably verified by real-world benchmarks has direct applicability in safety-system products for intelligent vehicles.

Automated Tutoring Systems. Optimal teaching and efficient teaching/learning environments can be applied to aid teaching in schools aiming both at increase the achievement levels and the reduce time needed. From a practical perspective, improved models could be saving millions of hours of students' time (and effort) in learning. These models should also predict the achievement levels of students in order to influence teaching practices.

5. Highlights of the Year

5.1. Highlights of the Year

- Clément Moulin-Frier was recruited as CRCN permanent research scientist.
- PY Oudeyer was invited to give plenary keynote talks at several international AI conferences, including ICLR 2019 in New Orleans (https://www.youtube.com/watch?v=7bJ0fnvPLaA) and ACM International Conference on Virtual Agents (ACM IVA 2019), Paris.
- The team published papers in several major machine learning conferences, including ICML [33], Neurips [32], CoRL [38] and IJCNN [36], [37], and one in a major educational technology conference, CHI 2019 [29].
- PY Oudeyer was awarded an individual "Chaire IA" in the context of the national plan on artificial intelligence.
- The Poppy Station association, initiated by the team from the Poppy Education project, and co-directed by Didier Roy, was created and gathers several major national and international educational associations. It aims at scaling up and disseminating the educational robotics kits designed by the Flowers team, and now used in many educational and artistic projects, see https://www.poppy-station.org.
- The work of the PhD of Sébastien Forestier (sup. by PY Oudeyer) on curiosity-driven learning of tool use in robots and children, was integrated as a video interview in the new permanent exhibition on robots at Cité des Sciences et de l'Industrie, Paris, see http://www.cite-sciences.fr/fr/au-programme/expos-permanentes/expos-permanentes-dexplora/robots/lexposition/.

5.1.1. Awards

- Y Oudeyer was awarded the Atos Joseph Fourier prize for his work on curiosity-driven machine learning.

6. New Software and Platforms

6.1. Explauto

an autonomous exploration library

KEYWORD: Exploration

SCIENTIFIC DESCRIPTION: An important challenge in developmental robotics is how robots can be intrinsically motivated to learn efficiently parametrized policies to solve parametrized multi-task reinforcement learning problems, i.e. learn the mappings between the actions and the problem they solve, or sensory effects they produce. This can be a robot learning how arm movements make physical objects move, or how movements of a virtual vocal tract modulates vocalization sounds. The way the robot will collects its own sensorimotor experience have a strong impact on learning efficiency because for most robotic systems the involved spaces are high dimensional, the mapping between them is non-linear and redundant, and there is limited time allowed for learning. If robots explore the world in an unorganized manner, e.g. randomly, learning algorithms will be often ineffective because very sparse data points will be collected. Data are precious due to the high dimensionality and the limited time, whereas data are not equally useful due to non-linearity and redundancy. This is why learning has to be guided using efficient exploration strategies, allowing the robot to actively drive its own interaction with the environment in order to gather maximally informative data to optimize the parametrized policies. In the recent year, work in developmental learning has explored various families of algorithmic principles which allow the efficient guiding of learning and exploration.

Explauto is a framework developed to study, model and simulate curiosity-driven learning and exploration in real and simulated robotic agents. Explauto's scientific roots trace back from Intelligent Adaptive Curiosity algorithmic architecture [127], which has been extended to a more general family of autonomous exploration architectures by [1] and recently expressed as a compact and unified formalism [119]. The library is detailed in [120]. In Explauto, interest models are implementing the strategies of active selection of particular problems / goals in a parametrized multi-task reinforcement learning setup to efficiently learn parametrized policies. The agent can have different available strategies, parametrized problems, models, sources of information, or learning mechanisms (for instance imitate by mimicking vs by emulation, or asking help to one teacher or to another), and chooses between them in order to optimize learning (a processus called strategic learning [124]). Given a set of parametrized problems, a particular exploration strategy is to randomly draw goals/ RL problems to solve in the motor or problem space. More efficient strategies are based on the active choice of learning experiments that maximize learning progress using bandit algorithms, e.g. maximizing improvement of predictions or of competences to solve RL problems [127]. This automatically drives the system to explore and learn first easy skills, and then explore skills of progressively increasing complexity. Both random and learning progress strategies can act either on the motor or on the problem space, resulting in motor babbling or goal babbling strategies.

- Motor babbling consists in sampling commands in the motor space according to a given strategy (random or learning progress), predicting the expected effect, executing the command through the environment and observing the actual effect. Both the parametrized policies and interest models are finally updated according to this experience.
- Goal babbling consists in sampling goals in the problem space and to use the current policies to infer a motor action supposed to solve the problem (inverse prediction). The robot/agent then executes the command through the environment and observes the actual effect. Both the parametrized policies and interest models are finally updated according to this experience.It has been shown that this second strategy allows a progressive solving of problems much more uniformly in the problem space than with a motor babbling strategy, where the agent samples directly in the motor space [1].

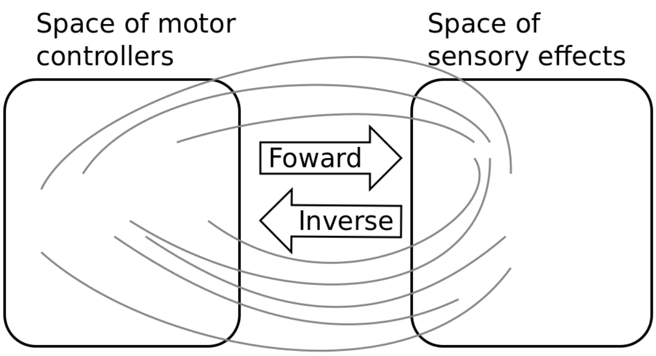


Figure 1. Complex parametrized policies involve high dimensional action and effect spaces. For the sake of visualization, the motor M and sensory S spaces are only 2D each in this example. The relationship between M and S is non-linear, dividing the sensorimotor space into regions of unequal stability: small regions of S can be reached very precisely by large regions of M, or large regions in S can be very sensitive to variations in M.: s as well as a non-linear and redundant relationship. This non-linearity can imply redundancy, where the same sensory effect can be attained using distinct regions in M.

FUNCTIONAL DESCRIPTION: This library provides high-level API for an easy definition of:

- Real and simulated robotic setups (Environment level),
- Incremental learning of parametrized policies (Sensorimotor level),
- Active selection of parametrized RL problems (Interest level).

The library comes with several built-in environments. Two of them corresponds to simulated environments: a multi-DoF arm acting on a 2D plan, and an under-actuated torque-controlled pendulum. The third one allows to control real robots based on Dynamixel actuators using the Pypot library. Learning parametrized policies involves machine learning algorithms, which are typically regression algorithms to learn forward models, from motor controllers to sensory effects, and optimization algorithms to learn inverse models, from sensory effects, or problems, to the motor programs allowing to reach them. We call these sensorimotor learning algorithms sensorimotor models. The library comes with several built-in sensorimotor models: simple nearest-neighbor look-up, non-parametric models combining classical regressions and optimization algorithms, online mixtures of Gaussians, and discrete Lidstone distributions. Explauto sensorimotor models are online learning algorithms, i.e. they are trained iteratively during the interaction of the robot in theenvironment in which it evolves. Explauto provides also a unified interface to define exploration strategies using the InterestModel class. The library comes with two built-in interest models: random sampling as well as sampling maximizing the learning progress in forward or inverse predictions.

Explauto environments now handle actions depending on a current context, as for instance in an environment where a robotic arm is trying to catch a ball: the arm trajectories will depend on the current position of the ball (context). Also, if the dynamic of the environment is changing over time, a new sensorimotor model (Non-Stationary Nearest Neighbor) is able to cope with those changes by taking more into account recent experiences. Those new features are explained in Jupyter notebooks.

This library has been used in many experiments including:

- the control of a 2D simulated arm,
- the exploration of the inverse kinematics of a poppy humanoid (both on the real robot and on the simulated version),
- acoustic model of a vocal tract.

Explauto is crossed-platform and has been tested on Linux, Windows and Mac OS. It has been released under the GPLv3 license.

- Contact: Sebastien Forestier
- URL: https://github.com/flowersteam/explauto

6.2. KidBreath

KEYWORD: Machine learning

FUNCTIONAL DESCRIPTION: KidBreath is a web responsive application composed by several interactive contents linked to asthma and displayed to different forms: learning activities with quiz, short games and videos. There are profil creation and personalization, and a part which describes historic and scoring of learning activities, to see evolution of Kidreath use. To test Kidlearn algorithm, it is iadapted and integrated on this platform. Development in PHP, HTML-5, CSS, MySQL, JQuery, Javascript. Hosting in APACHE, LINUX, PHP 5.5, MySQL, OVH.

- Partner: ItWell SAS
- Contact: Alexandra Delmas
- URL: http://www.kidbreath.fr

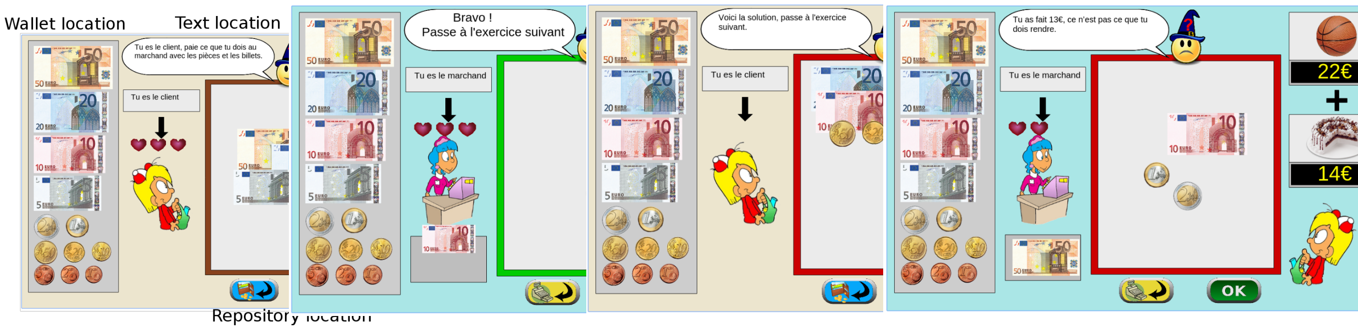


Figure 2. Four principal regions are defined in the graphical interface. The first is the wallet location where users can pick and drag the money items and drop them on the repository location to compose the correct price. The object and the price are present in the object location. Four different types of exercises exist: M : customer/one object, R : merchant/one object, MM : customer/two objects, RM : merchant/two objects.

6.3. Kidlearn: money game application

FUNCTIONAL DESCRIPTION: The games is instantiated in a browser environment where students are proposed exercises in the form of money/token games (see Figure 2). For an exercise type, one object is presented with a given tagged price and the learner has to choose which combination of bank notes, coins or abstract tokens need to be taken from the wallet to buy the object, with various constraints depending on exercises parameters. The games have been developed using web technologies, HTML5, javascript and Django.

- Contact: Benjamin Clement
- URL: https://flowers.inria.fr/research/kidlearn/

6.4. Kidlearn: script for Kidbreath use

KEYWORD: PHP

FUNCTIONAL DESCRIPTION: A new way to test Kidlearn algorithms is to use them on Kidbreath Plateform. The Kidbreath Plateform use apache/PHP server, so to facilitate the integration of our algorithm, a python script have been made to allow PHP code to use easily the python library already made which include our algorithms.

- Contact: Benjamin Clement
- URL: https://flowers.inria.fr/research/kidlearn/

6.5. KidLearn

KEYWORD: Automatic Learning

FUNCTIONAL DESCRIPTION: KidLearn is a software which adaptively personalize sequences of learning activities to the particularities of each individual student. It aims at proposing to the student the right activity at the right time, maximizing concurrently his learning progress and its motivation.

- Participants: Benjamin Clement, Didier Roy, Manuel Lopes and Pierre Yves Oudeyer
- Contact: Pierre-Yves Oudeyer
- URL: https://flowers.inria.fr/research/kidlearn/

6.6. Poppy

KEYWORDS: Robotics - Education

FUNCTIONAL DESCRIPTION: The Poppy Project team develops open-source 3D printed robots platforms based on robust, flexible, easy-to-use and reproduce hardware and software. In particular, the use of 3D printing and rapid prototyping technologies is a central aspect of this project, and makes it easy and fast not only to reproduce the platform, but also to explore morphological variants. Poppy targets three domains of use: science, education and art.

In the Poppy project we are working on the Poppy System which is a new modular and open-source robotic architecture. It is designed to help people create and build custom robots. It permits, in a similar approach as Lego, building robots or smart objects using standardized elements.

Poppy System is a unified system in which essential robotic components (actuators, sensors...) are independent modules connected with other modules through standardized interfaces:

- Unified mechanical interfaces, simplifying the assembly process and the design of 3D printable parts.
- Unified communication between elements using the same connector and bus for each module.
- Unified software, making it easy to program each module independently.

Our ambition is to create an ecosystem around this system so communities can develop custom modules, following the Poppy System standards, which can be compatible with all other Poppy robots.

- Participants: Jonathan Grizou, Matthieu Lapeyre, Pierre Rouanet and Pierre-Yves Oudeyer
- Contact: Pierre-Yves Oudeyer
- URL: https://www.poppy-project.org/

6.7. Poppy Ergo Jr

KEYWORDS: Robotics - Education

FUNCTIONAL DESCRIPTION: Poppy Ergo Jr is an open hardware robot developed by the Poppy Project to explore the use of robots in classrooms for learning robotic and computer science.

It is available as a 6 or 4 degrees of freedom arm designed to be both expressive and low-cost. This is achieved by the use of FDM 3D printing and low cost Robotis XL-320 actuators. A Raspberry Pi camera is attached to the robot so it can detect object, faces or QR codes.

The Ergo Jr is controlled by the Pypot library and runs on a Raspberry pi 2 or 3 board. Communication between the Raspberry Pi and the actuators is made possible by the Pixl board we have designed.

The Poppy Ergo Jr robot has several 3D printed tools extending its capabilities. There are currently the lampshade, the gripper and a pen holder.

With the release of a new Raspberry Pi board early 2016, the Poppy Ergo Jr disk image was updated to support Raspberry Pi 2 and 3 boards. The disk image can be used seamlessly with a board or the other.

- Contact: Theo Segonds
- URL: https://github.com/poppy-project/poppy-ergo-jr

6.8. S-RL Toolbox

Reinforcement Learning (RL) and State Representation Learning (SRL) for Robotics

KEYWORDS: Machine learning - Robotics

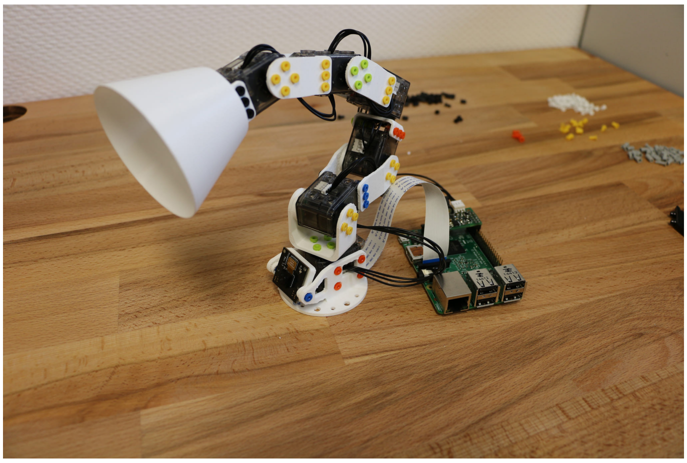


Figure 3. Poppy Ergo Jr, 6-DoFs arm robot for education

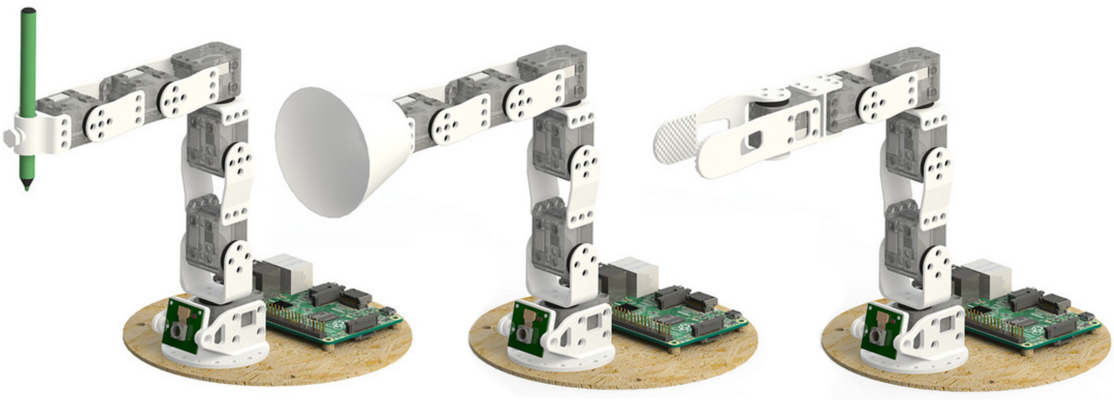


Figure 4. The available Ergo Jr tools: a pen holder, a lampshade and a gripper

FUNCTIONAL DESCRIPTION: This repository was made to evaluate State Representation Learning methods using Reinforcement Learning. It integrates (automatic logging, plotting, saving, loading of trained agent) various RL algorithms (PPO, A2C, ARS, ACKTR, DDPG, DQN, ACER, CMA-ES, SAC, TRPO) along with different SRL methods (see SRL Repo) in an efficient way (1 Million steps in 1 Hour with 8-core cpu and 1 Titan X GPU).

- Partner: ENSTA
- Contact: David Filliat
- URL: https://github.com/araffin/robotics-rl-srl

6.9. Deep-Explauto

KEYWORDS: Deep learning - Unsupervised learning - Learning - Experimentation

FUNCTIONAL DESCRIPTION: Until recently, curiosity driven exploration algorithms were based on classic learning algorithms, unable to handle large dimensional problems (see explauto). Recent advances in the field of deep learning offer new algorithms able to handle such situations.

Deep explauto is an experimental library, containing reference implementations of curiosity driven exploration algorithms. Given the experimental aspect of exploration algorithms, and the low maturity of the libraries and algorithms using deep learning, proposing black-box implementations of those algorithms, enabling a blind use of those, seem unrealistic.

Nevertheless, in order to quickly launch new experiments, this library offers an set of objects, functions and examples, allowing to kickstart new experiments.

- Contact: Alexandre Pere

6.10. Orchestra

KEYWORD: Experimental mechanics

FUNCTIONAL DESCRIPTION: Ochestra is a set of tools meant to help in performing experimental campaigns in computer science. It provides you with simple tools to:

+ Organize a manual experimental workflow, leveraging git and lfs through a simple interface. + Collaborate with other peoples on a single experimental campaign. + Execute pieces of code on remote hosts such as clusters or clouds, in one line. + Automate the execution of batches of experiments and the presentation of the results through a clean web ui.

A lot of advanced tools exists on the net to handle similar situations. Most of them target very complicated workflows, e.g. DAGs of tasks. Those tools are very powerful but lack the simplicity needed by newcomers. Here, we propose a limited but very simple tool to handle one of the most common situation of experimental campaigns: the repeated execution of an experiment on variations of parameters.

In particular, we include three tools: + expegit: a tool to organize your experimental campaign results in a git repository using git-lfs (large file storage). + runaway: a tool to execute code on distant hosts parameterized with easy to use file templates. + orchestra: a tool to automate the use of the two previous tools on large campaigns.

- Contact: Alexandre Pere

6.11. Curious

Curious: Intrinsically Motivated Modular Multi-Goal Reinforcement Learning

KEYWORDS: Exploration - Reinforcement learning - Artificial intelligence

FUNCTIONAL DESCRIPTION: This is an algorithm enabling to learn a controller for an agent in a modular multi-goal environment. In these types of environments, the agent faces multiple goals classified in different types (e.g. reaching goals, grasping goals for a manipulation robot).

- Contact: Cedric Colas

6.12. teachDeepRL

Teacher algorithms for curriculum learning of Deep RL in continuously parameterized environments

KEYWORDS: Machine learning - Git

FUNCTIONAL DESCRIPTION: Codebase from our CoRL2019 paper https://arxiv.org/abs/1910.07224

This github repository provides implementations for the following teacher algorithms: - Absolute Learning Progress-Gaussian Mixture Model (ALP-GMM), our proposed teacher algorithm - Robust Intelligent Adaptive Curiosity (RIAC), from Baranes and Oudeyer, R-IAC: robust intrinsically motivated exploration and active learning. - Covar-GMM, from Moulin-Frier et al., Self-organization of early vocal development in infants and machines: The role of intrinsic motivation.

- Contact: Remy Portelas
- URL: https://github.com/flowersteam/teachDeepRL

6.13. Automated Discovery of Lenia Patterns

KEYWORDS: Exploration - Cellular automaton - Deep learning - Unsupervised learning

SCIENTIFIC DESCRIPTION: In many complex dynamical systems, artificial or natural, one can observe selforganization of patterns emerging from local rules. Cellular automata, like the Game of Life (GOL), have been widely used as abstract models enabling the study of various aspects of self-organization and morphogenesis, such as the emergence of spatially localized patterns. However, findings of self-organized patterns in such models have so far relied on manual tuning of parameters and initial states, and on the human eye to identify “interesting” patterns. In this paper, we formulate the problem of automated discovery of diverse self-organized patterns in such high-dimensional complex dynamical systems, as well as a framework for experimentation and evaluation. Using a continuous GOL as a testbed, we show that recent intrinsically-motivated machine learning algorithms (POP-IMGEPs), initially developed for learning of inverse models in robotics, can be transposed and used in this novel application area. These algorithms combine intrinsically motivated goal exploration and unsupervised learning of goal space representations. Goal space representations describe the “interesting” features of patterns for which diverse variations should be discovered. In particular, we compare various approaches to define and learn goal space representations from the perspective of discovering diverse spatially localized patterns. Moreover, we introduce an extension of a state-of-the-art POP-IMGEP algorithm which incrementally learns a goal representation using a deep auto-encoder, and the use of CPPN primitives for generating initialization parameters. We show that it is more efficient than several baselines and equally efficient as a system pre-trained on a hand-made database of patterns identified by human experts.

FUNCTIONAL DESCRIPTION: Python source code of experiments and data analysis for the paper " Intrinsically Motivated Discovery of Diverse Patterns in Self-Organizing Systems" (Chris Reinke, Mayalen Echeverry, Pierre-Yves Oudeyer in Submitted to ICLR 2020). The software includes: Lenia environment, exploration algorithms (IMGEPs, random search), deep learning algorithms for unsupervised learning of goal spaces, tools and configurations to run experiments, and data analysis tools.

- Contact: Chris Reinke
- URL: https://github.com/flowersteam/automated_discovery_of_lenia_patterns

6.14. ZPDES_ts

ZPDES in typescript

KEYWORDS: Machine learning - Education

FUNCTIONAL DESCRIPTION: ZPDES is a machine learning-based algorithm that allows you to customize the content of training courses for each learner's level. It has already been implemented in the Kidlern software in python with other algorithms. Here, ZPDES is implemented in typescript.

- Authors: Benjamin Clement, Pierre-Yves Oudeyer, Didier Roy and Manuel Lopes
- Contact: Benjamin Clement
- URL: https://flowers.inria.fr/research/kidlearn/

6.15. GEP-PG

Goal Exploration Process - Policy Gradient

KEYWORDS: Machine learning - Deep learning

FUNCTIONAL DESCRIPTION: Reinforcement Learning algorithm working with OpenAI Gym environments. A first phase implements exploration using a Goal Exploration Process (GEP). Samples collected during exploration are then transferred to the memory of a deep reinforcement learning algorithm (deep deterministic policy gradient or DDPG). DDPG then starts learning from a pre-initialized memory so as to maximize the sum of discounted rewards given by the environment.

- Contact: Cedric Colas

7. New Results

7.1. Curiosity-Driven Learning in Humans

7.1.1. Computational Models Of Information-Seeking and Curiosity-Driven Learning in Human Adults

Participants: Pierre-Yves Oudeyer [correspondant], Sébastien Forestier, Alexandr Ten.

This project involves a collaboration between the Flowers team and the Cognitive Neuroscience Lab of J. Gottlieb at Columbia Univ. (NY, US), on the understanding and computational modeling of mechanisms of curiosity, attention and active intrinsically motivated exploration in humans.

It is organized around the study of the hypothesis that subjective meta-cognitive evaluation of information gain (or control gain or learning progress) could generate intrinsic reward in the brain (living or artificial), driving attention and exploration independently from material rewards, and allowing for autonomous lifelong acquisition of open repertoires of skills. The project combines expertise about attention and exploration in the brain and a strong methodological framework for conducting experimentations with monkeys, human adults and children together with computational modeling of curiosity/intrinsic motivation and learning.

Such a collaboration paves the way towards a central objective, which is now a central strategic objective of the Flowers team: designing and conducting experiments in animals and humans informed by computational/mathematical theories of information seeking, and allowing to test the predictions of these computational theories.

7.1.1.1. Context

Curiosity can be understood as a family of mechanisms that evolved to allow agents to maximize their knowledge (or their control) of the useful properties of the world - i.e., the regularities that exist in the world - using active, targeted investigations. In other words, we view curiosity as a decision process that maximizes learning/competence progress (rather than minimizing uncertainty) and assigns value ("interest") to competing tasks based on their epistemic qualities - i.e., their estimated potential allow discovery and learning about the structure of the world.

Because a curiosity-based system acts in conditions of extreme uncertainty (when the distributions of events may be entirely unknown) there is in general no optimal solution to the question of which exploratory action to take [108], [130], [141]. Therefore we hypothesize that, rather than using a single optimization process as it has been the case in most previous theoretical work [86], curiosity is comprised of a family of mechanisms that include simple heuristics related to novelty/surprise and measures of learning progress over longer time scales [128] [56], [118]. These different components are related to the subject's epistemic state (knowledge and beliefs) and may be integrated with fluctuating weights that vary according to the task context. Our aim is to quantitatively characterize this dynamic, multi-dimensional system in a computational framework based on models of intrinsically motivated exploration and learning.

Because of its reliance on epistemic currencies, curiosity is also very likely to be sensitive to individual differences in personality and cognitive functions. Humans show well-documented individual differences in curiosity and exploratory drives [106], [140], and rats show individual variation in learning styles and novelty seeking behaviors [80], but the basis of these differences is not understood. We postulate that an important component of this variation is related to differences in working memory capacity and executive control which, by affecting the encoding and retention of information, will impact the individual's assessment of learning, novelty and surprise and ultimately, the value they place on these factors [133], [149], [50], [155]. To start understanding these relationships, about which nothing is known, we will search for correlations between curiosity and measures of working memory and executive control in the population of children we test in our tasks, analyzed from the point of view of a computational models of the underlying mechanisms.

A final premise guiding our research is that essential elements of curiosity are shared by humans and non-human primates. Human beings have a superior capacity for abstract reasoning and building causal models, which is a prerequisite for sophisticated forms of curiosity such as scientific research. However, if the task is adequately simplified, essential elements of curiosity are also found in monkeys [106], [98] and, with adequate characterization, this species can become a useful model system for understanding the neurophysiological mechanisms.

7.1.1.2. Objectives

Our studies have several highly innovative aspects, both with respect to curiosity and to the traditional research field of each member team.

- Linking curiosity with quantitative theories of learning and decision making: While existing investigations examined curiosity in qualitative, descriptive terms, here we propose a novel approach that integrates quantitative behavioral and neuronal measures with computationally defined theories of learning and decision making.
- Linking curiosity in children and monkeys: While existing investigations examined curiosity in humans, here we propose a novel line of research that coordinates its study in humans and non-human primates. This will address key open questions about differences in curiosity between species, and allow access to its cellular mechanisms.
- Neurophysiology of intrinsic motivation: Whereas virtually all the animal studies of learning and decision making focus on operant tasks (where behavior is shaped by experimenter-determined primary rewards) our studies are among the very first to examine behaviors that are intrinsically motivated by the animals' own learning, beliefs or expectations.
- Neurophysiology of learning and attention: While multiple experiments have explored the single-neuron basis of visual attention in monkeys, all of these studies focused on vision and eye movement control. Our studies are the first to examine the links between attention and learning, which are recognized in psychophysical studies but have been neglected in physiological investigations.
- Computer science: biological basis for artificial exploration: While computer science has proposed and tested many algorithms that can guide intrinsically motivated exploration, our studies are the first to test the biological plausibility of these algorithms.
- Developmental psychology: linking curiosity with development: While it has long been appreciated that children learn selectively from some sources but not others, there has been no systematic investigation of the factors that engender curiosity, or how they depend on cognitive traits.

7.1.1.3. Current results: experiments in Active Categorization

In 2018, we have been occupied by analyzing data of the human adult experiment conducted in 2017. In this experiment we asked whether humans possess, and use, metacognitive abilities to guide task choices in two contexts motivational contexts, in which they could freely choose to learn about 4 competing tasks. Participants (n = 505, recruited via Amazon Mechanical Turk) were asked to play a categorization game with four distinct difficulty levels. Some participants had been explicitly prescribed a goal of maximizing their learning across the difficulty levels (across tasks), while others did not receive any specific instructions regarding the goal of the game. The experiment yielded a rich but complex set of data. The data includes records of participants' classification responses, task choices, reaction times, and post-task self-reports about various subjective evaluations of the competing tasks (e.g. subjective interest, progress, learning potential, etc.). We are now finalizing the results and a computational model of the underlying cognitive and motivational mechanisms in order to prepare them for public dissemination.

The central question going into the study was, how do active learners become interested in specific learning exercises: how do they decide which task to engage with, when none of the tasks provide external rewards. Last year, we identified some of the key behavioral observations that merited further attention. First, we saw a clear effect of an external goal prescription on the participants' overall task selection strategy. People who were explicitly instructed to try to maximize their learning across the 4 tasks challenged themselves more by giving preference towards harder tasks. In contrast, those who were simply familiarized with the rules of the game and not given any explicit suggestions from the experiments did not show this overchallenge bias and had a slight preference for easier tasks (see figure 5). Second, we observed that although strategies varied between the two instruction groups, there was some considerable within-group variability in learning. We found that in both groups, people had varying success in learning the classification task for each task family resulting in four distinct performance based groups: learners of 0, 1, 2, or 3 tasks (task 4 was unlearnable), as shown in figure 6. Importantly, successful 3-task learners in both instruction groups exhibited similar task preferences, suggesting that (1) even in the absence of external instruction, people can be motivated to explore the task space and (2) intrinsically motivated exploration is similar to strategies employed when a learner is trying to maximize her learning.

Assuming that task choice decisions are based on a subjective evaluative process that assigns value to choice candidates, we considered a simple choice model of task selection. In a classic conditional logit model [116], choices are made probabilistically and the choice probabilities are proportional to choice utilities (the inherent subjective value of a choice; also see ref [159]). We elaborated on the utility component of the basic choice model to consider two utility aspects of interest: a relative measure of learning progress (LP) and an absolute measure of proportion correct (PC). Although both measures are based on empirical feedback (correct / incorrect), the LP measure is considered relative, because it captures how performance changes over time by comparing performance estimates across different time scales, while PC is absolute in a sense that it only characterizes performance at a given instance. While PC alone does not differentiate between an unfamiliar (but potentially easy) task on which the performance might be low and a familiar but very hard task, the former can have markedly LP (due to the gradual improvement on that task) than the latter. Only the tasks characterized by high LP are then worthy of time and effort if the goal is to master tasks. The utility component in our model thus includes two principal quantities:

$$u_{i,t} = \alpha LP_{i,t} + \beta PC_{i,t}$$

where α and β are free parameters indexing the model's sensitivity to LP and PC, respectively. Index i designates the task, while t indexes time. Thus, in our model, utility is seen as a dual-component linear computation of both relative and absolute competence quantities. Task utilities enter the decision-making process that assigns relative preference to each task:

$$p(task_i) = \frac{e^{u_i/\tau}}{\sum_j e^{u_j/\tau}}$$

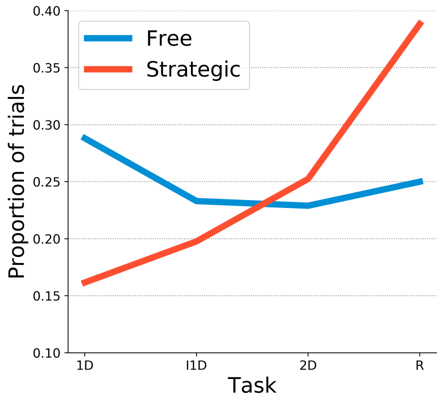


Figure 5. Proportion of trials on each task (1D, I1D, 2D, and R). The group with an externally prescribed learning maximization goal is referred to as "Strategic", and the unconstrained group is referred to as "Free". 1D was the task were categorization was determined by a single variable dimension. In I1D (ignore 1D), the stimuli varied across 2 dimensions, but only one determined the stimulus category. In 2D, there were 2 variable dimensions and both jointly determined the category. Finally in R, there were 2 variable dimensions, but none of them could reliably predict the stimulus class. The top plot shows data aggregated across experimental groups, shown separately in the bottom plot. In hte figure, task difficulty increases from left to right.

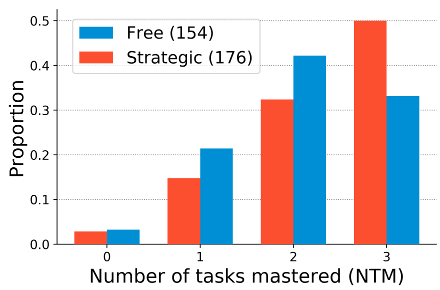


Figure 6. Learning outcomes by group. The group with an externally prescribed learning maximization goal is referred to as "Strategic", and the unconstrained group is referred to as "Free". Number of people in the groups are given in parentheses. The figure shows that some people seem to set and pursue learning maximization goals in the absence of external rewards and instructions. Additionally, learning goals have to be matched with appropriate behavioral strategies in order to be reached, which explains the failure to learn all 3 tasks by some people in the Strategic group.

where τ is another free parameter (known as temperature) that controls the stochasticity of utility-based decision. The sum over j elements, $\sum_j$ constitutes the total exponentiated utility of each task in the task space, thus normalizing each individual exponentiated task utility u_i.

The computation of the utility components is important for the model, because it ultimately determines how well the model can fit to choice data. We started exploring the model with a simple definition for both LP and PC. Both components are based on averaging binary feedback over multiple trials in the past. Since the familiarization stage of our experiment was 15-trials-long, the first free choice was made based on feedback data from 15 trials on each task. Accordingly, we defined PC to be the proportion of correct guesses in 15 trials. LP was defined as the absolute difference between the first 9 and the last 6 trials of the recent most 15 trials in the past. While a participant was engaged with one of the tasks, LP and PC for that task changed according to her dynamic performance, while LPs and PCs for other tasks remained unchanged. We acknowledge that there are probably multiple other components at play when it comes to utility computation, some of which may have little to do with task competence. We also submit that there are multiple ways of defining the PC and LP components that are more biologically rooted and plausible given what we know of memory and metacognition. Finally, we do not rule out the possibility of dynamic changes of free parameters themselves, corresponding to changes in motivation during the learning process. All of these considerations are worthy directions of future research, but in this study we focused on finding some necessary evidence for the sensitivity to learning progress.

We fitted the model to each individual's choice data using maximum likelihood estimation. Assuming that choice probabilities on each trial come from a categorical distribution (also called a generalized Bernoulli distribution), where the probability of choosing item i is given by:

$$P(\mathbf{x} \mid \mathbf{p}) = \prod_{i=1}^{k} p_i^{x_i}$$

where **p** is a vector of probabilities associated with k events, and **p** is a one-hot encoded vector representing discrete items x_i. We add a time index to indicate the dynamic quality of choice probabilities, so that:

$$P_t(\mathbf{x} \mid \mathbf{p}_t) = \prod_{i=1}^{k} p_{i,t}^{x_i}$$

Then, the likelihood of the choice model ($p(task_i \mid \alpha, \beta, \tau)$) at time t is equal to the product of choice probabilities given by that model for that time step:

$$L_t(\alpha, \beta, \tau \mid \mathbf{x}) = \prod_{i}^{k} p_{i,t}^{x_i}$$

and since the empirical choice data can be represented in a one-hot format, the likelihood of the model for a given time point boils down to the predicted probability of the actualy choice:

$$L_t(\alpha, \beta, \tau \mid choice = i) = p_{i,t} = \frac{e^{u_{i,t}/\tau}}{\sum_j e^{u_{j,t}/\tau}}$$

The likelihood of the model across all m trials is obtained by applying the product rule of probability:

$$L_{overall}(\alpha, \beta, \tau \mid choice = i) = \prod_{t}^{m} p_{i,t} = \frac{e^{u_{i,t}/\tau}}{\sum_j e^{u_{j,t}/\tau}}$$

For convenience, we use the negative log transformation to avoid computational precision problems and convert a likelihood maximization objective into negative likelihood minimization problem solvable by publicly accessible optimization tools:

$$-\log L_{overall}(\alpha, \beta, \tau \mid choice = i) = -\sum_{t}^{m} \log p_{i,t}$$

Having formulated the likelihood function, we optimized the free parameters to obtain a model that fits the individual data best. We thus fit an individual-level model to each participant's choice data. The fitted parameters can be interpreted as relative sensitivity to the competence quantities of interest (LP and PC), since these quantities share the same range of values (0 to 1). Finally, we performed some group-level analyses on these individual-level parameter estimates to evaluate certain group-level effects that might influence them (e.g. effect of instruction or learning proficiency).

The group with a learning maximization goal devalued tasks with higher positive feedback expectation. Qualitatively, this matched our prior observations showing their strong preference for harder tasks. However, the best learners (3-task learners) across both instruction groups showed a slight preference for learning progress and a relatively strong aversion to positive feedback. It appears that what separated better and worse learners among the learning maximizers was whether they followed learning progress, and not just the feedback heuristic. On the other hand, while less successful learners in the unconstrained group seemed to choose tasks according to learning progress, they valued positive feedback over it, which prevented them from exploring more challenging learnable tasks. This is reflected in group mean values of the fitted parameters summarized in table 1

Table 1. Fitted parameter values averaged within number of tasks learned and instruction groups. The group with an externally prescribed learning maximization goal is referred to as “Strategic”, and the unconstrained group is referred to as “Free”. NTM stands for the number of tasks mastered

Group	NTM	Learning progress	Proportion correct	Temperature
	1	0.27	0.56	6.92
	2	0.07	0.32	5.90
	3	0.12	-0.15	6.14
	1	-0.01	-0.56	7.14
	2	-0.15	-0.41	6.42
	3	0.11	-0.44	6.59

We also looked at the relative importance of the utility model parameters by performing model comparisons. We compared 4 models based on combinations of 2 factors: PC and LP. According to the AIC scores (see Table 2), the best model was the one which included both LP and PC factors, followed by the PC-only model, and then by the LP-only model. The random-choice model came in last with the highest AIC score. The results of this model comparison show that both learning progress and positive feedback expectation factors provide substantive improvement to model likelihood compared to when these factors are included alone, or when neither of them is present. This is potentially important, as it provides some evidence for the role of relative competence kind of measure in autonomous exploration. We are planning to submit the work described about to a high impact peer-reviewed journal focusing on computational modeling of human behavior.

7.1.2. Experimental study of the role of intrinsic motivation in developmental psychology experiments and in the development of tool use

Participants: Pierre-Yves Oudeyer, Sébastien Forestier [correspondant], Laurianne Rat-Fisher.

Children are so curious to explore their environment that it can be hard to focus their attention on one given activity. Many experiments in developmental psychology evaluate particular skills of children by setting up a task that the child is encouraged to solve. However, children may sometimes be following their own motivation

Table 2. Model comparisons.

Model	AIC	$AIC - AIC_{min}$
LP + PC	568.99	-
PC	593.51	24.52
LP	658.46	89.47
Random	693.60	124.61

to explore the experimental setup or other things in the environment. We suggest that considering the intrinsic motivations of children in those experiments could help understanding their role in the learning of related skills and on long-term child development. To illustrate this idea, we reanalyzed and reinterpretd a typical experiment aiming to evaluate particular skills in infants. In this experiment run by Lauriane Rat-Fischer et al, 32 21-month old infants have to retrieve a toy stuck inside a tube, by inserting several blocks in sequence into the tube. In order to understand the mechanisms of the motivations of babies, we studied in detail their behaviors, goals and strategies in this experiment. We showed that their motivations are diverse and do not always coincide with the target goal expected and made salient by the experimenter. Intrinsically motivated exploration seems to play an important role in the observed behaviors and to interfere with the measured success rates. This new interpretation provides a motivation for studying curiosity and intrinsic motivations in robotic models.

7.2. Intrinsically Motivated Learning in Artificial Intelligence

7.2.1. Intrinsically Motivated Goal Exploration and Goal-Parameterized Reinforcement Learning

Participants: Sébastien Forestier, Pierre-Yves Oudeyer [correspondant], Olivier Sigaud, Cédric Colas, Adrien Laversanne-Finot, Rémy Portelas, Grgur Kovac.

7.2.1.1. Intrinsically Motivated Exploration of Modular Goal Spaces and the Emergence of Tool use

A major challenge in robotics is to learn goal-parametrized policies to solve multi-task reinforcement learning problems in high-dimensional continuous action and effect spaces. Of particular interest is the acquisition of inverse models which map a space of sensorimotor goals to a space of motor programs that solve them. For example, this could be a robot learning which movements of the arm and hand can push or throw an object in each of several target locations, or which arm movements allow to produce which displacements of several objects potentially interacting with each other, e.g. in the case of tool use. Specifically, acquiring such repertoires of skills through incremental exploration of the environment has been argued to be a key target for life-long developmental learning [54].

Recently, we developed a formal framework called "Intrinsically motivated goal exploration processes" (IMGEPs), enabling study agents that generate and sequence their own goals to learn world models and skill repertoirs, that is both more compact and more general than our previous models [82]. We experimented several implementations of these processes in a complex robotic setup with multiple objects (see Fig. 7), associated to multiple spaces of parameterized reinforcement learning problems, and where the robot can learn how to use certain objects as tools to manipulate other objects. We analyzed how curriculum learning is automated in this unsupervised multi-goal exploration process, and compared the trajectory of exploration and learning of these spaces of problems with the one generated by other mechanisms such as hand-designed learning curriculum, or exploration targeting a single space of problems, and random motor exploration. We showed that learning several spaces of diverse problems can be more efficient for learning complex skills than only trying to directly learn these complex skills. We illustrated the computational efficiency of IMGEPs as these robotic experiments use a simple memory-based low-level policy representations and search algorithm, enabling the whole system to learn online and incrementally on a Raspberry Pi 3.

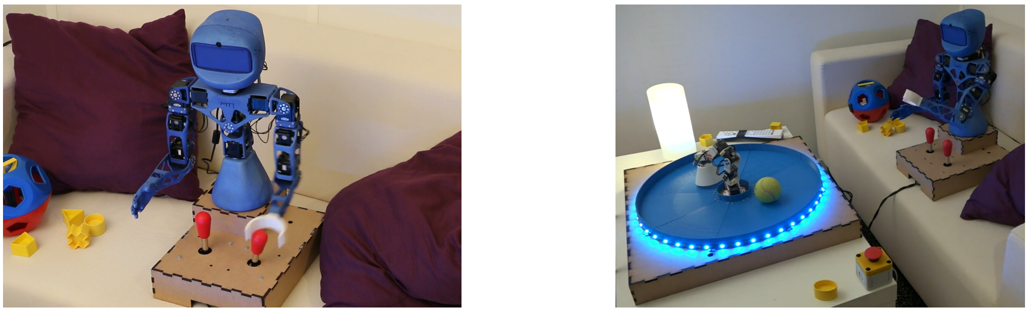


Figure 7. Robotic setup. Left: a Poppy Torso robot (the learning agent) is mounted in front of two joysticks. Right: full setup: a Poppy Ergo robot (seen as a robotic toy) is controlled by the right joystick and can hit a tennis ball in the arena which changes some lights and sounds.

In order to run many systematic scientific experiments in a shorter time, we scaled up this experimental setup to a platform of 6 identical Poppy Torso robots, each of them having the same environment to interact with. Every robot can run a different task with a specific algorithm and parameters each (see Fig. 8). Moreover, each Poppy Torso can also perceives the motion of a second Poppy Ergo robot, than can be used, this time, as a distractor performing random motions to complicate the learning problem. 12 top cameras and 6 head cameras can dump video streams during experiments, in order to record video datasets. This setup is now used to perform more experiments to compare different variants of curiosity-driven learning algorithms.

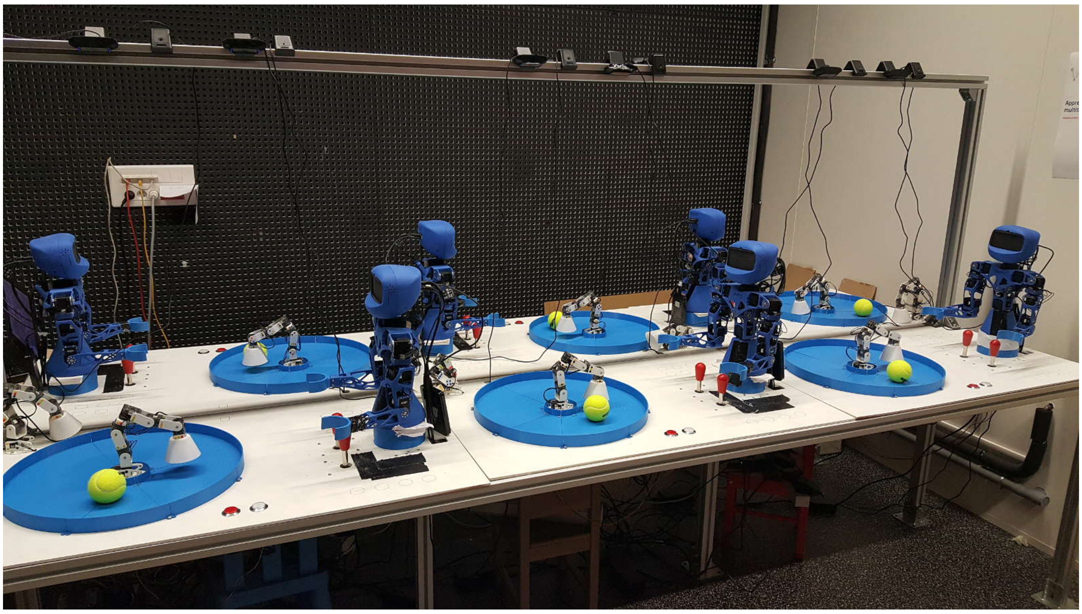


Figure 8. Platform of 6 robots with identical environment: joysticks, Poppy Ergo, ball in an arena, and a distractor. The central bar supports the 12 top cameras.

7.2.1.2. Leveraging the Malmo Minecraft platform to study IMGEP in rich simulations

We continued to leverage the Malmo platform to study curiosity-driven learning applied to multi-goal reinforcement learning tasks (https://github.com/Microsoft/malmo). The first step was to implement an environment called Malmo Mountain Cart (MMC), designed to be well suited to study multi-goal reinforcement learning (see figure [9]). We then showed that IMGEP methods could efficiently explore the MMC environment without any extrinsic rewards. We further showed that, even in the presence of distractors in the goal space, IMGEP methods still managed to discover complex behaviors such as reaching and swinging the cart, especially Active Model Babbling which ignored distractors by monitoring learning progress.

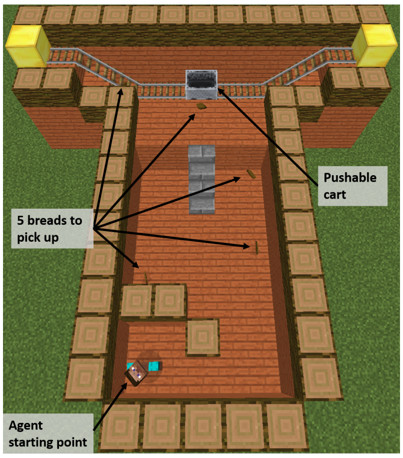


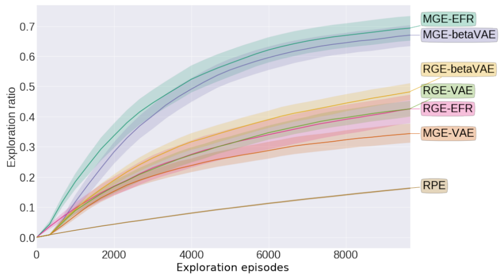
Figure 9. Malmo Mountain Cart. In this episodic environment the agent starts at the bottom left corner of the arena and is able to act on the environment using 2 continuous action commands: move and strafe. If the agent manages to get out of its starting area it may be able to collect items dispatched within the arena. If the agent manages to climb the stairs it may get close enough to the cart to move it along its railroad.

7.2.1.3. Unsupervised Learning of Modular Goal Spaces for Intrinsically Motivated Goal Exploration

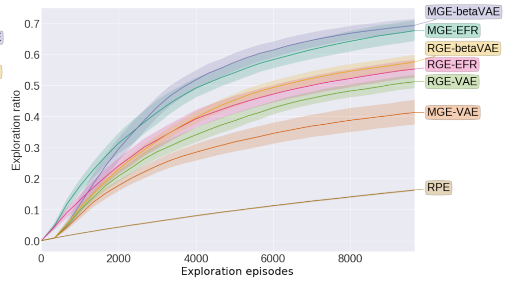
Intrinsically motivated goal exploration algorithms enable machines to discover repertoires of policies that produce a diversity of effects in complex environments. These exploration algorithms have been shown to allow real world robots to acquire skills such as tool use in high-dimensional continuous state and action spaces, as shown in previous sections. However, they have so far assumed that self-generated goals are sampled in a specifically engineered feature space, limiting their autonomy. We have proposed an approach using deep representation learning algorithms to learn an adequate goal space. This is a developmental 2-stage approach: first, in a perceptual learning stage, deep learning algorithms use passive raw sensor observations of world changes to learn a corresponding latent space; then goal exploration happens in a second stage by sampling goals in this latent space. We made experiments with a simulated robot arm interacting with an object, and we show that exploration algorithms using such learned representations can closely match, and even sometimes improve, the performance obtained using engineered representations. This work was presented at ICLR 2018 [136].

However, in the case of more complex environments containing multiple objects or distractors, an efficient exploration requires that the structure of the goal space reflects the one of the environment. We studied how the structure of the learned goal space using a representation learning algorithm impacts the exploration phase. In particular, we studied how disentangled representations compare to their entangled counterparts in a paper published at CoRL 2019 [101], associated with a blog post available at: https://openlab-flowers.inria.fr/t/discovery-of-independently-controllable-features-through-autonomous-goal-setting/494.

Those ideas were evaluated on a simple benchmark where a seven joints robotic arm evolves in an environment containing two balls. One of the ball can be grasped by the arm and moved around whereas the second one acts as a distractor: it cannot be grasped by the robotic arm and moves randomly across the environment.



(a) Small exploration noise ($\sigma = 0.05$)



(b) Large exploration noise ($\sigma = 0.1$)

Figure 10. Exploration ratio during exploration for different exploration noises. Architectures with disentangled representations as a goal space (βVAE) explore more than those with entangled representations (VAE). Similarly modular architectures (MGE) explore more than flat architecture (RGE).

Our results showed that using a disentangled goal space leads to better exploration performances than an entangled goal space: the goal exploration algorithm discovers a wider variety of outcomes in less exploration steps (see Figure 10). We further showed that when the representation is disentangled, one can leverage it by sampling goals that maximize learning progress in a modular manner. Lastly, we have shown that the measure of learning progress, used to drive curiosity-driven exploration, can be used simultaneously to discover abstract independently controllable features of the environment.

Finally, we experimented the applicability of those principles on a real-world robotic setup, where a 6-joint robotic arm learns to manipulate a ball inside an arena, by choosing goals in a space learned from its past experience, presented in this technical report: https://arxiv.org/abs/1906.03967.

7.2.1.4. Monolithic Intrinsically Motivated Modular Multi-Goal Reinforcement Learning

In this project we merged two families of algorithms. The first family is the population-based Intrinsically Motivated Goal Exploration Processes (IMGEP) developped in the team (see [83] for a presentation). In this family, autonomous learning agents sets their own goals and learn to reach them. Intrinsic motivation under the form of absolute learning progress is used to guide the selection of goals to target. In some variations of this framework, goals can be represented as coming from different *modules* or *tasks*. Intrinsic motivations are then used to guide the choice of the next task to target.

The second family encompasses goal-parameterized reinforcement learning algorithms. The first algorithm of this category used an architecture called Universal Value Function Approximators (UVFA), and enabled to train a single policy on an infinite number of goals (continuous goal spaces) [144] by appending the current goal to the input of the neural network used to approximate the value function and the policy. Using a single network allows to share weights among the different goals, which results in faster learning (shared representations). Later, HER [51] introduced a goal replay policy: the actual goal aimed at, could be replaced by a fictive goal when learning. This could be thought of as if the agent were pretending it wanted to reach a goal that it actually reached later on in the trajectory, in place of the true goal. This enables cross-goal learning and speeds up training. Finally, UNICORN [111] proposed to use UVFA to achieve multi-task learning with a discrete task-set.

In this project, we developed CURIOUS [33] (ICML 2019), an intrinsically motivated reinforcement learning algorithm able to achieve both multiple tasks and multiple goals with a single neural policy. It was tested on a custom multi-task, multi-goal environment adapted from the OpenAI Gym Fetch environments [61], see Figure 11. CURIOUS is inspired from the second family as it proposes an extension of the UVFA architecture. Here, the current task is encoded by a one-hot code corresponding to the task id. The goal is of size $\sum_{i=1}^{N} dim(\mathcal{G}_i)$ where $\mathcal{G}_i$ is the goal space corresponding to task T_i. All components are zeroed except the ones corresponding to the current goal g_i of the current task T_i, see Figure 12.

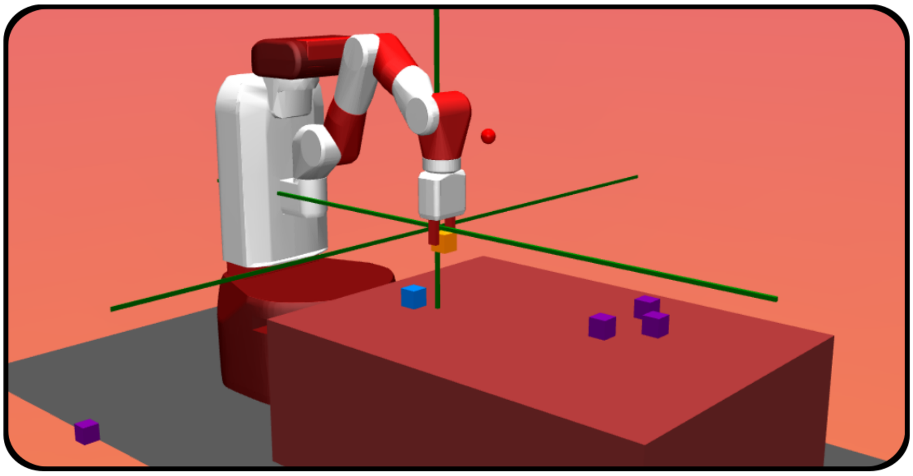


Figure 11. Custom multi-task and multi-goal environment to test the CURIOUS algorithm.

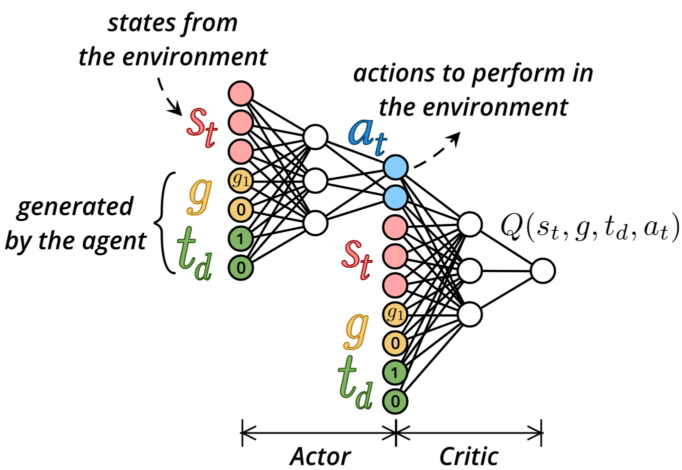


Figure 12. Architecture extended from Universal Value Function Approximators. In this example, the agent is targeting task T_1 among two tasks, each corresponding to a 1 dimension goal.

CURIOUS is also inspired from the first family, as it self-generates its own tasks and goals and uses a measure of learning progress to decide which task to target at any given moment. The learning progress is computed as the absolute value of the difference of non-overlapping window average of the successes or failures

$$LP_i(t) = \frac{|\sum_{\tau=t-2l}^{t-l} S_\tau - \sum_{\tau=t-l}^{t} S_\tau|}{2l},$$

where S_τ describes a success (1) or a failure (0) and l is a time window length. The learning progress is then used in two ways: it guides the selection of the next task to attempt, and it guides the selection of the task to replay. Cross-goal and cross-task learning are achieved by replacing the goal and/or task in the transition by another. When training on one combination of task and goal, the agent can therefore use this sample to learn about other tasks and goals. Here, we decide to replay and learn more on tasks for which the absolute learning progress is high. This helps for several reasons: 1) the agent does not focus on already learned tasks, as the corresponding learning progress is null, 2) the agent does not focus on impossible tasks for the same reason. The agent focuses more on tasks that are being learned (therefore maximizing learning progress), and on tasks that are being forgotten (therefore fighting the problem of forgetting). Indeed, when many tasks are learned in a same network, chances are tasks that are not being attempted often will be forgotten after a while.

In this project, we compare CURIOUS to two baselines: 1) a flat representation algorithm where goals are set from a multi dimensional space including all tasks (equivalent to HER); 2) a task-expert algorithm where a multi-goal UVFA expert policy is trained for each task. The results are shown in Figure 13.

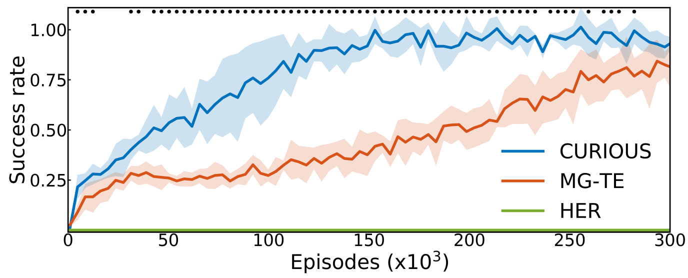


Figure 13. Comparison of CURIOUS to alternative algorithms.

7.2.1.5. Autonomous Multi-Goal Reinforcement Learning with Natural Language

This project follows the CURIOUS project on intrinsically motivated modular multi-goal reinforcement learning [33]. In the CURIOUS algorithm, we presented an agent able to tackle multiple goals of multiple types using a single controller. However, the agent needed to have access to the description of each of the goal types, and their associated reward functions. This represents a considerable amount of prior knowledge for the engineer to encode into the agent. In our new project, the agent builds its own representations of goals, can tackle a growing set of goals, and learns its own reward function, all this through interactions in natural language with a social partner.

The agent does not know any potential goal at first, and act randomly. As it reaches outcomes that are meaningful for the social partner, the social partner provides descriptions of the scene in natural language. The agent stores descriptions and corresponding states for two purposes. First it builds a list of potential goals, reaching back these outcomes that the social partner described. Second, it uses the combination of state and state description to learn a reward function, mapping current state and language descriptions to a binary feedback: 1 if the description is satisfied by the current state, 0 if not.

The agent sets goals to itself from the set of previously discovered descriptions, and is able to learn how to reach them thanks to its learned internal reward function. Concretely, the agent learns a set of 50+ goals from these interactions. We showed co-learning of the reward function and the policy did not produce consequent overhead compared to using an oracle reward function (see Figure 14). This project led to an article accepted at the NeurIPS workshop Visually Grounded Interaction and Language [35]. Current work aims at learning the language model mapping the description into a continuous goal space used as input to the policy and reward function using recurrent networks.

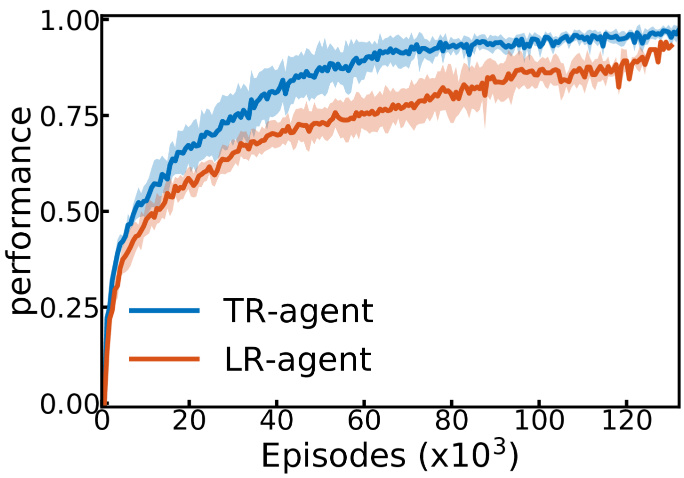


Figure 14. Comparison of performance of agents having access to the true oracle reward function (TR-agent), and agents co-learning policy and reward function (LR-agent).

7.2.1.6. Intrinsically Motivated Exploration and Multi-Goal RL with First-Person Images

The aim of this project is to create an exploration process in first-person 3D environments. Following the work presented in [121], [135], [157] the current algorithm is setup in a similar manner. The agent observes the environment in a first person manner and is given a goal to reach. Furthermore, the goal policy samples goals that encourage the agent to explore the environment.

Currently, there are two ways of representing and sampling goals. Following [157] the goal policy has a buffer of states previously visited by the agent and samples from this buffer the next goals as first person observations. In this setting a goal conditioned reward function is also learned in the form of a reachability network introduced in [142]. On the other hand, following [136], [121] and [135] one can learn a latent representation of a goal using an autoencoder (VAE) and then sample from this generative model or in the latent space. Then, we can use the L2 distance in the latent space as a reward function. The experiments are conducted on a set of Unity environments created in the team.

7.2.2. Teacher algorithms for curriculum learning of Deep RL in continuously parameterized environments

Participants: Remy Portelas [correspondant], Katja Hoffman, Pierre-Yves Oudeyer.

In this work we considered the problem of how a teacher algorithm can enable an unknown Deep Reinforcement Learning (DRL) student to become good at a skill over a wide range of diverse environments. To do so, we studied how a teacher algorithm can learn to generate a learning curriculum, whereby it sequentially samples parameters controlling a stochastic procedural generation of environments. Because it does not initially know the capacities of its student, a key challenge for the teacher is to discover which environments are easy, difficult or unlearnable, and in what order to propose them to maximize the efficiency of learning over the learnable ones. To achieve this, this problem is transformed into a surrogate continuous bandit problem where the teacher samples environments in order to maximize absolute learning progress of its student. We presented ALP-GMM (see figure 15), a new algorithm modeling absolute learning progress with Gaussian mixture models. We also adapted existing algorithms and provided a complete study in the context of DRL. Using parameterized variants of the BipedalWalker environment, we studied their efficiency to personalize a learning curriculum for different learners (embodiments), their robustness to the ratio of learnable/unlearnable environments, and their scalability to non-linear and high-dimensional parameter spaces. Videos and code are available at https://github.com/flowersteam/teachDeepRL.

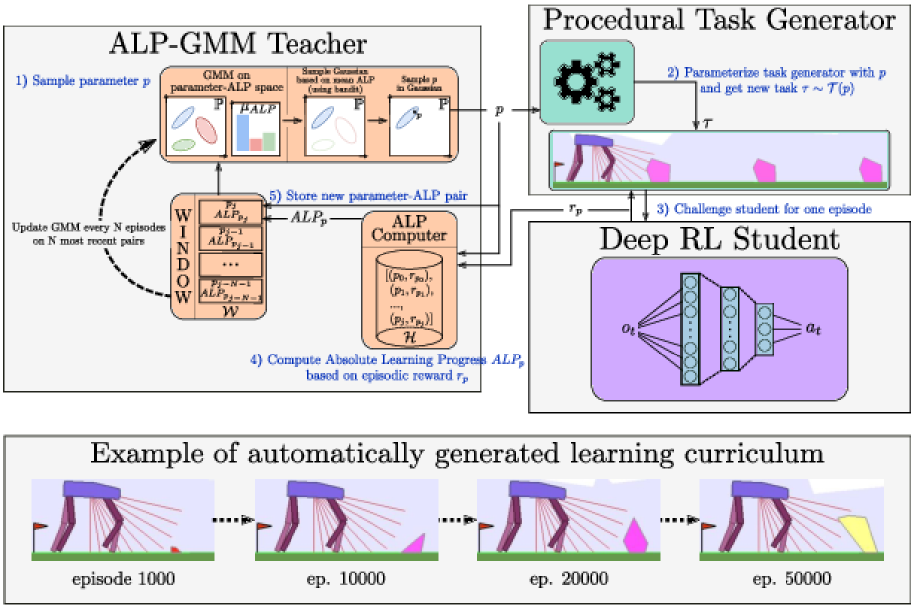


Figure 15. Schematic view of an ALP-GMM teacher's workflow

Overall, this work demonstrated that LP-based teacher algorithms could successfully guide DRL agents to learn in difficult continuously parameterized environments with irrelevant dimensions and large proportions of unfeasible tasks. With no prior knowledge of its student's abilities and only loose boundaries on the task space, ALP-GMM, our proposed teacher, consistently outperformed random heuristics and occasionally even expert-designed curricula (see figure 16). This work was presented at CoRL 2019 [38].

ALP-GMM, which is conceptually simple and has very few crucial hyperparameters, opens-up exciting perspectives inside and outside DRL for curriculum learning problems. Within DRL, it could be applied to previous work on autonomous goal exploration through incremental building of goal spaces [101]. In this case several ALP-GMM instances could scaffold the learning agent in each of its autonomously discovered goal spaces. Another domain of applicability is assisted education, for which current state of the art relies heavily on expert knowledge [68] and is mostly applied to discrete task sets.

7.3. Automated Discovery in Self-Organizing Systems

7.3.1. Curiosity-driven Learning for Automated Discovery of Physico-Chemical Structures

Participants: Chris Reinke [correspondant], Mayalen Etcheverry, Pierre-Yves Oudeyer.

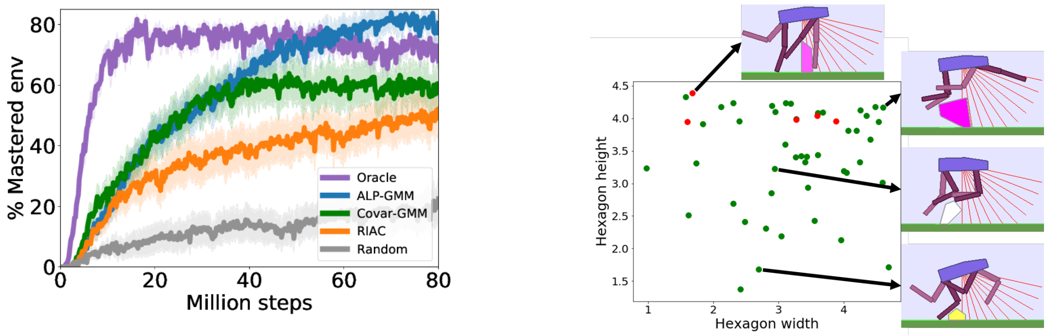


Figure 16. ***Teacher-Student approaches in Hexagon Tracks.Left:*** *Evolution of mastered tracks for Teacher-Student approaches in Hexagon Tracks. 32 seeded runs (25 for Random) of 80 Millions steps where performed for each condition. The mean performance is plotted with shaded areas representing the standard error of the mean.* ***Right:*** *A visualization of which track distributions of the test-set are mastered (i.e $r_t > 230$, shown by green dots) by an ALP-GMM run after 80 million steps.*

7.3.1.1. Introduction

Intrinsically motivated goal exploration algorithms (IMGEPs) enable machines to discover repertoires of action policies that produce a diversity of effects in complex environments. In robotics, these exploration algorithms have been shown to allow real world robots to acquire skills such as tool use [81] [55]. In other domains such as chemistry and physics, they open the possibility to automate the discovery of novel chemical or physical structures produced by complex dynamical systems [134]. However, they have so far assumed that self-generated goals are sampled in a specifically engineered feature space, limiting their autonomy. Recent work has shown how unsupervised deep learning approaches could be used to learn goal space representations [136] but they have used precollected data to learn the representations. This project studies how IMGEPs can be extended and used for automated discovery of behaviours of dynamical systems in physics or chemistry without using assumptions or knowledge about such systems.

As a first step towards this goal we choose Lenia [66], a simulated high-dimensional complex dynamical system, as a target system. Lenia is a continuous cellular automaton where diverse visual structures can self-organize (Fig.17, c). It consists of a two-dimensional grid of cells $A \in [0,1]^{256\times 256}$ where the state of each cell is a real-valued scalar activity $A^t(x) \in [0,1]$. The state of cells evolves over discrete time steps t. The activity change is computed by integrating the activity of neighbouring cells. Lenia's behavior is controlled by its initial pattern $A^{t=1}$ and several settings that control the dynamics of the activity change. Lenia can produce diverse patterns with different dynamics. Most interesting, spatially localized coherent patterns that resemble in their shapes microscopic *animals* can emerge. Our goal was to develop methods that allow to explore a high diversity of such animal patterns.

We could successfully accomplish this goal [30] based on two key contributions of our research: 1) the usage of compositional pattern producing networks (CPPNs) for the generation of initial states for Lenia, and 2) the development of a novel IMGEP algorithm that learns goal representations online during the exploration of the system.

7.3.1.2. 1) CPPNs for the generation of initial states

A key role in the generation of patterns in dynamical systems is their initial state $A^{t=1}$. IMGEPs sample these initial states and apply random perturbations to them during the exploration. For Lenia this state is a two-dimensional grid with 256×256 cells. Performing directly a random sampling of the 256×256 grid cells results in initial patterns that resemble white noise. Such random states result mainly in the emergence of global patterns that spread over the whole state space, complicating the search for spatially localized patterns.

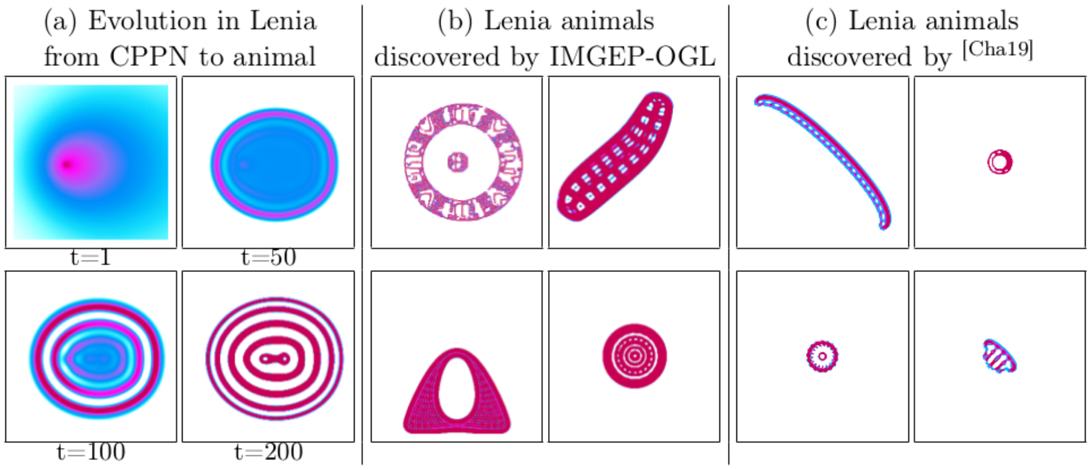


Figure 17. Example patterns produced by the Lenia system. Illustration of the dynamical morphing from an initial CPPN image to an animal (a). The automated discovery (b) is able to find similar complex animals as a human-expert manual search (c) by [66].

We solved the sampling problem for the initial states by using compositional pattern producing networks (CPPNs) [148]. CPPNs are recurrent neural networks that allow the generation of structured initial states (Fig.17, a). The CPPNs are used as part of the system parameters which are explored by the algorithms. They are defined by their network structure (number of neurons, connections between neurons) and their connection weights. They include a mechanism for random mutation of the weights and structure.

7.3.1.3. 2) IMGEP for Online Learning of Goal Space Representations

We proposed an online goal space learning IMGEP (IMGEP-OGL), which learns the goal space incrementally during the exploration process. A variational autoencoder (VAE) is used to encode Lenia patterns into a 8-dimensional latent representation used as goal space. The training procedure of the VAE is integrated in the goal sampling exploration process by first initializing the VAE with random weights. The VAE network is then trained every K explorations for E epochs on the previously idetnfied patterns during the exploration.

7.3.1.4. Experiments

We evaluated the performance of the novel IMGEP-OGL to other exploration algorithms by comparing the diversity of their identified patterns. Diversity is measured by the spread of the exploration in an *analytic behavior space*. This space is defined by a latent representation space that was build through the training of a VAE to learn the important features over a very large dataset of Lenia patterns identified during the many experiments over all evaluated algorithms. We then augmented that space by concatenating hand-defined features. Each identified Lenia pattern is represented by a specific point in this space. The space was then discretized in a fixed number of areas/bins of equal size. The final diversity measure of each algorithm is the number of areas/bins in which at least one explored pattern exists.

We compared different exploration algorithms to the novel IMGEP-OGL: 1) Random exploration of system parameters, 2) IMGEP-HGS: IMGEP with a hand-defined goal space, 3) IMGEP-PGL: IMGEP with a learned goal space via an VAE by a precollected dataset of Lenia patterns, and 4) IMGEP-RGS: IMGEP with a VAE with random weights that defines the goal space.

The system parameters θ consisted of a CPPN that generates the initial state $A^{t=1}$ for Lenia and 6 further settings defining Lenia's dynamics: $\theta = [\text{CPPN} \rightarrow A^{t=1}, R, T, \mu, \sigma, \beta_1, \beta_2, \beta_3]$. The CPPNs were initialized and mutated by a random process that defines their structure and connection weights as done. The random initialization of the other Lenia settings was done by an uniform distribution and their mutation by a Gaussian distribution around the original values.

7.3.1.5. Results

The diversity of identified patterns in the analytic behavior space show that IMGEP approaches with learned goal spaces via VAEs (PGL, OGL) could identify the highest diversity of patterns overall (Fig. 18, a). They were followed by the IMGEP with a hand-defined goal space (HGS). The lowest performance had the random exploration and the IMGEP with a random goal space (RGS). The advantage of learned goals space approaches (PGL, OGL) over all other approaches was even stronger for the diversity of animal patterns, i.e. the main goal of our exploration (Fig. 18, b).

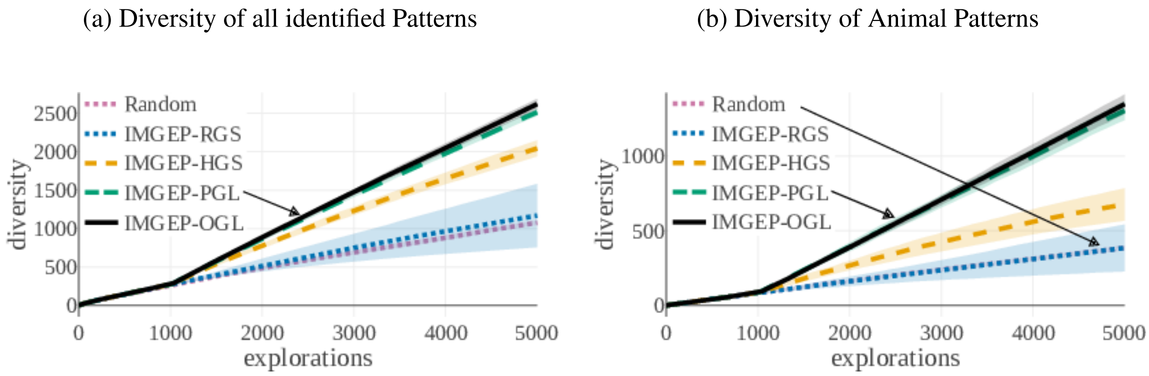


Figure 18. (a) All IMGEPs reach a higher diversity in the analytic behavior space over all patterns than random search. (b) IMGEPs with a learned goal space are especially successful in identifying a diversity of animal patterns. Depicted is the average diversity ($n = 10$) with the standard deviation as shaded area (for some not visible because it is too small).

7.3.1.6. Conclusion

Our goal was to investigate new techniques based on intrinsically motivated goal exploration for the automated discovery of patterns and behaviors in complex dynamical systems. We introduced a new algorithm (IMGEP-OGL) which is capable of learning unsupervised goal space representations during the exploration of an unknown system. Our results for Lenia, a high-dimensional complex dynamical system, show its superior performance over hand-defined goal spaces or random exploration. It shows the same performance as a learned goal space based on precollected data, showing that such a precollection of data is not necessary. We furthermore introduced the usage of CPPNs for the successful initialization of the intial states of the dynamical systems. Both advances allowed us to explore an unknown and high-dimensional dynamical system which shares many similarities with different physical or chemical systems.

7.4. Representation Learning

7.4.1. State Representation Learning in the Context of Robotics

Participants: David Filliat [correspondant], Natalia Diaz Rodriguez, Timothee Lesort, Antonin Raffin, René Traoré, Ashley Hill, Te Sun, Lu Lin, Guanghang Cai, Bunthet Say.

During the DREAM project, we participated in the development of a conceptual framework of open-ended lifelong learning [77] based on the idea of representational re-description that can discover and adapt the states, actions and skills across unbounded sequences of tasks.

In this context, State Representation Learning (SRL) is the process of learning without explicit supervision a representation that is sufficient to support policy learning for a robot. We have finalized and published a large state-of-the-art survey analyzing the existing strategies in robotics control [103], and we developed unsupervised methods to build representations with the objective to be minimal, sufficient, and that encode the relevant information to solve the task. More concretely, we used the developed and open sourced[0] the S-RL toolbox [137] containing baseline algorithms, data generating environments, metrics and visualization tools for assessing SRL methods. Part of this study is the [105] where we present a robustness analysis on Deep unsupervised state representation learning with robotic priors loss functions.

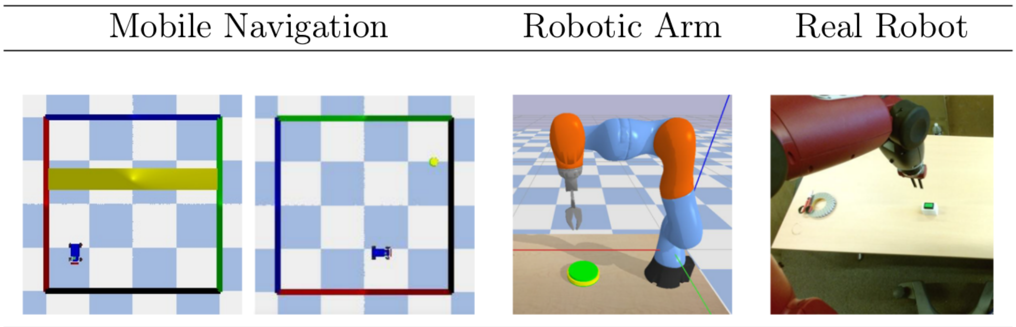


Figure 19. Environments and datasets for state representation learning.

The environments proposed in Fig. 19 are variations of two environments: a 2D environment with a mobile robot and a 3D environment with a robotic arm. In all settings, there is a controlled robot and one or more targets (that can be static, randomly initialized or moving). Each environment can either have a continuous or discrete action space, and the reward can be sparse or shaped, allowing us to cover many different situations.

The evaluation and visualization tools are presented in Fig. 20 and make it possible to qualitatively verify the learned state space behavior (e.g., the state representation of the robotic arm dataset is expected to have a continuous and correlated change with respect to the arm tip position).

We also proposed a new approach that consists of learning a state representation that is split into several parts where each optimizes a fraction of the objectives. In order to encode both target and robot positions, auto-encoders, reward and inverse model losses are used.

The latest work on decoupling feature extraction from policy learning, was presented at the SPIRL workshop at ICLR2019 in New Orleans, LA [138]. We assessed the benefits of state representation learning in goal based robotic tasks, using different self-supervised objectives.

Because combining objectives into a single embedding is not the only option to have features that are *sufficient* to solve the tasks, by stacking representations, we favor *disentanglement* of the representation and prevent objectives that can be opposed from cancelling out. This allows a more stable optimization. Fig. 21 shows the split model where each loss is only applied to part of the state representation.

As using the learned state representations in a Reinforcement Learning setting is the most relevant approach to evaluate the SRL methods, we use the developed S-RL framework integrated algorithms (A2C, ACKTR, ACER, DQN, DDPG, PPO1, PPO2, TRPO) from Stable-Baselines [92], Augmented Random Search (ARS), Covariance Matrix Adaptation Evolutionary Strategy (CMA-ES) and Soft Actor Critic (SAC). Due to its stability, we perform extensive experiments on the proposed datasets using PPO and states learned with the approaches described in [137] along with ground truth (GT).

[0] https://github.com/araffin/robotics-rl-srl

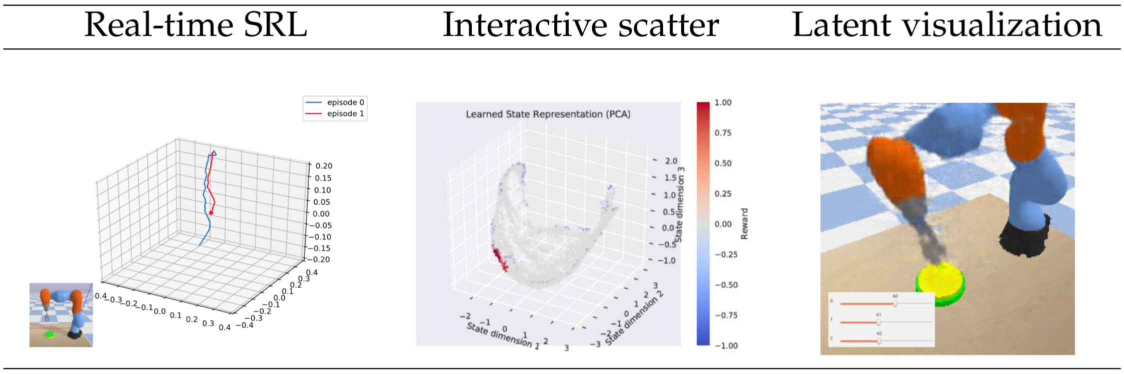


Figure 20. Visual tools for analysing SRL; Left: Live trajectory of the robot in the state space. Center: 3D scatter plot of a state space; clicking on any point displays the corresponding observation. Right: reconstruction of the point in the state space defined by the sliders.

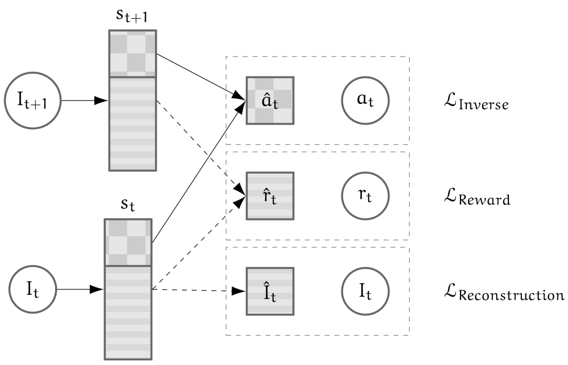


Figure 21. SRL Splits model: combines a reconstruction of an image I, a reward (r) prediction and an inverse dynamic models losses, using two splits of the state representation s. Arrows represent model learning and inference, dashed frames represent losses computation, rectangles are state representations, circles are real observed data, and squares are model predictions.

Ground Truth States	Learned States	RL Performance

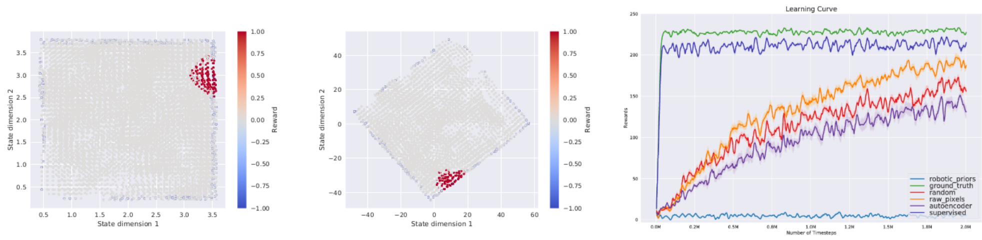


Figure 22. Ground truth states (left), states learned (Inverse and Forward) (center), and RL performance evaluation (PPO) (right) for different baselines in the mobile robot environment. Colour denotes the reward, red for positive, blue for negative and grey for null reward (left and center).

Table 22 illustrates the qualitative evaluation of a state space learned by combining forward and inverse models on the mobile robot environment. It also shows the performance of PPO algorithm based on the states learned by several baseline approaches.

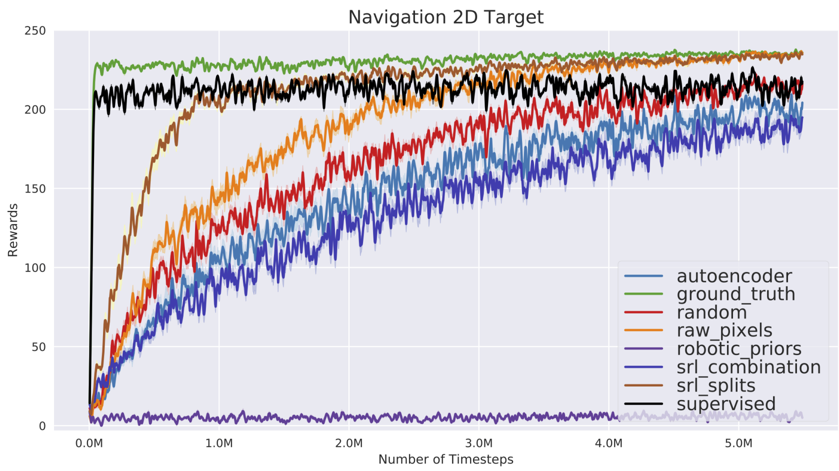


Figure 23. Performance (mean and standard error for 10 runs) for PPO algorithm for different state representations learned in Navigation 2D random target environment.

We verified that our new approach (described in Task 2.1) makes it possible for reinforcement learning to converge faster towards the optimal performance in both environments with the same amount of budget timesteps. Learning curve in Fig. 23 shows that our unsupervised state representation learned with the split model even improves on the supervised case.

7.4.2. Continual learning

Participants: David Filliat [correspondant], Natalia Díaz Rodríguez, Timothee Lesort, Hugo Caselles-Dupré.

Continual Learning (CL) algorithms learn from a stream of data/tasks continuously and adaptively through time to better enable the incremental development of ever more complex knowledge and skills. The main problem that CL aims at tackling is catastrophic forgetting [115], i.e., the well-known phenomenon of a neural network experiencing a rapid overriding of previously learned knowledge when trained sequentially on new data. This is an important objective quantified for assessing the quality of CL approaches, however, the almost exclusive focus on catastrophic forgetting by continual learning strategies, lead us to propose a set of comprehensive, implementation independent metrics accounting for factors we believe have practical implications worth considering with respect to the deployment of real AI systems that learn continually, and in "Non-static" machine learning settings. In this context we developed a framework and a set of comprehensive metrics [78] to tame the lack of consensus in evaluating CL algorithms. They measure Accuracy (A), Forward and Backward (*/remembering*) knowledge transfer (FWT, BWT, REM), Memory Size (MS) efficiency, Samples Storage Size (SSS), and Computational Efficiency (CE). Results on iCIFAR-100 classification sequential class learning is in Table 24.

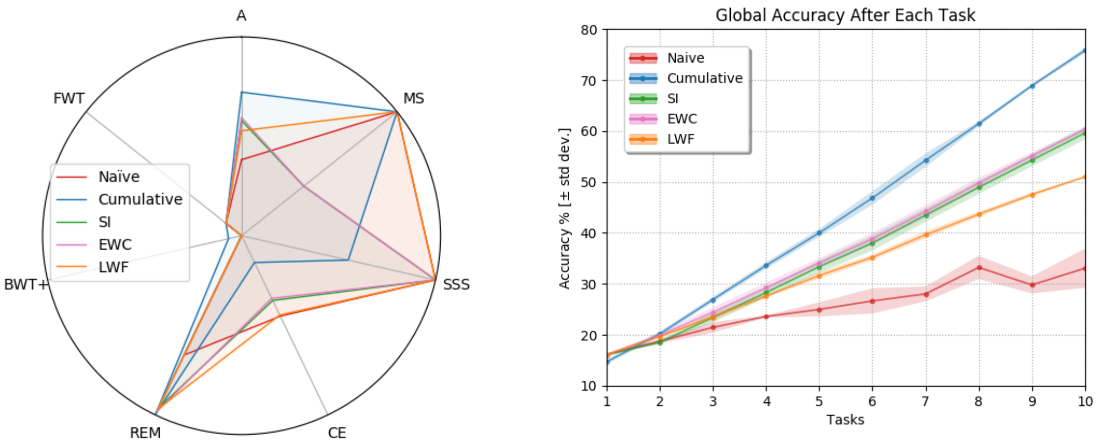


Figure 24. (left) Spider chart: CL metrics per strategy (larger area is better) and (right) Accuracy per CL strategy computed over the fixed test set.

Generative models can also be evaluated from the perspective of Continual learning which we investigated in our work [102]. This work aims at evaluating and comparing generative models on disjoint sequential image generation tasks. We study the ability of Generative Adversarial Networks (GANS) and Variational Auto-Encoders (VAEs) and many of their variants to learn sequentially in continual learning tasks. We investigate how these models learn and forget, considering various strategies: rehearsal, regularization, generative replay and fine-tuning. We used two quantitative metrics to estimate the generation quality and memory ability. We experiment with sequential tasks on three commonly used benchmarks for Continual Learning (MNIST, Fashion MNIST and CIFAR10). We found (see Figure 26) that among all models, the original GAN performs best and among Continual Learning strategies, generative replay outperforms all other methods. Even if we found satisfactory combinations on MNIST and Fashion MNIST, training generative models sequentially on CIFAR10 is particularly instable, and remains a challenge. This work has been published at the NIPS workshop on Continual Learning 2018.

Another extension of previous section on state representation learning (SRL) to the continual learning setting is in our paper [65]. This work proposes a method to avoid catastrophic forgetting when the environment changes using generative replay, i.e., using generated samples to maintain past knowledge. State representations are learned with variational autoencoders and automatic environment change is detected through VAE

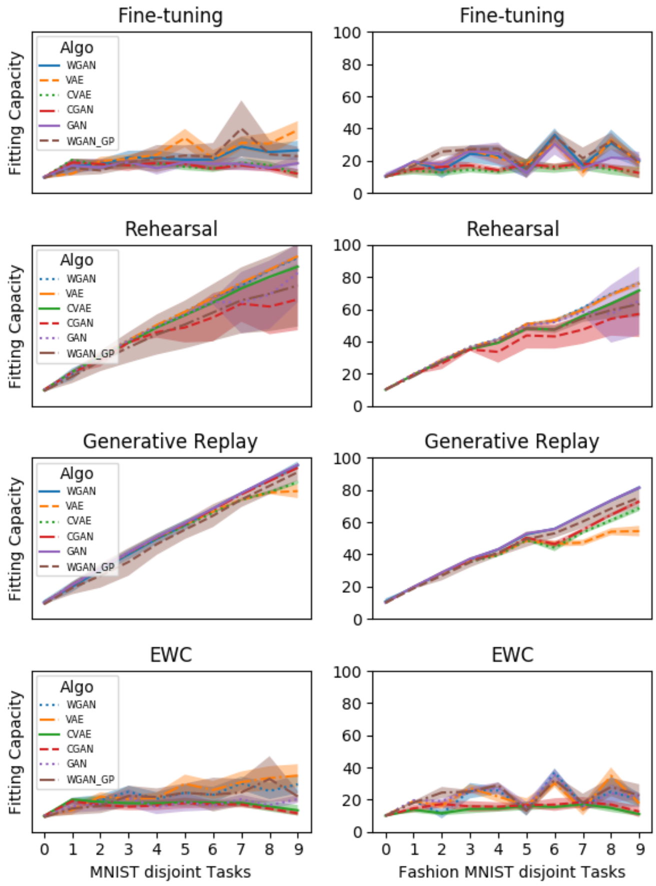


Figure 25. Means and standard deviations over 8 seeds of Fitting Capacity metric evaluation of VAE, CVAE, GAN, CGAN and WGAN. The four considered CL strategies are: Fine Tuning, Generative Replay, Rehearsal and EWC. The setting is 10 disjoint tasks on MNIST and Fashion MNIST.

reconstruction error. Results show that using a state representation model learned continually for RL experiments is beneficial in terms of sample efficiency and final performance, as seen in Figure 26. This work has been published at the NIPS workshop on Continual Learning 2018 and is currently being extended.

The experiments were conducted in an environment built in the lab, called Flatland [64]. This is a lightweight first-person 2-D environment for Reinforcement Learning (RL), designed especially to be convenient for Continual Learning experiments. Agents perceive the world through 1D images, act with 3 discrete actions, and the goal is to learn to collect edible items with RL. This work has been published at the ICDL-Epirob workshop on Continual Unsupervised Sensorimotor Learning 2018, and was accepted as oral presentation.

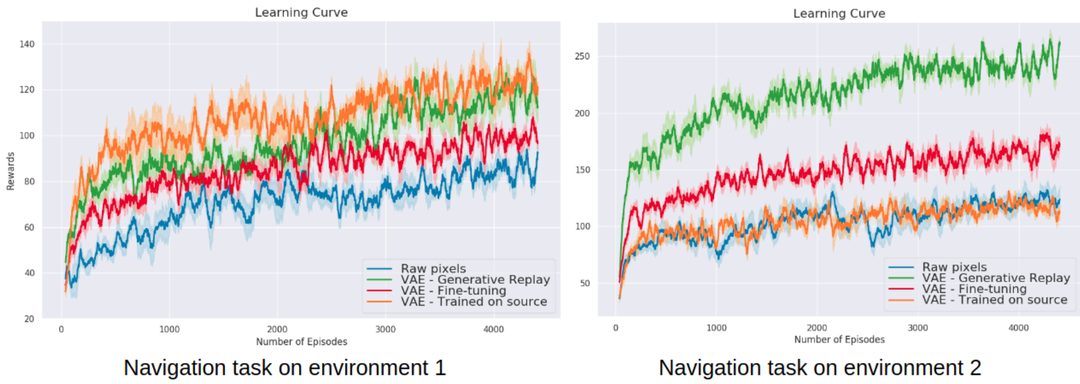


Figure 26. Mean reward and standard error over 5 runs of RL evaluation using PPO with different types of inputs. Fine-tuning and Generative Replay models are trained sequentially on the first and second environment, and then used to train a policy for both tasks. Generative Replay outperforms all other methods. It shows the need for continually learning features in State Representation Learning in settings where the environment changes.

In the last year, we published a survey on continual learning models, metrics and contributed a CL framework to categorize the approaches on this area [104]. Figure 27 shows the different approaches cited and the strategies proposed and a small subset of examples analyzed.

We also worked on validating a distillation approach for multitask learning in a continual learning reinforcement learning setting [152], [153].

Applying State Representation Learning (SRL) into a continual learning setting of reinforcement learning was possible by learning a compact and efficient representation of data that facilitates learning a policy. The proposed a CL algorithm based on distillation does not manually need to be given a task indicator at test time, but learns to infer the task from observations only. This allows to successfully apply the learned policy on a real robot.

We present 3 different 2D navigation tasks to a 3 wheel omni-directional robot to be learned to be solved sequentially. The robot has first access to task 1 only, and then to task 2 only, and so on. It should learn a single policy that solves all tasks and be applicable in a real life scenario. The robot can perform 4 high level discrete actions (move left/right, move up/down). The tasks where the method was validated are in Fig. 28:

Task 1: Target Reaching (TR): Reaching a red target randomly positioned.

Task 2: Target Circling (TC): Circling around a fixed blue target.

Task 3: Target Escaping (TE): Escaping a moving robot.

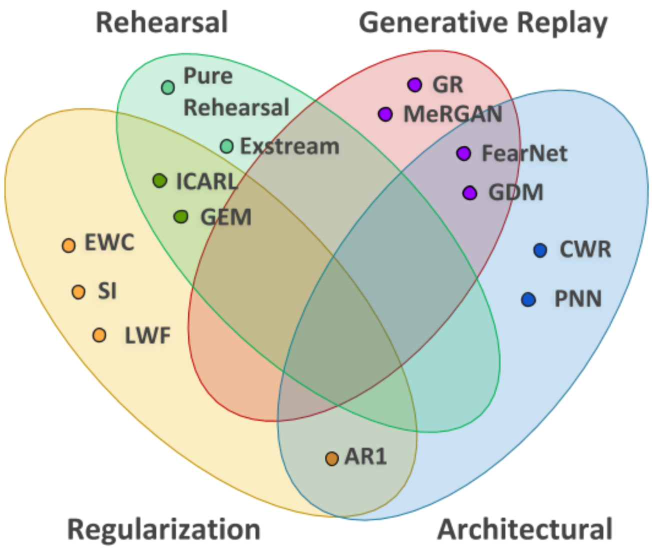


Figure 27. Venn diagram of some of the most popular CL strategies w.r.t the main approaches in the literature (CWR,PNN EWC, SI, LWF, ICARL, GEM, FearNet, GDM, ExStream, GR, MeRGAN, and AR1. Rehearsal and Generative Replay upper categories can be seen as a subset of replay strategies. Better viewed in color [104].

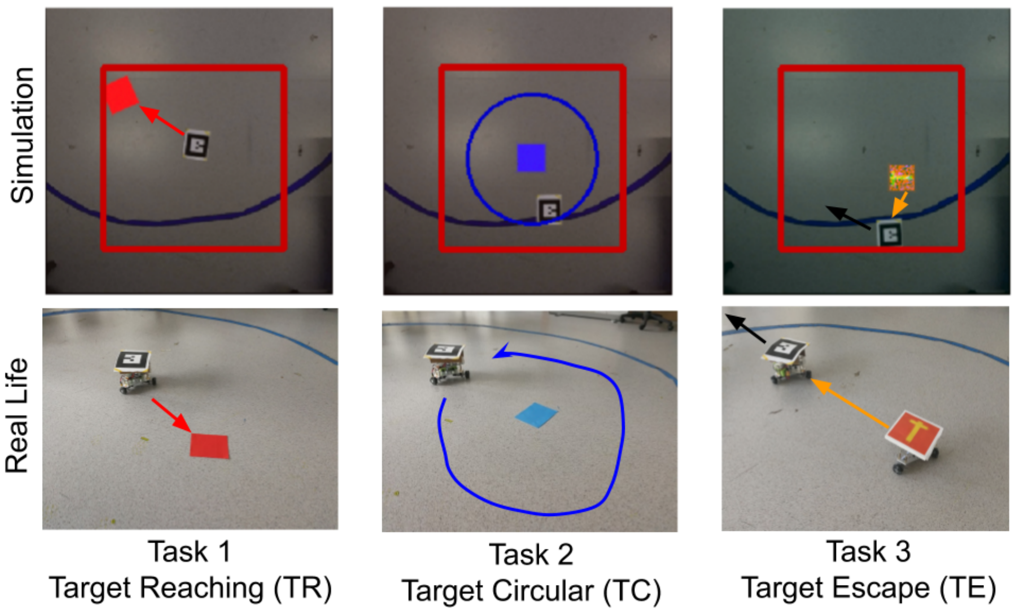


Figure 28. The three tasks, in simulation (top) and in real life (bottom), sequentially experienced. Learning is performed in simulation, the real life setting is only used at test time.

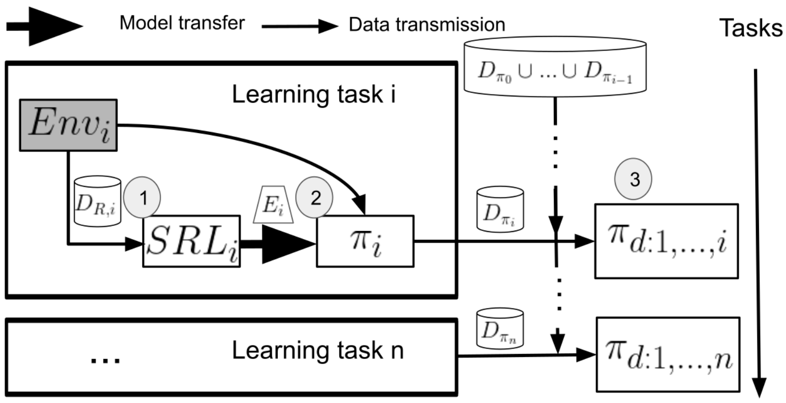


Figure 29. White cylinders are for datasets, gray squares for environments, and white squares for learning algorithms, whose name correspond to the model trained. Each task i is learned sequentially and independently by first generating a dataset $D_{R,i}$ with a random policy to learn a state representation with an encoder E_i with an SRL method (1), then we use E_i and the environment to learn a policy π_i in the state space (2). Once trained, π_i is used to create a distillation dataset D_{π_i} that acts as a memory of the learned behaviour. All policies are finally compressed into a single policy $\pi_{d:1,...,i}$ by merging the current dataset D_{π_i} with datasets from previous tasks $D_{\pi_1} \cup ... \cup D_{\pi_{i-1}}$ and using distillation (3).

DisCoRL (Distillation for Continual Reinforcement learning) is a modular, effective and scalable pipeline for continual RL. This pipeline uses policy distillation for learning without forgetting, without access to previous environments, and without task labels in order to transfer policies into real life scenarios [152]. It was presented as an approach for continual reinforcement learning that sequentially summarizes different learned policies into a dataset to distill them into a student model. Some loss in performance may occur while transferring knowledge from teacher to student, or while transferring a policy from simulation to real life. Nevertheless, the experiments show promising results when learning tasks sequentially, in simulated environments and real life settings.

The overview of DisCoRL full pipeline for Continual Reinforcement Learning is in Fig. 29.

7.4.3. Disentangled Representation Learning for agents

Participants: Hugo Caselles-Dupré [correspondant], David Filliat.

Finding a generally accepted formal definition of a disentangled representation in the context of an agent behaving in an environment is an important challenge towards the construction of data-efficient autonomous agents. Higgins et al. (2018) recently proposed Symmetry-Based Disentangled Representation Learning, a definition based on a characterization of symmetries in the environment using group theory. We build on their work and make observations, theoretical and empirical, that lead us to argue that Symmetry-Based Disentangled Representation Learning cannot only be based on static observations: agents should interact with the environment to discover its symmetries.

Our research was published in NeuRIPS 2019 [32] at Vancouver, Canada.

7.5. Tools for Understanding Deep Learning Systems

7.5.1. Explainable Deep Learning

Participants: Natalia Díaz Rodríguez [correspondant], Adrien Bennetot.

Together with Segula Technologies and Sorbonne Université, ENSTA Paris has been working on eXplainable Artificial Intelligence (XAI) in order to make machine learning more interpretable. While opaque decision systems such as Deep Neural Networks have great generalization and prediction skills, their functioning does not allow obtaining detailed explanations of their behaviour. The objective is to fight the trade-off between performance and explainability by combining connectionist and symbolic paradigms [47].

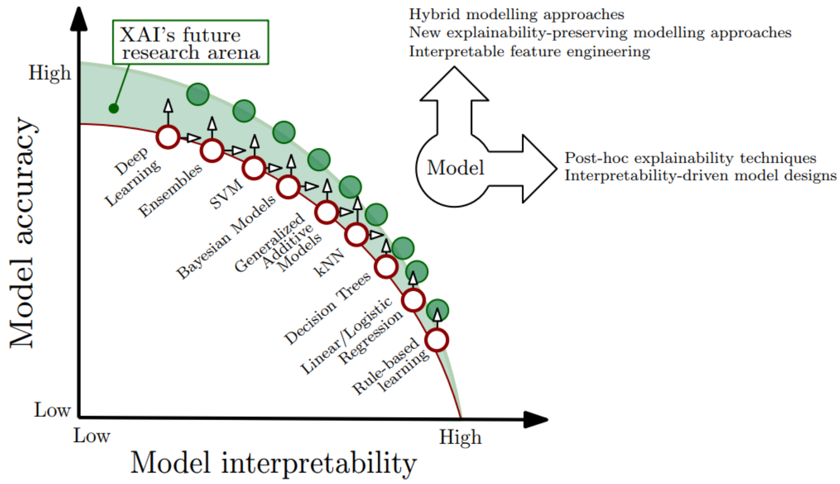


Figure 30. Trade-off between model interpretability and performance, and a representation of the area of improvement where the potential of XAI techniques and tools resides [46].

Broad consensus exists on the importance of interpretability for AI models. However, since the domain has only recently become popular, there is no collective agreement on the different definitions and challenges that constitute XAI. The first step is therefore to summarize previous efforts made in this field. We presented a taxonomy of XAI techniques in [46] and we are currently working on a prediction model that generates itself an explanation of its rationale in natural language while keeping performance as close as possible to the the state of the art [47].

7.5.2. Methods for Statistical Comparison of RL Algorithms

Participants: Cédric Colas [correspondant], Pierre-Yves Oudeyer, Olivier Sigaud.

Following a first article in 2018 [71], we pursued the objective of providing key tools to robustly compare reinforcement learning (RL) algorithms to practioners and researchers. In this year's extension, we compiled a hitchhicker's guide for statistical comparisons of RL algorithms. In particular, we provide a list of statistical tests adapted to compare RL algorithms and compare them in terms of false positive rate and statistial power. In particular, we study the robustness of these tests when their assumptions are violated (non-normal distributions of performances, different distributions, unknown variance, unequal variances etc). We provided an extended study using data from synthetic performance distributions, as well as empirical distributions obtained from running state-of-the-art RL algorithms (TD3 [84] and SAC [88]). From these results we draw a selection of advice for researchers. This study led to an article accepted at the ICLR conference workshop on Reproducibility in Machine Learning [34], to be sumitted to the Neural Networks journal.

7.5.3. Knowledge engineering tools for neural-symbolic learning

Participants: Natalia Díaz Rodríguez [correspondant], Adrien Bennetot.

Symbolic artificial intelligence methods are experiencing a come-back in order to provide deep representation methods the explainability they lack. In this area, a survey on RDF stores to handle ontology-based triple databases has been contributed [97], as well as the use of neural-symbolic tools that aim at integrating both neural and symbolic representations [58].

7.6. Applications in Educational Technologies

7.6.1. Machine Learning for Adaptive Personalization in Intelligent Tutoring Systems

Participants: Pierre-Yves Oudeyer [correspondant], Benjamin Clément, Didier Roy, Helene Sauzeon.

7.6.1.1. The Kidlearn project

Kidlearn is a research project studying how machine learning can be applied to intelligent tutoring systems. It aims at developing methodologies and software which adaptively personalize sequences of learning activities to the particularities of each individual student. Our systems aim at proposing to the student the right activity at the right time, maximizing concurrently his learning progress and its motivation. In addition to contributing to the efficiency of learning and motivation, the approach is also made to reduce the time needed to design ITS systems.

We continued to develop an approach to Intelligent Tutoring Systems which adaptively personalizes sequences of learning activities to maximize skills acquired by students, taking into account the limited time and motivational resources. At a given point in time, the system proposes to the students the activity which makes them progress faster. We introduced two algorithms that rely on the empirical estimation of the learning progress, **RiARiT** that uses information about the difficulty of each exercise and **ZPDES** that uses much less knowledge about the problem.

The system is based on the combination of three approaches. First, it leverages recent models of intrinsically motivated learning by transposing them to active teaching, relying on empirical estimation of learning progress provided by specific activities to particular students. Second, it uses state-of-the-art Multi-Arm Bandit (MAB) techniques to efficiently manage the exploration/exploitation challenge of this optimization process. Third, it leverages expert knowledge to constrain and bootstrap initial exploration of the MAB, while requiring only coarse guidance information of the expert and allowing the system to deal with didactic gaps in its knowledge. The system was evaluated in several large-scale experiments relying on a scenario where 7-8 year old schoolchildren learn how to decompose numbers while manipulating money [68]. Systematic experiments were also presented with simulated students.

7.6.1.2. Kidlearn Experiments 2018-2019: Evaluating the impact of ZPDES and choice on learning efficiency and motivation

An experiment was held between mars 2018 and July 2019 in order to test the Kidlearn framework in classrooms in Bordeaux Metropole. 600 students from Bordeaux Metropole participated in the experiment. This study had several goals. The first goal was to evaluate the impact of the Kidlearn framework on motivation and learning compared to an Expert Sequence without machine learning. The second goal was to observe the impact of using learning progress to select exercise types within the ZPDES algorithm compared to a random policy. The third goal was to observe the impact of combining ZPDES with the ability to let children make different kinds of choices during the use of the ITS. The last goal was to use the psychological and contextual data measures to see if correlation can be observed between the students psychological state evolution, their profile, their motivation and their learning. The different observations showed that generally, algorithms based on ZPDES provided a better learning experience than an expert sequence. In particular, they provide a better motivating and enriching experience to self-determined students. Details of these new results, as well as the overall results of this project, are presented in Benjamin Clément PhD thesis [69] and are currently being processed to be published.

7.6.1.3. *Kidlearn and Adaptiv'Math*

The algorithms developed during the Kidlearn project and Benjamin Clement thesis [69] are being used in an innovation partnership for the development of a pedagogical assistant based on artificial intelligence intended for teachers and students of cycle 2. The algorithms are being written in typescript for the need of the project. The expertise of the team in creating the pedagogical graph and defining the graph parameters used for the algorithms is also a crucial part of the role of the team for the project. One of the main goal of the team here is to transfer technologies developed in the team in a project with the perspective of industrial scaling and see the impact and the feasibility of such scaling.

7.6.1.4. *Kidlearn for numeracy skills with individuals with autism spectrum disorders*

Few digital interventions targeting numeracy skills have been evaluated with individuals with autism spectrum disorder (ASD) [114]. Yet, some children and adolescents with ASD have learning difficulties and/or a significant academic delay in mathematics. While ITS are successfully developed for typically developed students to personnalize learning curriculum and then to foster the motivation-learning coupling, they are not or fewly proposed today to student with specific needs. The objective of this pilot study is to test the feasibility of a digital intervention using an STI with high school students with ASD and/or intellectual disability. This application (KidLearn) provides calculation training through currency exchange activities, with a dynamic exercise sequence selection algorithm (ZPDES). 24 students with ASD and/or DI enrolled in specialized classrooms were recruited and divided into two groups: 14 students used the KidLearn application, and 10 students received a control application. Pre-post evaluations show that students using KidLearn improved their calaculation performance, and had a higher level of motivation at the end of the intervention than the control group. These results encourage the use of an STI with students with specific needs to teach numeracy skills, , but need to be replicated on a larger scale. Suggestions for adjusting the interface and teaching method are suggested to improve the impact of the application on students with autism. (Paper is in progress).

7.6.2. *Curiosity-driven interaction systems for education*

Participants: Pierre-Yves Oudeyer, Hélène Sauzéon [correspondant], Mehdi Alami, Didier Roy, Edith Law.

Three studies have been developed and conducted to newly design curiosity-driven interaction systems aiming to foster learning performance across lifespan : the first two studies include children and the last one includes the older adults.

The first study regards a new interactive robotic system to foster curiosity-driven learning. This led to an article in CHI 2019 [29]. In this work, we explored whether a social peer robot's verbal expression of curiosity can be perceived by participants, produce emotional or behavioural contagion effects, and impact learning. In a between-subject experiment involving 30 participants, a peer robot was manipulated to verbally express: curiosity, curiosity plus rationale, or no curiosity (neutral), within the context of LinkedIt!, a cooperative game we designed for teaching students how to classify rocks. Results show that participants were able to reliably recognize curiosity in the robot and curious robots can be used to elicit significantly more curiosity-driven behaviours among participants.

The second study regards a new interactive educational application to foster curiosity-driven question-asking in children. This study has been performed during the Master 2 internship of Mehdi Alaimi co-supervised by H. Sauzéon, E. Law and PY Oudeyer. The paper submission to CHI'20 is just accepted in december 2019 (« Pedagogical Agents for Fostering Question-Asking Skills in Children »). It addresses a key challenge for 21st-century schools, i.e., teaching diverse students with varied abilities and motivations for learning, such as curiosity within educational settings. Among variables eliciting curiosity state, one is known as « knowledge gap », which is a motor for curiosity-driven exploration and learning. It leads to question-asking which is an important factor in the curiosity process and the construction of academic knowledge. However, children questions in classroom are not really frequent and don't really necessitate deep reasoning. Determined to improve children's curiosity, we developed a digital application aiming to foster curiosity-related question-asking from texts and their perception of curiosity. To assess its efficiency, we conducted a study with 95 fifth grade students of Bordeaux elementary schools. Two types of interventions were designed, one trying to focus children on the construction of low-level question (i.e. convergent) and one focusing them on high-level questions (i.e. divergent) with the help of prompts or questions starters models. We observed that both interventions increased the number of divergent questions, the question fluency performance, while they did not significantly improve the curiosity perception despite high intrinsic motivation scores they have elicited in children. The curiosity-trait score positively impacted the divergent question score under divergent condition, but not under convergent condition. The overall results supported the efficiency and usefulness of digital applications for fostering children's curiosity that we need to explore further.

Finaly, the third study investigates the role of intrinsic motivation in spatial learning in late adulthood [25]. We investigated age differences in memory for spatial routes that were either actively (i.e., intinsic motivation condition) or passively (i.e., control condition) encoded. A series of virtual environments were created and presented to 20 younger (Mean age = 19.71) and 20 older (Mean age = 74.55) adults, through a cardboard viewer. During encoding, participants explored routes presented within city, park, and mall virtual environments, and were later asked to re-trace their travelled routes. Critically, participants encoded half the virtual environments by passively viewing a guided tour along a pre-selected route, and half through active exploration with volitional control of their movements by using a button press on the viewer. During retrieval, participants were placed in the same starting location and asked to retrace the previously traveled route. We calculated the percentage overlap in the paths travelled at encoding and retrieval, as an indicator of spatial memory accuracy, and examined various measures indexing individual differences in their cognitive approach and visuo-spatial processing abilities. Results showed that active navigation, compared to passive viewing during encoding, resulted in a higher accuracy in spatial memory, with the magnitude of this memory enhancement being significantly larger in older than in younger adults. Results suggest that age-related deficits in spatial memory can be reduced by active encoding. In other words, this means that conditions where intrinsic motivation is involved, reduce negative effects of aging on spatial learning.

7.6.3. Poppy Education: Designing and Evaluating Educational Robotics Kits

Participants: Pierre-Yves Oudeyer, Didier Roy [correspondant], Thibault Desprez.

The Poppy Education project aims to create, evaluate and disseminate all-inclusive pedagogical kits, open-source and low cost, for teaching computer science and robotics in secondary education and higher education, scientific literacy centers and Fablabs.

It is designed to help young people to take ownership with concepts and technologies of the digital world, and provide the tools they need to allow them to become actors of this world, with a considerable socio-economic potential. It is carried out in collaboration with teachers and several official french structures (French National Education, High schools, engineering schools, ...).

Poppy Education is based on the robotic platform poppy (open-source platform for the creation, use and sharing of interactive 3D printed robots), including:

- web interface connection (see figure 31)
- Poppy Humanoid, a robust and complete robotics platform designed for genuine experiments in the real world and that can be adapted to specific user needs.
- Poppy Torso, a variant of Poppy Humanoid that can be easily installed on any flat support.
- Ergo Jr, a robotic arm. Durable and inexpensive, it is perfect to be used in class. It can be programmed in Python, directly from a web browser, using Ipython notebooks (an interactive terminal, in a web interface for the Python Programming Language).
- Snap. The visual programming system Snap (see figure 32), which is a variant of Scratch. Its features allow a thorough introduction of information technology. Several specific "blocks" have been developed for this.
- C++, Java, Matlab, Ruby, Javascript, etc. thanks to a REST API that allows you to send commands and receive information from the robot with simple HTTP requests.
- Virtual robots (Poppy Humanoid, Torso and Ergo) can be simulated with the free simulator V-REP (see figure 33). It is possible in the classroom to work on the simulated model and then allow students to run their program on the physical robot.
- Virtual robots (Poppy Ergo) can also be simulated with a 3D web viewer (see figure 34).

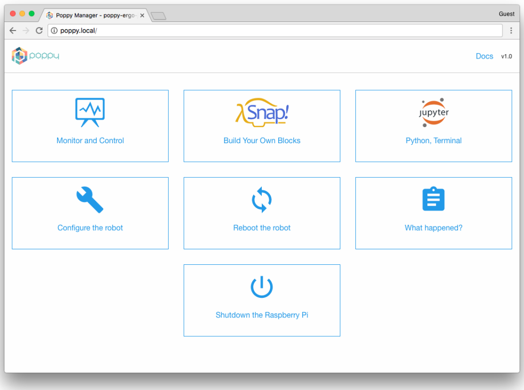


Figure 31. Home page on http://poppy.local

Figure 32. The visual programming system Snap

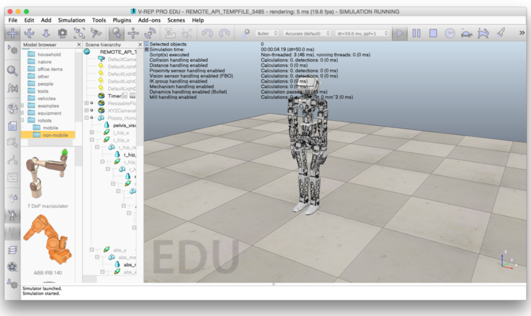


Figure 33. V-rep

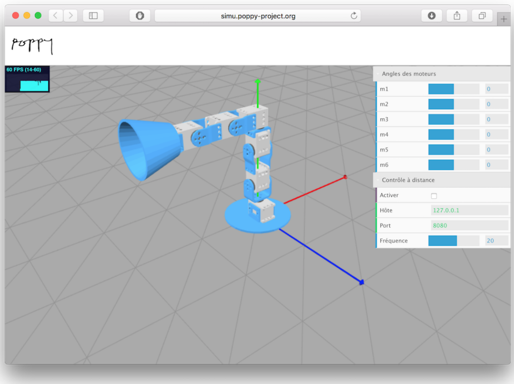


Figure 34. 3D viewer

7.6.3.1. Pedagogical experimentations : Design and experiment robots and the pedagogical activities in classroom.

The robots are designed with the final users in mind. The pedagogical tools of the project (robots and resources) are being created directly with the users and evaluated in real life by experiments. So teachers and researchers co-create activities, test them with students in class-room, share their experience and develop the platform as needed [126].

The activities were designed mainly with Snap! and Python. Most activities use Poppy Ergo Jr, but some use Poppy Torso (mostly in higher school due to its cost).

The pedagogical experiments in classroom carried out during the first year of the project notably allowed to create and experiment many robotic activities. These activities are designed as pedagogical resources introducing robotics. The main objective of the second year was to make all the activities and resources reusable (with description, documentation and illustration) easily and accessible while continuing the experiments and the diffusion of the robotic kits.

Figure 35. Experiment robots and pedagogical activities in classroom

- Pedagogical working group : the teacher partners continued to use the robots in the classroom and to create and test new classroom activities. We organized some training to help them to discover and learn how to use the robotics platform. Also, an engineer of the Poppy Education team went to visit the teachers in their school to see and to evaluate the pedagogical tools (robots and activities) in a real context of use.
  Five meetings have been organized during the year including all teachers part of the project as well as the Poppy Education team in order to exchange about their experience using the robots as a pedagogical tool, to understand their need and to get some feedback from them. This is helping us to understand better the educational needs, to create and improve the pedagogical tools.
  You can see the videos of pedagogical robotics activities here:
  https://www.youtube.com/playlist?list=PLdX8RO6QsgB7hM_7SQNLvyp2QjDAkkzLn

7.6.3.2. Pedagogical documents and resources

- We continued to improve the documentation of the robotic platform Poppy (https://docs.poppy-project.org/en/) and the documentation has been translated into French (https://docs.poppy-project.org/fr/.
  We configured a professional platform to manage the translation of the documentation (https://crowdin.com/project/poppy-docs. This platforms allows anybody to participate in the translation of the documentation to the language of their choice.
- To complete the pedagogical booklet [125] that provides guided activities and small challenges to become familiar with Poppy Ergo Jr robot and the Programming language Snap! (https://hal.inria.fr/hal-01384649/document) we provided a list of Education projects. Educational projects have been written for each activity carried out and tested in class. Each project has its own web page including resources allowing any teacher to carry out the activity (description, pedagogical sheet, photos / videos, pupil's sheet, teacher's sheet with correction etc.).
  The activities are available here:
  https://www.poppy-education.org/activites/activites-lycee
  The pedagogical activities are also available on the Poppy project forum where everyone is invited to comment and create new ones:
  https://forum.poppy-project.org/t/liste-dactivites-pedagogiques-avec-les-robots-poppy/2305

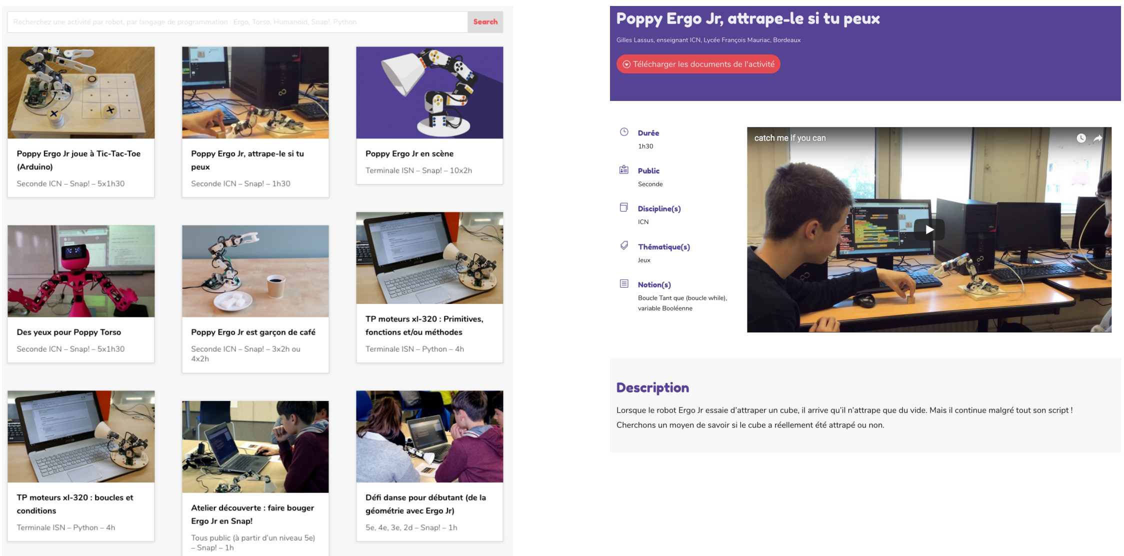


Figure 36. Open-source educational activities with Poppy robots are available on Poppy-Education.org

- A FAQ have been written with the most frequents questions to help the users: https://www.poppy-education.org/aide/
- A website has been created to present the project and to share all resources and activities. https://www.poppy-education.org/

7.6.3.3. Evaluation of the pedagogical kits

The impact of educational tools created in the lab and experimented in class had to be evaluated qualitatively and quantitatively. First, the usability, efficiency and user satisfaction must be evaluated. We must therefore assess, at first, if these tools offer good usability (i.e. effectiveness, efficiency, satisfaction). Then, in a second step, select items that can be influenced by the use of these tools. For example, students' representations of robotics, their motivation to perform this type of activity, or the evolution of their skills in these areas. In 2017 we conducted experiments to evaluate the usability of kits. We also collected data on students' perceptions of robotics.

- Population

  Our sample is made up of 28 teachers and 146 students from the region Nouvelle Aquitaine. Each subject completed an online survey in June 2017. Here, we study several groups of individuals: teachers and students. Among the students we are interested in those who practiced classroom activities with the Ergo Jr kit during the school year 2016 - 2017 (N = 68) (age = 16, std = 2.44). Among these students, 37 where High School students following the "Computer Science and Digital Sciences" stream (BAC S option ISN), 12 followed the stream "Computer and Digital Creation" (BAC S option ICN) and 18 where in Middle School.

  Among the 68 students, 13 declared having used the educational booklet provided in the kit and 16 declared having used other robotic kits. Concerning the time resource dedicated to activities with the robot, 30 students declared having spent less than 6 hours, 22 declared between 6 and 25 hours, and 16 declared having spent more than 25 hours.

  have practiced less than 6 hours of activity with the robot (N = 30), between 6 and 25 hours (N = 22) or more than 25 hours (N = 16); having built the robot (N = 12); have used the visual programming language Snap! (N = 46), the language of Python textual programming (N = 21), both (N = 8) or none (N = 9), it should be noted that these two languages are directly accessible via the main interface of the robot.
- Evaluation of the tool

  We have selected two standardized surveys dealing with this issue: SUS (The Systeme Usability Scales) [62] and The AttrakDiff [100]. These two surveys are complementary and allow to identify the design problems and to account for the perception of the user during the activities. The results of these surveys are available in the article (in French) [76] published at the conference Didapro (Lausanne Feb, 2018). Figures 37 and 38 show the averages of the 96 respondents (68 students + 28 teachers) for each of the 10 statements from the SUS and 28 pairs of antonyms to be scored on a scale of 1 to 5 and a 7-point scale, respectively.

- Evaluation of impact on learner

  One of the objectives of the integration of digital sciences in school is to allow students to have a better understanding of the technological tools that surround them daily (i.e. web, data, algorithm, connected object, etc.). So, we wanted to measure how the practice of activities with ErgoJr robot had changed this apprehension; especially towards robots. For that, we used a standardized survey: "attitude towards robot" *EuroBarometer 382* originally distributed in 2012 to more than 1000 people in each country of the European Union. On the one hand, we sought to establish whether there had been a change in response between 2012 and 2017, and secondly whether there was an impact on the responses of 2017 according to the participation, or not, in educational activities with ErgoJr robot. The analysis of the results is in progress and will be published in 2019.
- Web page for the experimentations

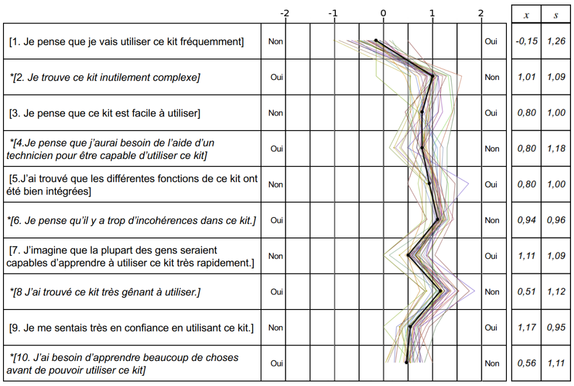


Figure 37. Result of SUS survey

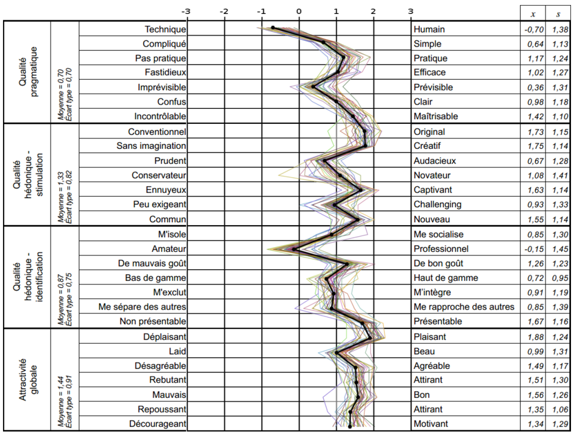


Figure 38. Result of AttrakDiff survey

To facilitate the storage of documents, their availability, and to highlight some information and news, a page dedicated to the experimentations is now available on the website. https://www.poppy-education.org/evaluation/

7.6.3.4. Partnership on education projects

- Ensam

  The Arts and Métiers campus at Bordeaux-Talence in partnership with Inria wishes to contribute to its educational and scientific expertise to the development of new teaching methods and tools. The objective is to develop teaching sequences based on a project approach, relying on an attractive multidisciplinary technological system: the humanoid Inria Poppy robot.

  The humanoid Inria Poppy robot offers an open platform capable of providing an unifying thread for the different subjects covered during the 3-years of the Bachelor training: mechanics, manufacturing (3D printing), electrical, mecha-tronics, computer sciences, design.

- Poppy entre dans la danse (Poppy enters the dance)

  The project "Poppy enters the dance" (Canope 33) took place for the second year. It uses the humanoid robot Poppy. This robot is able to move and experience the dance. The purpose of this project is to allow children to understand the interactions between science and choreography, to play with the random and programmable, to experience movement in dialogue with the machine. At the beginning of the project they attended two days of training on the humanoid robot (Inria - Poppy Education). During the project, they met the choreographer Eric Minh Cuong Castaing and the engineer Segonds Theo (Inria - Poppy Education).

  You can see a description and an overview of the project here:
  https://www.youtube.com/watch?v=XfxXaq899kY

- DANE

  The Academic Delegation for Digital Educational is in charge of supporting the development of digital uses for pedagogy. It implements the educational digital policy of the academy in partnership with local authorities. She accompanies institutions daily, encourages innovations and participates in their dissemination.

- RobotCup Junior

  RoboCupJunior OnStage invites teams to develop a creative stage performance using autonomous robots that they have designed, built and programmed. The objective is to create a robotic performance between 1 to 2 minutes that uses technology to engage an audience. The challenge is intended to be open-ended. This includes a whole range of possible performances, for example dance, storytelling, theatre or an art installation. The performance may involve music but this is optional. Teams are encouraged to be as creative, innovative and entertaining, in both the design of the robots and in the design of the overall performance.

7.7. Other applications

7.7.1. Applications in Robotic myoelectric prostheses

Participants: Pierre-Yves Oudeyer [correspondant], Aymar de Rugy, Daniel Cattaert, Mick Sebastien.

Together with the Hybrid team at INCIA, CNRS (Sébastien Mick, Daniel Cattaert, Florent Paclet, Aymar de Rugy) and Pollen Robotics (Matthieu Lapeyre, Pierre Rouanet), the Flowers team continued to work on a project related to the design and study of myoelectric robotic prosthesis. The ultimate goal of this project is to enable an amputee to produce natural movements with a robotic prosthetic arm (open-source, cheap, easily reconfigurable, and that can learn the particularities/preferences of each user). This will be achieved by 1) using the natural mapping between neural (muscle) activity and limb movements in healthy users, 2) developing a low-cost, modular robotic prosthetic arm and 3) enabling the user and the prosthesis to co-adapt to each other, using machine learning and error signals from the brain, with incremental learning algorithms inspired from the field of developmental and human-robot interaction.

7.7.1.1. Reachy, a 3D-printed Human-like Robotic Arm as a Test Bed for Prosthesis Control Strategies

To this day, despite the increasing motor capability of robotic prostheses, elaborating efficient control strategies is still a key challenge for their design. To provide an amputee with efficient ways to drive a prosthesis, this task requires thorough testing prior to integration into finished products. To preserve consistency with prosthetic applications, employing an actual robot for such testing requires it to show human-like features. To fulfill this need for a biomimetic test platform, we developed the Reachy robotic platform, a seven-joint human-like robotic arm that can emulate a prosthesis. Although it does not include an articulated hand and is therefore more suitable for studying reaching than manipulation, a robotic hand from available research prototypes could be integrated to Reachy. Its 3D-printed structure and off-the-shelf actuators make it inexpensive relatively to the price of a genuine prosthesis. Using an open-source architecture, its design makes it broadly connectable and customizable, so it can be integrated into many applications. To illustrate how Reachy can connect to external devices, we developed several proofs of concept where it is operated with various control strategies, such as tele- operation or vision-driven control. In this way, Reachy can help researchers to develop and test innovative control strategies on a human-like robot.

7.7.2. Ship Motion estimation from sea wave vision

Participants: David Filliat [correspondant], Natalia Díaz Rodríguez, Zhi Zhou, Manuel Cortés-Batet, Nazar-Mykola Kaminskyi.

Together with Naval Group, ENSTA Paris has been working on a set of software tools for simulating sea waves and motion estimation from images. The objective is predicting variables of interest in order to compensate the position and inclination of large boats at deep sea, seconds ahead of time to preserve stability. Work being currently done in partnership with Abo Akademi University (Turku, Finland) will validate the soon to be published Blender wave generator and machine learning algorithms, with real data gathered from the Baltic Sea archipelago.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

8.1.1. Autonomous Driving Commuter Car

Participants: David Filliat [correspondant], Emmanuel Battesti.

We developed planning algorithms for a autonomous electric car for Renault SAS in the continuation of the previous ADCC project. We improved our planning algorithm in order to go toward navigation on open roads, in particular with the ability to reach higher speed than previously possible, deal with more road intersection case (roundabouts), and with multiple lane roads (overtake, insertion...).

8.2. Bilateral Grants with Industry

8.2.1. Perception Techniques and Sensor Fusion for Level 4 Autonomous Vehicles

Participants: David Filliat [correspondant], Vyshakh Palli-Thazha.

Financing of the CIFRE PhD grant of Vyshakh Palli-Thazha by Renault.

8.2.2. Incremental Methods of Deep Learning for detection and classification in an robotics environment

Participants: David Filliat [correspondant], Timothée Lesort.

Financing of the CIFRE PhD grant of Timothée Lesort by Thales.

8.2.3. Exploration of reinforcement learning algorithms for drone visual perception and control

Participants: David Filliat [correspondant], Florence Carton.

Financing of the CIFRE PhD grant of Florence Carton by CEA.

8.2.4. Incremental learning for sensori-motor control

Participants: David Filliat [correspondant], Hugo Caselles Dupré.

Financing of the CIFRE PhD grant of Hugo Caselles-Dupré by Softbank Robotics.

8.2.5. Curiosity-driven Learning Algorithms for Exploration of Video Game Environments

Participant: Pierre-Yves Oudeyer [correspondant].

Financing of a postdoc grant for a 2 year project with Ubisoft and Région Aquitaine.

8.2.6. Intrinsically Motivated Exploration for Lifelong Deep Reinforcement Learning in the Malmo Environment

Participants: Pierre-Yves Oudeyer [correspondant], Remy Portelas.

Financing of the PhD grant of Rémy Portelas by Microsoft Research.

8.2.7. Explainable continual learning for autonomous driving

Participants: Natalia Díaz Rodríguez [correspondant], Adrien Bennetot.

Financing of the CIFRE PhD grant of Adrien Bennetot by Segula Technologies.

9. Partnerships and Cooperations

9.1. Regional Initiatives

9.1.1. Perseverons

Perseverons

Program: eFran

Duration: January 2016 - December 2019

Coordinator: PY Oudeyer, Inria Flowers

Partners: Inria Flowers

Funding: 140 keuros

The Perseverons project (Perseverance with / by digital objects), coordinated by the university via the ESPE (Higher School of Teaching and Education) of Aquitaine, and by the Rectorat of Bordeaux via the DANE (Academic Delegation digital education), aims to measure the real effectiveness of digital techniques in education to improve school motivation and perseverance, and, in the long term, reduce dropout. The project proposes to analyze the real effects of the use of two types of objects, robots, tablets, by comparing the school and non-school contexts of the *fablabs*. It is one of the 22 winners http://www.gouvernement.fr/efran-les-22-laureats of the "E-Fran" call for projects (training, research and digital animation spaces), following the Monteil mission on digital education, as part of the Investissement d'Avenir 2 program http://ecolenumerique.education.gouv.fr/2016/09/23/1244/. Formed of 12 sub-projects, "perseverons" has many partnerships, especially with the Poppy Education project of Inria Flowers. It is funding the PhD of Thibault Desprez.

Attachement	Type	Name	Adresse	Tel	Web
Poppy Éducation	High School	Alfred Kastler	14 Avenue de l'Université,33402 Talence, France	+33 5 57 35 40 70	http://www.lyceekastler.fr/
Poppy Éducation	Middle School	Anatole France	28 Rue des Micocouliers,33410 Cadillac, France	+33 5 56 62 98 42	http://www.afcadillac.net/
PERSEVERONS	High School	André Malraux	3 Rue du 8 Mai 1945,64200 Biarritz, France	+33 5 59 01 20 40	http://lycee-malraux-biarritz.fr/
Poppy Éducation	High School	Camille Jullian	29 Rue de la Croix Blanche,33000 Bordeaux, France	+33 5 56 01 47 47	http://www.camillejullian.com/
Poppy Éducation	Middle School	de France	Rue du Cimetière Saint-Benoist,75005 Paris, France	+33 1 44 27 12 11	http://www.college-de-france.fr/
Poppy Éducation	High School	des Graves	238 Cours du Général de Gaulle,33170 Gradignan, France	+33 5 56 75 77 56	http://www.grandlebrun.com/
PERSEVERONS	High School	Élie Faure	63 Avenue de la Libération,33310 Lormont, France	+33 5 56 38 23 23	http://www.lyc-eliefaure.fr/
PERSEVERONS	High School	Elisée Reclus	7 Avenue de Verdun,33220 Pineuilh, France	+33 5 57 41 92 50	http://lycee-foyen.fr/
Poppy Éducation	High School	François Mauriac	1 Rue Henri Dunant,33000 Bordeaux, France	+33 5 56 38 52 82	http://lyceemauriac.fr/
PERSEVERONS	High School	Gaston Febus	20 Avenue Georges Moutet,64300 Orthez, France	+33 5 59 67 07 26	http://webetab.ac-bordeaux.fr/cite-gaston-febus-orthez/
PERSEVERONS	Middle School	Giraud de Borneil	10 Boulevard André Dupuy,24160 Excideuil, France	+33 5 53 62 21 16	http://www.gdeborneil.fr/
PERSEVERONS	High School	Grand Air	Avenue du Docteur Lorentz Monod,33120 Arcachon, France	+33 5 56 22 38 00	http://webetab.ac-bordeaux.fr/lycee-grand-air/
PERSEVERONS	High School	Gustave Eiffel	143 Rue Ferbos,33000 Bordeaux, France	+33 5 56 33 83 00	http://www.eiffel-bordeaux.org/
PERSEVERONS	High School	Jacques Monod	10 Rue du Parvis,64230 Lescar, France	+33 5 59 77 92 00	http://lyceejacquesmonod.fr/
Poppy Éducation	High School	Jean Moulin	Avenue de la République,33210 Langon, France	+33 5 56 63 62 30	http://webetab.ac-bordeaux.fr/lycee-jean-moulin-langon/
Poppy Éducation	Middle School	Jean Zay	41 Rue Henri Cochet,33380 Biganos, France	+33 5 57 17 01 70	http://collegebiganos.fr/
Poppy Éducation	High School	La Morlette	62 Rue du Docteur Roux,33150 Cenon, France	+33 5 57 80 37 00	http://lycee-lamorlette.fr/
PERSEVERONS	High School	Les Iris	13 Rue Sourbès,33310 Lormont, France	+33 5 57 80 10 60	http://www.lyceelesiris.fr/
PERSEVERONS	High School	Louis Barthou	2 Boulevard Barbanègre,64000 Pau, France	+33 5 59 98 98 00	http://www.cyberlycee.fr/
PERSEVERONS	High School	Louis de Foix	4 Avenue Jean Rostand,64100 Bayonne/Bayona/Baiona, France	+33 5 59 63 31 10	http://www.louisdefoix.com/
PERSEVERONS	High School	Maine de Biran	108 Rue Valette,24100 Bergerac, France	+33 5 53 74 50 00	http://webetab.ac-bordeaux.fr/lycee-maine-de-biran/
Poppy Éducation	Middle School	Mios	Route du Pujeau,33380 Mios, France	+33 5 56 03 00 77	http://www.villemios.fr/enfance-jeunesse/college/
PERSEVERONS	High School	Nord Bassin	128 Avenue de Bordeaux,33510 Andernos-les-Bains, France	+33 5 56 82 20 77	http://www.lyceenordbassin.com/
Forum Poppy	Primary School	Notre-Dame du Mur	19 Rue de Kermadiou,29600 Morlaix, France	+33 2 98 88 18 69	http://lycee.ecmorlaix.fr/
PERSEVERONS	High School	Pape Clément	1 Rue Léo Lagrange,33600 Pessac, France	+33 5 57 26 63 00	http://lyceepapeclement.fr/
PERSEVERONS	High School	Pays de Soule	Avenue Jean Monnet,64130 Chéraute, France	+33 5 59 28 22 28	http://www.lyceedupaysdesoule.fr/index.php
PERSEVERONS	High School	Pré De Cordy	5 Avenue Joséphine Baker,24200 Sarlat-la-Canéda, France	+33 5 53 31 70 70	http://lycee-predecordy-sarlat.com/
Poppy Éducation	High School	Raoul Follereau	9 Boulevard Saint-Exupéry,58000 Nevers, France	+33 3 86 60 36 00	http://lyc58-renardfollereau.ac-dijon.fr/
PERSEVERONS	High School	René Cassin	2 Rue de Lasseguette,64100 Bayonne/Bayona/Baiona, France	+33 5 59 58 42 00	http://webetab.ac-bordeaux.fr/lycee-rene-cassin/
PERSEVERONS	High School	Saint-Cricq	4 Piste Cyclable,64000 Pau, France	+33 5 59 30 50 55	http://www.lycee-saint-cricq.org/
Poppy Éducation	High School	Saint-Genès	160 Rue de Saint-Genès,33000 Bordeaux, France	+33 5 56 33 84 84	http://www.saint-genes.com/
PERSEVERONS	High School	Saint-John Perse	2 Chemin de Barincou,64000 Pau, France	+33 5 59 62 73 11	http://www.lycee-saint-john-perse.fr/
Poppy Éducation	High School	Sainte-Marie Grand Lebrun	164 Rue François Mauriac,33200 Bordeaux, France	+33 5 56 08 32 13	http://www.grandlebrun.com/
inria	High School	Sainte-Saintonge	12 Rue de Saintonge,33000 Bordeaux, France	+33 5 56 99 39 29	http://www.lyceesaintefamille.com/
Poppy Éducation	High School	Sud-Médoc	Piste du Médoc Bleu,33320 Le Taillan-Médoc, France	+33 5 56 70 10 10	http://www.lyceesudmedoc.fr/
Poppy Éducation	High School	Victor Louis	2 Rue de Mégret,33400 Talence, France	+33 5 56 80 76 40	http://lyceevictorlouis.fr/

Figure 39. List of partner schools

9.1.1.1. Partner schools

In 2018, we have 36 partner schools (show Fig 39). 15 directly from the Poppy Education project. 19 new establishments were equipped in September 2017 by the Perseverons project. 21 of these establishments are located in Gironde. We have 27 high schools, 5 middle school.

9.2. National Initiatives

9.2.1. Myoelectric prosthesis - PEPS CNRS

PY Oudeyer collaborated with Aymar de Rugy, Daniel Cattaert, Mathilde Couraud, Sébastien Mick and Florent Paclet (INCIA, CNRS/Univ. Bordeaux) about the design of myoelectric robotic prostheses based on the Poppy platform, and on the design of algorithms for co-adaptation learning between the human user and the prosthesis. This was funded by a PEPS CNRS grant.

9.2.2. Poppy Station structure

- Since 1 september 2017 until february 2019, PerPoppy and Poppy Station Projects : D. Roy, P.-Y. Oudeyer. These projects aim to perpetuate the Poppy robot ecosystem by creating an external structure from outside Inria, with various partners. After the Poppy Robot Project, the Poppy Education Project has ended and Poppy Station structure is born. PerPoppy is the project which is building the new structure, and Poppy Station is the name of the new structure. Poppy Station, which includes Poppy robot ecosystem (hardware, software, community) from the beginning, is a place of excellence to build future educational robots and to design pedagogical activities to teach computer science, robotics and Artificial Intelligence. https://www.poppy-station.org
- Partners of Poppy Station : Inria, La Ligue de l'Enseignement, HESAM Université, SNCF Développement, IFÉ-ENS Lyon, MOBOTS – EPFL, Génération Robots, Pollen Robotics, KONEX-Inc, Mobsya, CERN Microclub, LINE Lab (Université Nice), Stripes, Canopé Martinique, Rights Tech Women, Editions Nathan.

9.2.3. Adaptiv'Math

Adaptiv'Math

Program: PIA

Duration: 2019 - 2020

Coordinator: EvidenceB

Partners:

EvidenceB

Nathan

APMEP

LIP6

Inria

ISOGRAD

Daesign

Schoolab

BlueFrog

The solution Adaptiv'Math comes from an innovation partnership for the development of a pedagogical assistant based on artificial intelligence. This partnership is realized in the context of a call for projects from the Ministry of Education to develop a pedagogical plateform to propose and manage mathematical activities intended for teachers and students of cycle 2. The role of Flowers team is to work on the AI of the proposed solution to personalize the pedagogical content to each student. This contribution is based on the work done during the Kidlearn Project and the thesis of Benjamin Clement [69], in which algorithms have been developed to manage and personalize sequence of pedagogical activities. One of the main goal of the team here is to transfer technologies developed in the team in a project with the perspective of industrial scaling.

9.3. European Initiatives

9.3.1. Collaborations in European Programs, except FP7 & H2020

9.3.1.1. IGLU

Title: Interactive Grounded Language Understanding (IGLU)

Programm: CHIST-ERA

Duration: October 2015 - September 2018

Coordinator: University of Sherbrooke, Canada

Partners:

University of Sherbrooke, Canada

Inria Bordeaux, France

University of Mons, Belgium

KTH Royal Institute of Technology, Sweden

University of Zaragoza, Spain

University of Lille 1 , France

University of Montreal, Canada

Inria contact: Pierre-Yves Oudeyer

Language is an ability that develops in young children through joint interaction with their caretakers and their physical environment. At this level, human language understanding could be referred as interpreting and expressing semantic concepts (e.g. objects, actions and relations) through what can be perceived (or inferred) from current context in the environment. Previous work in the field of artificial intelligence has failed to address the acquisition of such perceptually-grounded knowledge in virtual agents (avatars), mainly because of the lack of physical embodiment (ability to interact physically) and dialogue, communication skills (ability to interact verbally). We believe that robotic agents are more appropriate for this task, and that interaction is a so important aspect of human language learning and understanding that pragmatic knowledge (identifying or conveying intention) must be present to complement semantic knowledge. Through a developmental approach where knowledge grows in complexity while driven by multimodal experience and language interaction with a human, we propose an agent that will incorporate models of dialogues, human emotions and intentions as part of its decision-making process. This will lead anticipation and reaction not only based on its internal state (own goal and intention, perception of the environment), but also on the perceived state and intention of the human interactant. This will be possible through the development of advanced machine learning methods (combining developmental, deep and reinforcement learning) to handle large-scale multimodal inputs, besides leveraging state-of-the-art technological components involved in a language-based dialog system available within the consortium. Evaluations of learned skills and knowledge will be performed using an integrated architecture in a culinary use-case, and novel databases enabling research in grounded human language understanding will be released. IGLU will gather an interdisciplinary consortium composed of committed and experienced researchers in machine learning, neurosciences and cognitive sciences, developmental robotics, speech and language technologies, and multimodal/multimedia signal processing. We expect to have key impacts in the development of more interactive and adaptable systems sharing our environment in everyday life. http://iglu-chistera.github.io/

9.4. International Initiatives

9.4.1. Inria Associate Teams Not Involved in an Inria International Labs

9.4.1.1. NEUROCURIOSITY

Title: NeuroCuriosity

International Partner (Institution - Laboratory - Researcher):

Columbia Neuroscience (United States) - Cognitive Neuroscience - JACQUELINE GOTTLIEB

Start year: 2016

See also: https://flowers.inria.fr/neurocuriosityproject/

Curiosity can be understood as a family of mechanisms that evolved to allow agents to maximize their knowledge of the useful properties of the world. In this project we will study how different internal drives of an animal, e.g. for novelty, for action, for liking, are combined to generate the rich variety of behaviors found in nature. We will approach such challenge by studying monkeys, children and by developing new computational tools.

9.4.1.2. Idex Bordeaux-Univ. Waterloo collaborative project on curiosity in HCI

Title: Curiosity

International Partner (Institution - Laboratory - Researcher):

University of Waterloo (Canada), Edith Law's HCI Lab and Dana Kulic's Robotics lab.

Start year: 2018

Pierre-Yves Oudeyer collaborated with Edith Law's HCI research group at University of Waterloo on the topic of "Curiosity in HCI system". They obtained a grant from Univ. Bordeaux to set up a project with Inria Potioc team and with Dana Kulic, Robotics lab, Univ. Waterloo. They organized several cross visits and collaborated on the design and experimentation of an educational interactive robotic system to foster curiosity-driven learning. This led to two articles accepted at CHI 2019 and CHI2020 (see new results section).

To continue this collaborative research, a new proposal on « Curiosity-driven learning and personalized (re-)education technologies across the lifespan » have been successfully submitted to UB-UW IDEX call regarding the projects in the field of AI and health sciences (PI: E. Law, PY Oudeyer ; co-PI : M. Fernandes, H. Sauzéon & F. Lotte)

9.4.1.3. Idex Bordeaux-Univ. Waterloo collaborative project on Virtual realty-based study on spatial learning in aging

Title: Spatial learning with aging

International Partner (Institution - Laboratory - Researcher):

University of Waterloo (Canada), Myra Fernandes, Cognitive neurosciences Lab.

Start year: 2016 (end year 2019)

Helene Sauzéon collaborated with Myra Fernandes's cognitive neuroscience Lab at University of Waterloo on the topic of "VR based study of spatial learning in older adults". They obtained a grant from Univ. Bordeaux to set up a project with Quincy Almeida, head of Movement Disorders Research and Rehabilitation Centre, Laurier University. They organized several cross visits and collaborated on the design and experimentation of a virtual reality application allowing to investigate intrinsic motivation (i.e., Active exploration) as cognitive support for older adults' spatial learning. This led to an article published in Brain Science in 2019 (see new results section).

9.4.1.4. Informal International Partners

Pierre-Yves Oudeyer and Didier Roy have created a collaboration with LSRO EPFL and Pr Francesco Mondada, about Robotics and education. The two teams co-organize the annual conference "Robotics and Education"in Bordeaux. Didier Roy teaches "Robotics and Education" in EPFL several times a year.

Didier Roy has created a collaboration with HEP Vaud (Teachers High School) and Bernard Baumberger and Morgane Chevalier, about Robotics and education. Scientific discussions and shared professional training.

Didier Roy has created a collaboration with Biorob - EPFL, LEARN - EPFL, and Canton de Vaud, about Robotics and Computer Science education. Scientific discussions and shared professional training.

Didier Roy has created a collaboration with Mauritius Research Council, Mauritius Education Institute and AUF, about Robotics, AI and Computer Science projects, teaching and learning. Scientific discussions and shared professional training. With Gérard Giraudon (Advisor to the President of Inria, with in particular a mission on "Digital & Training").

A collaboration with Johan Lilius and Sebastien Lafond from Abo Akademi University, Turku (Finland) is ongoing to sign an Erasmus contract for researchers and students visits on the topic of autonomous boats.

Funding applications have been submitted jointly with Davide Maltoni and Vincenzo Lomonaco from University of Bologna (Italy) on the topic of continual learning. Also the project https://www.continualai.org/ is being further developed jointly and on the way to become a non-profit organization.

9.4.2. Participation in Other International Programs

David Filliat participates in the ITEA3 DANGUN project with Renault S.A.S. in france and partners in Korea. The purpose of the DANGUN project is to develop a Traffic Jam Pilot function with autonomous capabilities using low-cost automotive components operating in France and Korea. By incorporating low-cost advanced sensors and simplifying the vehicle designs as well as testing in different scenarios (France & Korea), a solution that is the result of technical cooperation between both countries should lead to more affordable propositions to respond to client needs in the fast moving market of intelligent mobility.

Natalia Díaz Rodríguez collaborates with the Abo Akademi University in Turku, Finland on the autonomous navigation systems project, involving the sailing schools of Novia and Naval Group (France). She also collaborates with the Andalusian Research Institute in Data Science and Computational Intelligence https://dasci.es (DaSCI) and the University of Granada (Spain) on explainable AI.

9.5. International Research Visitors

9.5.1. Visits of International Scientists

- Kevvyn Collins-Thompson, Univ. Michigan (sept.-dec. 2019)
- Franck Guerin, Univ. Aberyswith (dec 2019)
- Justus Piater, Univ. Innsbrucj (dec 2019)
- Verena Hafner, Univ. Berlin (dec 2019)
- Jochen Triesch, Univ. Frankfurt (dec 2019)
- Nivedita Mani, Univ. Gottingen (dec 2019)
- Oksana Hagen, Plymouth University (Oct. 2019)

9.5.2. Internships

- Medhi Alaimi [Inria, until Jul 2019]
- Timothee Anne [Inria, from Feb 2019 until Jun 2019]
- Anouche Banikyan [Inria, from Feb 2019 until Jul 2019]
- Lucie Galland [Ecole Normale Supérieure Paris, from Jun 2019 until Aug 2019]
- Tallulah Gilliard [Inria, from Feb 2019 until Jul 2019]
- Marion Schaeffer [Inria, from Jul 2019 until Sep 2019]
- Martin Serret [Inria, from Feb 2019 until Aug 2019]
- Maria Teodorescu [Inria, from Sep 2019]

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events: Organisation

10.1.1.1. Member of the Organizing Committees

PY Oudeyer was co-organizer of the Workshop on Exploration in Reinforcement Learning (ICML 19), https://sites.google.com/view/erl-2019/organizers.

10.1.2. Scientific Events: Selection

10.1.2.1. Member of the Conference Program Committees

PY Oudeyer was member of the program committee of IEEE International Conference on Developmental Learning and Epigenetic Robotics (ICDL-Epirob).

Natalia Díaz Rodríguez, steering committee and reviewer of CONTLEARN Workshop at CVPR2020 Workshop on Continual Learning in Computer Vision, Seattle, US.

10.1.2.2. Reviewer

PY Oudeyer was a reviewer for: Workshop on Exploration in Reinforcement Learning (ICML 19).

Hélène Sauzéon reviewed a conference paper for CHI 2020.

10.1.3. Journal

10.1.3.1. Member of the Editorial Boards

PY Oudeyer was editor of the IEEE Newsletter on Cognitive and Developmental Systems.

PY Oudeyer was associate editor of: IEEE Transactions on Cognitive and Developmental Systems and Frontiers in Neurorobotics.

10.1.3.2. Reviewer - Reviewing Activities

Clément Moulin-Frier reviewed an article for *Journal of Artificial Intelligence Research (JAIR)*.

PY Oudeyer reviewed for the journals: Journal of Artificial Intelligence Research, Cognitive Science, Nature Science Reports.

Hélène Sauzéon reviewed 6 articles for Memory & Cognition (M&C), Annals of Physical and Rehabilitative Medecine (APRM), Psychonomic Bulletin, Motivation & Cognition (MC); Cognition & Emotion (CE)

Natalia Díaz Rodríguez reviewed at Frontiers in Robotics and AI, Transactions on Emerging Telecommunications Technologies, IEEE Robotics & Automation Magazine, Neurocomputing, Robotics and Autonomous Systems.

Cédric Colas reviewed an article for the Robotics Science and Systems (RSS) conference.

10.1.4. Invited Talks

Clément Moulin-Frier gave invited talks at the *Journées Nationales de Recherche en Robotics (JNRR)* in Vittel (France) and in the *Journée GT8 "Robotique et Neurosciences"* du GDR Robotique in Bordeaux (France).

Clément Moulin-Frier and Natalia Díaz-Rodríguez gave a talk and participated, resp. in the workshop *Open Artificial Intelligence: From big data to smart data* at the *Centre de Recherche Interdisciplinaire (CRI)* in Paris (France) 13-15 Nov. 2019.

PY Oudeyer gave a keynote talk at International Conference on Learning Representations (ICLR 2019), New-Orleans, May 2019, https://iclr.cc/Conferences/2019/Schedule?showEvent=1141.

PY Oudeyer gave a keynote talk at ACM International Conference on Virtual Agents (ACM IVA 2019), Paris, on developmental machine learning https://iva2019.sciencesconf.org/.

PY Oudeyer gave an invited talk at the Deep Learning Summit (ReWork 2019), London, on curiosity-driven artificial intelligence, https://www.re-work.co/events/deep-learning-summit-london-2019/speakers/.

PY Oudeyer gave an invited talk at the conference on Reinforcement Learning and Decision Making (RLDM 2019), Montreal, on curiosity-driven developmental learning, http://rldm.org/invited-speakers/.

PY Oudeyer gave an invited talk at the Workshop on Curiosity for Decision Making at RLDM 2019, Montreal, https://sites.google.com/view/rldm-curiosity.

PY Oudeyer gave an invited talk at the HUMAINT conference in Séville, on "Developmental Autonomous Learning: AI, Cognitive Sciences and EdTech", 2019.

PY Oudeyer gave an invited talk at the workshop "AI and cognitive systems in Aquitaine", ENSC/Chaire STAH, Bordeaux, 2019.

PY Oudeyer gave an invited talk at the workshop "Task-agnostic reinforcement learning" at ICLR 2019, https://tarl2019.github.io, on developmental autonomous learning.

PY Oudeyer gave an invited talk at the workshop on Curiosity, Explanation and Exploration at Princeton University, 2019, on models of curiosity-driven learning in humans and machines.

PY Oudeyer gave an invited talk at the workshop on AI and Machine Learning, Telecom ParisTech, 2019, on developmental machine learning, https://workshopmlai.wp.imt.fr.

PY Oudeyer gave an invited talk at Académie de Médecine, Paris, 2019, on models of curiosity-driven learning and educational technologies.

PY Oudeyer gave an invited talk at workshop on Self and Sense of Agency, University Paris Descartes, nov. 2019, on models of curiosity-driven learning in humans and machines.

Hélène Sauzéon gave three invited talks at : 1) the conference on « Neuropsychologie clinique et technologies » - SNLF 2019, Paris, dec., 2-5 ; 2) Annual cycle of conference of Hôpital Salpêtrière, dec., 3; 3) Computer science Dpt. Of the University of Beijing, Beijing, July, 22-23.

Chris Reinke gave three invited talks at: 1) Okinawa Institute of Science and Technology, May 2019, on machine learning methods for the automated discovery of behaviors in physical and chemical systems; 2) LOMA Theory Day at Bordeaux, July 2019, on machine learning in physics; 3) Inria Grenoble, December 2019, on using cognitive models for artificial intelligence

N. Díaz Rodríguez gave an invited keynote (Continual Learning and Robotics: An Overview) and was a panelist at the ICLR workshop on multi-task and lifelong reinforcement learning https://sites.google.com/view/mtlrl

N. Díaz Rodríguez gave a guest talk at the Network of Young Researchers - Neuro Day NYR, Continual learning and Robotics, Paris 7th June 2019[0].

N. Díaz Rodríguez moderated a round table tomorrow in Paris: *WHEN AI AND BIG DATA MEET LIFE SCIENCES: ADVANCES IN RESEARCH AND ETHICAL QUESTIONS*https://yrls.fr/roundtable/ at Institut Imagine, Paris.

10.1.5. Leadership within the Scientific Community

Hélène Sauzéon was member of the ANR committe of « Technologie & Health »

10.1.6. Scientific Expertise

PY Oudeyer was a reviewer for the European Commission (FET program).

Hélène Sauzéon was a reviewer for the ANR call on International and european and scientific networks.

10.1.7. Research Administration

PY Oudeyer has been head of the Flowers team and member of piloting committees of consortium projects Adaptiv'Maths and Perseverons (eFran) on educational technologies.

Hélène Sauzéon was head of HACS team (BPH Lab, Inserm-UB), and thus member of directory committe of « Handicap » IFR (Inserm).

Helène Sauzéon is member of directory committe of the « centre d'excellence BIND », and she managed the Industrial Innovation and transfer sub-committee.

[0]https://ifm-institute.fr/fr/accueil/actualites/470-network-of-young-researchers-neuro-day-7th-june-20?fbclid=IwAR03u8T-opoede5hnCQx_QSphsJPC77YCrmnuNZH8c5XiBoRH9kgotLvYyw

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

PY Oudeyer gave a course on developmental reinforcement learning at ENSEIRB master on AI and machine learning (3h), nov. 2019.

PY Oudeyer gave a course on developmental learning at CogMaster cognitive science master (3h), nov. 2019.

PY Oudeyer gave a course on developmental learning at ENSC/ENSEIRB "option robot" master (3h), dec. 2019.

During the latest academic year, Hélène Sauzéon teached 96h in the BS. and master degrees in cognitive science (Department of Mathematics & interaction, University of Bordeaux). She was (co-)responsible of 9 teaching units (3 in BS et 6 in Master).

N Díaz Rodríguez taught, at ENSTA, a total of 3.25 h in ROB313, 27h at IN104, 10.5 at IN102, 21h at IA301. She also gave 42h at IG.2410 at the engineering school ISEP, and 3h course on Continual Learning and State Representation Learning at the reinforcement learning course at ENSEIRB master on AI and machine learning (3h), nov. 2019.

Didier Roy gave courses on computer science basics, and on computer science, robotics and AI activities for education at Canton de Vaud teachers.

10.2.2. Supervision

- PhD defended: Sébastien Forestier, "Intrinsically Motivated Goal Exploration in Child Development and Artificial Intelligence: Learning and Development of Speech and Tool Use", University of Bordeaux (supervised by PY Oudeyer).
- PhD defended: Thibault Desprez, "Conception et évaluation de kits robotiques pédagogiques", University of Bordeaux (supervisors: PY. Oudeyer and D. Roy)
- PhD in progress : Rémy Portelas, "Teacher algorithms for curriculum learning in Deep RL", beg. in sept. 2018 (supervisors: PY Oudeyer and K Hoffmann)
- PhD in progress: Cédric Colas, "Intrinsically Motivated Deep RL", beg. in sept. 2017 (supervisors: PY Oudeyer and O Sigaud)
- PhD in progress: Tristan Karch, "Language acquisition in curiosity-driven Deep RL", beg. in sept. 2019 (supervisors: PY Oudeyer and C Moulin-Frier)
- PhD in progress: Alexandr Ten, "Models of human curiosity-driven learning and exploration", beg. in sept. 2018 (supervisor: PY Oudeyer)
- PhD defended: Cécile Mazon, "Des Technologies Numériques Pour L'inclusion Scolaire Des Collégiens Avec TSA : des approches individuelles aux approches écosystémiques pour soutenir l'individu et ses aidants ", University of Bordeaux (supervised by H. Sauzéon).
- PhD defended: Pierre-Antoine Cinquin, "Conception, intégration et validation de systèmes numériques d'enseignement accessibles aux personnes en situation de handicap cognitif ", University of Bordeaux (supervised by H. Sauzéon & P. Guitton).
- PhD in progress: Adrien Bennetot, "Explainable continual learning for autonomous driving", Sorbonne University and ENSTA Paris (supervised by N Díaz Rodríguez & R Chatila).
- Master thesis defended: Anouche Banikyian "Curiosity, intrinsic motivation and spatial learning in children", University of Bordeaux (supervised by H. Sauzéon).
- Master thesis defended: Mehdi Alaimi "New educational application for fostering curiosity-related question-asking in children", University of Bordeaux (supervised by H. Sauzéon & PY Oudeyer).
- Master thesis defended: Juewan Wang "Can an accessible MOOC player improve the retention of disabled students? A MOOC accessibility assessment based on analytic method ", University of Bordeaux (supervised by H. Sauzéon & P. Guitton).

10.2.3. Juries

PY Oudeyer was reviewer of the PhD of Simon Hangl, entitled « Autonomous Robotics: an Integrated Approach from Controllers to Cognitive Capabilities », University of Innsbruck, Austria, 2019.

PY Oudeyer was reviewer of the PhD of Yannick Bourrier, titled "Diagnostic et prise de décision pédagogique pour la construction de compétences non- techniques en situation critique", from university Paris-Sorbonne, 2019.

PY Oudeyer was reviewer of the PhD of Leni Kenneth Le Goff, titled "Bootstrapping robotic ecological perceptin with exploration and interactions", from University Pierre et Marie Curie, 2019.

PY Oudeyer was examiner of the PhD of Jelena Mladenovic, titled "Modélisation computationnelle des compétences et des états de l'utilisateur pour optimiser les taches d'entraînement aux Interfaces Cerveaux-Ordinateur", University of Bordeaux, 2019.

PY Oudeyer was examiner of the PhD of Pierre Fournier, titled "Intrinsically Motivated and Interactive Reinforcement Learning: a Developmental Approach", University Pierre and Marie Curie, 2019.

PY Oudeyer was examiner of the PhD of Lisa Jacquey, titled "La sensibilité aux contingences sensorimotrices chez le bébé et son rôle dans le développement du savoir-faire corporel", from University of Paris, 2019.

PY Oudeyer was examiner in the PhD jury of Svetlana Meyer, on the topic "Entraînement de l'attention visuelle pour l'apprentissage de la lecture : l'apport du jeu vidéo d'action", University of Grenoble (feb. 2019).

Hélène Sauzéon organized a selection commitee for recruitment of Assistant professor in Rehabilitative science (University of de Bordeaux).

Hélène Sauzéon was external member of a selection commitee for recruitment of Assistant professor in cognitive psychology (University of Toulouse – LeMirail).

Hélène Sauzéon performed several scientific expertises for application requests such as HDR (ED SP2, University of Bordeaux) or local careers advancement (University of Bordeaux).

N. Díaz Rodríguez was invited jury (President) of the PhD thesis "Deep Learning for Abnormal Movement Detection using Wearable Sensors: Case Studies on Stereotypical Motor Movements in Autism and Freezing of Gait in Parkinson's Disease" in the University of Trento, Italy May 2019.

10.3. Popularization

10.3.1. Internal or external Inria responsibilities

Pierre-Yves Oudeyer has been member of the scientific committee for the permanent exhibition "Robots" at Cité des Sciences et de l'Industrie, Paris: http://www.cite-sciences.fr/fr/au-programme/expos-permanentes/expos-permanentes-dexplora/robots/lexposition/. See also https://www.inria.fr/fr/la-robotique-a-la-cite-des-sciences.

Pierre-Yves Oudeyer has been member of the scientific committee for the exhibition "Robots" at Cap Sciences, http://www.cap-sciences.net/au-programme/exposition/robots.

Pierre-Yves Oudeyer was member of the jury of the popular science competition Creathon in Poitiers.

Didier Roy is member of the team "Livre blanc Inria EdTech", with Gérard Giraudon, Pascal Guitton, Thierry Viéville and Margarida Romero.

Didier Roy is member of the Class'code and Class'code AI teams.

Didier Roy has been member of the organization committee for the public workshop/exhibition "Robots" at Cité des Sciences et de l'Industrie, Paris.

Didier Roy is vice-president of Poppy Station Structure. Poppy Station, which includes Poppy robot ecosystem (hardware, software, community) from the beginning, is a place of excellence to build future educational robots and to design pedagogical activities to teach computer science, robotics and Artificial Intelligence. https://www.poppy-station.org. Partners of Poppy Station : Inria, La Ligue de l'Enseignement, HESAM Université, SNCF Développement, IFÉ-ENS Lyon, MOBOTS – EPFL, Génération Robots, Pollen Robotics, KONEXInc, Mobsya, CERN Microclub, LINE Lab (Université Nice), Stripes, Canopé Martinique, Rights Tech Women, Editions Nathan.

10.3.2. Articles and contents

Sébastien Forestier and Pierre-Yves Oudeyer were interviewed for a video documentary on curiosity-driven learning in robots, now permanently displayed in the exhibition "Robots" at Cité des Sciences et de l'Industrie, Paris: http://www.cite-sciences.fr/fr/au-programme/expos-permanentes/expos-permanentes-dexplora/robots/lexposition/. The video is available here: https://www.youtube.com/watch?v=Kw724djJpUs.

PY Oudeyer was interviewed in RFI radio program "Autour de la question" on artificial intelligence and society (feb. 2019), http://www.rfi.fr/emission/20190211-comment-vivre-bonne-intelligence-toutes-intelligences.

Didier Roy and PY Oudeyer wrote an illustrated book on artificial intelligence and robotics for 7-8 years old children, to be published by Nathan.

10.3.3. Education

Hélène Sauzéon, as co-designer (with P. Guitton) of "Digital Accessibility" MOOC displayed on FUN platform, has interacted with the learners during the permanent session in 2019.

N Díaz Rodríguez participated on the Future Fest organized by the director and deans of School of AI with the objective of creating and self fund the first free degree on AI (April 2019, Granada, Spain. theSchool.ai).

Didier Roy is organizing an International R2T2 Robotics Mission Event for the EduCamp (RoboCup Junior 2020 at Bordeaux).

10.3.4. Interventions

Pierre-Yves Oudeyer gave a popular science conference at Lycée Montaigne, Bordeaux, on machine learning and AI (17th jan. 2019).

PY Oudeyer participated to a popular science debate on science-fiction movies and artificial intelligence at cinema Utopia, Bordeaux (jan. 2019).

PY Oudeyer gave an invited popular science talk at Collège des Bernardins, Paris, 2019, on affective machine learning and educational technologies, https://www.collegedesbernardins.fr/content/affects-numeriques-et-education and video at https://www.youtube.com/watch?v=WYd6RzaCQDc.

PY Oudeyer gave a popular science conference to 2nde students from Lycée La Sauque, Bordeaux.

PY Oudeyer gave a popular science presentation on artificial intelligence in the event "AI and education" organized at Inria Bordeaux by Didier Roy and Nicolas Rougier.

Hélène Sauzéon participated to several talks targetted disability-related professionals, students or industries : 1) Technologies educatives & Handicap Conference, organised by ESPE of Academy of Nantes, Mar., 20 ; 2) Journée d'étude de l'Observatoire des ressources numériques adaptées (Orna) « Autisme et outils numériques : de la recherche aux applications », May, 3at INSHE , Paris. ; 3) Colloque « Augmentation de l'humain » STAH Industrial Chair of Nouvelle Aquitaine, Mar., 28

Didier Roy gave an invited talk at CERN, Geneve, Switzerland, november 2019, on Educational Power of International R2T2 Robotics Missions

Didier Roy gave an invited talk at LEARN DAY, Bern, Switzerland, november 2019, on Strategies for introducing Robotics and Computer science activities at school.

Didier Roy organized the APEIA DAY (Artificial Intelligence & Education), at Inria BSO, Inria Sophia and open video-conference. Talks and workshop about unplugged and plugged activities for teaching AI from primary school to high education. With teachers, animators, education experts and AI researchers.

10.3.5. Internal action

Hélène Sauzéon has presented the « Collège + » and Kidlearn projects to Sophie Cluzel, Secretary of State for Disability, during the launch day of the Disability Plan of Inria (November, 16).

10.3.6. Creation of media or tools for science outreach

10.3.6.1. AIANA: an accessible multimedia player

Hélène Sauzéon is co-designer with P. Guitton of the accessible AIANA multimedia player for MOOCs. The V1 was developed by Learning Lab Inria in 2016 and the V2 by Damien Caseli (ADT engineer) as part of the POTIOC-Inria team in 2019. This player offers a flexible interface, configurable in terms of sensory and motor alternatives for the communication of people with physical disabilities, and of cognitive alternatives (attention load, reading aid, note-taking, etc.) for people with cognitive disabilities. The most convincing result is that it has increased the number of disabled learners completing a MOOC course (16%) on FUN platform compared to the available benchmark (10

10.3.6.2. Poppy Station: Robotics and AI for Education, Arts and Research with the Poppy platform

Didier Roy continued to promote and co-manage the Poppy Station Association.

Among the recent actions of poppy station, there were the training provided at the 2nd chance school created in Saintes by SNCF Development, the training given at the Institut Pasteur in Paris, on IT, robotics and artificial intelligence. Lasting collaborations have taken hold.

There is also a new artistic collaboration with the artist Clara Maïda and her project "(a)utom@ton" of contemporary musical and robotic creation (work for electroacoustic device and two humanoid robots).

Poppy Station has also participated in various events concerning educational robotics and artificial intelligence : APEIA Day at Inria Bordeaux, National Educational Robotics Colloquium at French Institute of education (ENS Lyon), Educatec Educatice exhibition in Paris, Ludovia Summer university in Ax-les-thermes.

A new open source wheeled robot printed in 3d was created for poppy Station by Pollen robotics, partner of poppy Station.

Poppy Station is also involved in European calls for projects with the Institut Pasteur around the continuous training of scientific staff on IT, robotics and AI.

Poppy Station Association brings together players from the world of business, research, training, culture and education and aims to develop and preserve robotic ecosystems and associated open source or free technologies, in all areas where their use can allow this development and preservation. The association pays particular attention to the fields of education, training, arts and research. Poppy Station is the result of a transfer of Inria research from its open-source robotics ecosystem Poppy to an external multi-partners structure. The Poppy ecosystem includes software and hardware tools to create and program robots, as well as educational content for education and training, and a large interdisciplinary community of users. This ecosystem was created and developed by the Inria Flowers team, with the aim of facilitating the experimentation and creation of innovative robotic tools in the fields of education, research and the arts. http://www.poppy-station.org.

10.3.6.3. IniRobot: Educational Robotics in Primary Schools

Didier Roy and PY Oudeyer continued to promote and disseminate the IniRobot pedagogical toolkit. Irirobot, a project done in collaboration with EPFL/Mobsya, aims to create, evaluate and disseminate a pedagogical kit which uses Thymio robot, an open-source and low cost robot, for teaching computer science and robotics.

IniRobot Project aims to produce and diffuse a pedagogical kit for teachers and animators, to help them and to train them directly or by the way of external structures. The aim of the kit is to initiate children to computer science and robotics. The kit provides a micro-world for learning, and takes an inquiry-based educational approach, where kids are led to construct their understanding through practicing an active investigation methodology within teams. See https://dm1r.inria.fr/c/kits-pedagogiques/inirobot or http://www.inirobot.fr.

Deployment: After 4 years of activity, IniRobot is used by more than 3000 adults, 30 000 children in France. Inirobot is also used in higher education, for example in Master 2 "Neurosciences, human and animal cognition" at the Paul Sabatier University in Toulouse. Inirobot is additionally used to train the management and elected officials of the Bordeaux metropolitan area (20 people). The digital mediators of the 8 Inria centers are trained to Inirobot and use it in their activities.

10.3.6.3.1. Partnership

The project continues to be carried out in main collaboration with the LSRO Laboratory from EPFL (Lausanne) and others collaborations such as the French National Education/Rectorat d'Aquitaine, the Canopé Educational Network, the ESPE (teacher's school) Aquitaine, the ESPE Martinique, the ESPE Poitiers and the National Directorate of Digital Education.

10.3.6.3.2. Created pedagogical documents and resources

- The inirobot pedagogical kit [87]: This pedagogical booklet provides activities scenarized as missions to do. An updated version of the Inirobot pedagogical kit is available at: https://dm1r.inria.fr/uploads/default/original/1X/70037bdd5c290e48c7ec4cb4f26f0e426a4b4cf6.pdf. Another pedagogical booklet has been also created by three pedagogical advisers for primary school, with pedagogical instructions and aims, under our supervision. The new pedagogical kit,"Inirobot Scolaire, Langages et robotique", which extends Inirobot to a full primary school approach is available at https://blogacabdx.ac-bordeaux.fr/numerique33/2018/10/04/robotique-sequence-inirobot-scolaire/
- Inirobot website and forum: https://dm1r.inria.fr/c/kits-pedagogiques/inirobot or http://www.inirobot.fr On this website, teachers, animators and general public can download documents, exchange about their use of inirobot's kit.

10.3.6.3.3. Scientific mediation

Inirobot is very popular and often presented in events (conferences, workshops, ...) by us and others.

10.3.6.3.4. Spread of Inirobot activities

Inirobot activities are used by several projects: Dossier 123 codez from Main à la Pâte Fundation, Classcode project, ...

10.3.6.3.5. MOOC Thymio

The MOOC Thymio, released in october 2018, in collaboration with Inria Learning Lab and EPFL (Lausanne, Switzerland), on FUN platform and edX EPFL Platform), use Inirobot activities to teach how to use Thymio robot in education.

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Project-Team GEOSTAT

Geometry and Statistics in acquisition data

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Optimization, machine learning and statistical methods

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Project-Team GEOSTAT

Creation of the Team: 2009 November 01, updated into Project-Team: 2011 January 01

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2. Overall Objectives

2.1. Overall Objectives

GEOSTAT is a research project which investigates the analysis of some classes of natural complex signals (physiological time series, turbulent universe and earth observation data sets) by determining, in acquired signals, the properties that are predicted by commonly admitted or new physical models best fitting the phenomenon. Consequently, when statistical properties discovered in the signals do not match closely enough those predicted by accepted physical models, we question the validity of existing models or propose, whenever possible, modifications or extensions of existing models. We will give, in the sequel, a detailed example of this approach and methodology.

An important aspect of this methodological approach is that we don't rely on a predetermined "universal" signal processing model to analyze natural complex signals. Instead, we take into consideration existing approaches in nonlinear signal processing (wavelets, multifractal analysis tools such as log-cumulants or micro-canonical multifractal formalism, time frequency analysis etc.) which are used to determine the micro structures or other micro features inside the acquired signals. Then, statistical analysis of these micro data are determined and compared to expected behaviour from theoretical physical models used to describe the phenomenon from which the data is acquired. From there different possibilities can be contemplated:

- The statistics match behaviour predicted by the model: complexity parameters predicted by the model are extracted from signals to analyze the dynamics of underlying phenomena. Examples: analysis of turbulent data sets in Oceanography and Astronomy.
- The signals displays statistics that cannot be attainable by the common lore of accepted models: how to extend or modify the models according to the behaviour of observed signals ? Example: electrical activity of heart signal analysis (see infra).

GEOSTAT is a research project in nonlinear signal processing which develops on these considerations: it considers the signals as the realizations of complex extended dynamical systems. The driving approach is to describe the relations between complexity (or information content) and the geometric organization of information in a signal. For instance, for signals which are acquisitions of turbulent fluids, the organization of information may be related to the effective presence of a multiscale hierarchy of coherent structures, of multifractal nature, which is strongly related to intermittency and multiplicative cascade phenomena ; the determination of this geometric organization unlocks key nonlinear parameters and features associated to these signals; it helps understand their dynamical properties and their analysis. We use this approach to derive novel solution methods for super-resolution and data fusion in Universe Sciences acquisitions [12]. Another example can be found in signal analysis of the electrical activity of the heart, where we find the distribution of activation points in a signal during episodes of atrial fibrilation (with strengthening from feature selection and Bayesian learning see below). Specific advances are obtained in GEOSTAT in using this type of statistical/geometric approach to get validated dynamical information of signals acquired in Universe Sciences, e.g. Oceanography or Astronomy. The research in GEOSTAT encompasses nonlinear signal processing and the study of emergence in complex systems, with a strong emphasis on geometric approaches to complexity. Consequently, research in GEOSTAT is oriented towards the determination, in real signals, of quantities or phenomena, usually unattainable through linear methods, that are known to play an important role both in the evolution of dynamical systems whose acquisitions are the signals under study, and in the compact representations of the signals themselves.

2.1.1.

Signals studied in GEOSTAT belong to two broad classes:

- Acquisitions in Astronomy and Earth Observation.
- Physiological time series.

3. Research Program

3.1. General methodology

Fully Developed Turbulence (FDT) Turbulence at very high Reynolds numbers; systems in FDT are beyond deterministic chaos, and symmetries are restored in a statistical sense only, and multi-scale correlated structures are landmarks. Generalizing to more random uncorrelated multi-scale structured turbulent fields.

Compact Representation Reduced representation of a complex signal (dimensionality reduction) from which the whole signal can be reconstructed. The reduced representation can correspond to points randomly chosen, such as in Compressive Sensing, or to geometric localization related to statistical information content (framework of reconstructible systems).

Sparse representation The representation of a signal as a linear combination of elements taken in a dictionary (frame or Hilbertian basis), with the aim of finding as less as possible non-zero coefficients for a large class of signals.

Universality class In theoretical physics, the observation of the coincidence of the critical exponents (behaviour near a second order phase transition) in different phenomena and systems is called universality. Universality is explained by the theory of the renormalization group, allowing for the determination of the changes followed by structured fluctuations under rescaling, a physical system is the stage of. The notion is applicable with caution and some differences to generalized out-of-equilibrium or disordered systems. Non-universal exponents (without definite classes) exist in some universal slowing dynamical phenomena like the glass transition and kindred. As a consequence, different macroscopic phenomena displaying multiscale structures (and their acquisition in the form of complex signals) may be grouped into different sets of generalized classes.

Every signal conveys, as a measure experiment, information on the physical system whose signal is an acquisition of. As a consequence, it seems natural that signal analysis or compression should make use of physical modelling of phenomena: the goal is to find new methodologies in signal processing that goes beyond the simple problem of interpretation. Physics of disordered systems, and specifically physics of (spin) glasses is putting forward new algorithmic resolution methods in various domains such as optimization, compressive sensing etc. with significant success notably for NP hard problem heuristics. Similarly, physics of turbulence introduces phenomenological approaches involving multifractality. Energy cascades are indeed closely related to geometrical manifolds defined through random processes. At these structures' scales, information in the process is lost by dissipation (close to the lower bound of inertial range). However, all the cascade is encoded in the geometric manifolds, through long or short distance correlations depending on cases. How do these geometrical manifold structures organize in space and time, in other words, how does the scale entropy cascades itself ? To unify these two notions, a description in term of free energy of a generic physical model is sometimes possible, such as an elastic interface model in a random nonlinear energy landscape : This is for instance the correspondence between compressible stochastic Burgers equation and directed polymers in a disordered medium. Thus, trying to unlock the fingerprints of cascade-like structures in acquired natural signals becomes a fundamental problem, from both theoretical and applicative viewpoints.

To illustrate the general methodology undertaken, let us focus on an example conducted in the study of physiological time series: the analysis of signals recorded from the electrical activity of the heart in the general setting of Atrial Fibrillation (AF). AF is a cardiac arrhythmia characterized by rapid and irregular atrial electrical activity with a high clinical impact on stroke incidence. Best available therapeutic strategies combine pharmacological and surgical means. But when successful, they do not always prevent long-term relapses. Initial success becomes all the more tricky to achieve as the arrhythmia maintains itself and the pathology evolves into sustained or chronic AF. This raises the open crucial issue of deciphering the mechanisms that govern the onset of AF as well as its perpetuation. We have developed a wavelet-based multi-scale strategy to analyze the electrical activity of human hearts recorded by catheter electrodes, positioned in the coronary sinus (CS), during episodes of chronic AF. We have computed the so-called multifractal spectra using two variants of the wavelet transform modulus maxima method, the moment (partition function) method and the magnitude cumulant method (checking confidence intervals with surrogate data). Application of these methods to long time series recorded in a patient with chronic AF provides quantitative evidence of the multifractal intermittent nature of the electric energy of passing cardiac impulses at low frequencies, *i.e.* for times ($>\sim 0.5$ s) longer than the mean interbeat ($\simeq 10^{-1}$s). We have also reported the results of a two-point magnitude correlation analysis which infers the absence of a multiplicative time-scale structure underlying multifractal scaling. The electric energy dynamics looks like a “multifractal white noise” with quadratic (log-normal) multifractal spectra. *These observations challenge concepts of functional reentrant circuits in mechanistic theories of AF*. A transition is observed in the computed multifractal spectra which group according to two distinct areas, consistently with the anatomical substrate binding to the CS, namely the left atrial posterior wall, and the ligament of Marshall which is innervated by the ANS. These negative results challenge also the existing models, which by principle cannot explain such results. As a consequence, we go beyond the existing models and propose a mathematical model of a denervated heart where the kinetics of gap junction conductance alone induces a desynchronization of the myocardial excitable cells, accounting for the multifractal spectra found experimentally in the left atrial posterior wall area (devoid of ANS influence).

3.2. Turbulence in insterstellar clouds and Earth observation data

The research described in this section is a collaboration effort of GEOSTAT, CNRS LEGOS (Toulouse), CNRS LAM (Marseille Laboratory for Astrophysics), MERCATOR (Toulouse), IIT Roorkee, Moroccan Royal Center for Teledetection (CRST), Moroccan Center for Science CNRST, Rabat University, University of Heidelberg. Researchers involved:

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The analysis and modeling of natural phenomena, specially those observed in geophysical sciences and in astronomy, are influenced by statistical and multiscale phenomenological descriptions of turbulence; indeed these descriptions are able to explain the partition of energy within a certain range of scales. A particularly important aspect of the statistical theory of turbulence lies in the discovery that the support of the energy transfer is spatially highly non uniform, in other terms it is *intermittent* [70]. Because of the absence of localization of the Fourier transform, linear methods are not successful to unlock the multiscale structures and cascading properties of variables which are of primary importance as stated by the physics of the phenomena. This is the reason why new approaches, such as DFA (Detrented Fluctuation Analysis), Time-frequency analysis, variations on curvelets [66] etc. have appeared during the last decades. Recent advances in dimensionality reduction, and notably in Compressive Sensing, go beyond the Nyquist rate in sampling theory using nonlinear reconstruction, but data reduction occur at random places, independently of geometric localization of information content, which can be very useful for acquisition purposes, but of lower impact in signal analysis. We are successfully making use of a microcanonical formulation of the multifractal theory, based on predictability and reconstruction, to study the turbulent nature of interstellar molecular or atomic clouds. Another important result obtained in GEOSTAT is the effective use of multiresolution analysis associated to optimal inference along the scales of a complex system. The multiresolution analysis is performed on dimensionless quantities given by the *singularity exponents* which encode properly the geometrical structures associated to multiscale organization. This is applied successfully in the derivation of high resolution ocean dynamics, or the high resolution mapping of gaseous exchanges between the ocean and the atmosphere; the latter is of primary importance for a quantitative evaluation of global warming. Understanding the dynamics of complex systems is recognized as a new discipline, which makes use of theoretical and methodological foundations coming from nonlinear physics, the study of dynamical systems and many aspects of computer science. One of the challenges is related to the question of *emergence* in complex systems: large-scale effects measurable macroscopically from a system made of huge numbers of interactive agents [31], [61]. Some quantities related to nonlinearity, such as Lyapunov exponents, Kolmogorov-Sinai entropy etc. can be computed at least in the phase space [32]. Consequently, knowledge from acquisitions of complex systems (which include *complex signals*) could be obtained from information about the phase space. A result from F. Takens [67] about strange attractors in turbulence has motivated the theoretical determination of nonlinear characteristics associated to complex acquisitions. Emergence phenomena can also be traced inside complex signals themselves, by trying to localize information content geometrically. Fundamentally, in the nonlinear analysis of complex signals there are broadly two approaches: characterization by attractors (embedding and bifurcation) and time-frequency, multiscale/multiresolution approaches. In real situations, the phase space associated to the acquisition of a complex phenomenon is unknown. It is however possible to relate, inside the signal's domain, local predictability to local reconstruction [13] and to deduce relevant information associated to multiscale geophysical signals [14]. A multiscale organization is a fundamental feature of a complex system, it can be for example related to the cascading properties in turbulent systems. We make use of this kind of description when analyzing turbulent signals: intermittency is observed within the inertial range and is related to the fact that, in the case of FDT (fully developed turbulence), symmetry is restored only in a statistical sense, a fact that has consequences on the quality of any nonlinear signal representation by frames or dictionaries.

The example of FDT as a standard "template" for developing general methods that apply to a vast class of complex systems and signals is of fundamental interest because, in FDT, the existence of a multiscale hierarchy $\mathcal{F}_h$ which is of multifractal nature and geometrically localized can be derived from physical considerations. This geometric hierarchy of sets is responsible for the shape of the computed singularity spectra, which in turn is related to the statistical organization of information content in a signal. It explains scale invariance, a characteristic feature of complex signals. The analogy from statistical physics comes from the fact that singularity exponents are direct generalizations of *critical exponents* which explain the macroscopic properties of a system around critical points, and the quantitative characterization of *universality classes*, which allow the definition of methods and algorithms that apply to general complex signals and systems, and not only turbulent signals: signals which belong to a same universality class share common statistical organization. During the past decades, canonical approaches permitted the development of a well-established analogy taken from thermodynamics in the analysis of complex signals: if $\mathcal{F}$ is the free energy, $\mathcal{T}$ the temperature measured in energy units, $\mathcal{U}$ the internal energy per volume unit $\mathcal{S}$ the entropy and $\widehat{\beta} = 1/\mathcal{T}$, then the scaling exponents associated to moments of intensive variables $p \to \tau_p$ corresponds to $\widehat{\beta}\mathcal{F}$, $\mathcal{U}(\widehat{\beta})$ corresponds to the singularity exponents values, and $\mathcal{S}(\mathcal{U})$ to the singularity spectrum [27]. The research goal is to be able to determine universality classes associated to acquired signals, independently of microscopic properties in the phase space of various complex systems, and beyond the particular case of turbulent data [53].

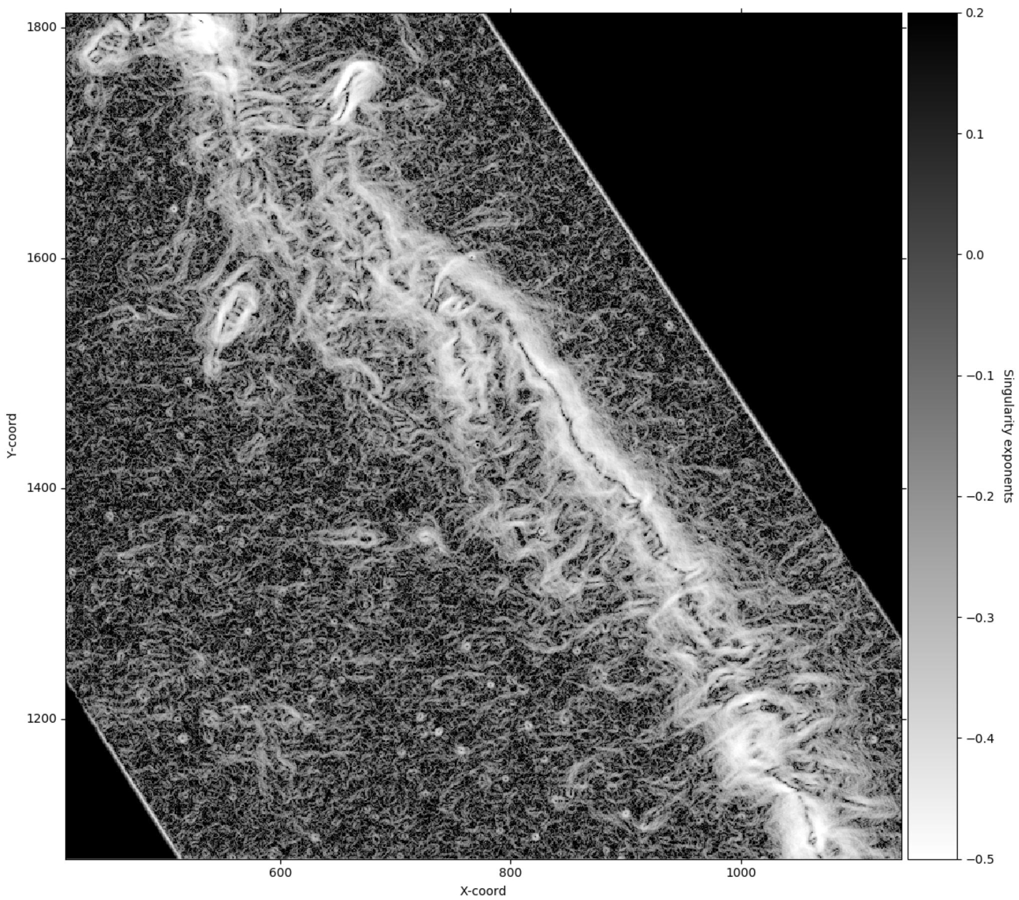

Figure 1. Visualization of the singularity exponents, computed on a edge-aware filtered Musca Herschel observation map .

We show in figure 1 the result of the computation of singularity exponents on an *Herschel* astronomical observation map (the Musca galactic cloud) which has been edge-aware filtered using sparse L^1 filtering to eliminate the cosmic infrared background (or CIB), a type of noise that can modify the singularity spectrum of a signal.

3.3. Causal modeling

The team is working on a new class of models for modeling physical systems, starting from measured data and accounting for their dynamics [40]. The idea is to statistically describe the evolution of a system in terms of causally-equivalent states; states that lead to the same predictions [33]. Transitions between these states can be reconstructed from data, leading to a theoretically-optimal predictive model [63]. In practice, however, no algorithm is currently able to reconstruct these models from data in a reasonable time and without substantial discrete approximations. Recent progress now allows a continuous formulation of predictive causal models. Within this framework, more efficient algorithms may be found. The broadened class of predictive models promises a new perspective on structural complexity in many applications.

3.4. Speech analysis

Phonetic and sub-phonetic analysis: We developed a novel algorithm for automatic detection of Glottal Closure Instants (GCI) from speech signals using the Microcanonical Multiscale Formalism (MMF). This state of the art algorithm is considered as a reference in this field. We made a Matlab code implementing it available to the community (link). Our approach is based on the Microcanonical Multiscale Formalism. We showed that in the case of clean speech, our algorithm performs almost as well as a recent state-of-the-art method. In presence of different types of noises, we showed that our method is considerably more accurate (particularly for very low SNRs). Moreover, our method has lower computational times does not rely on an estimate of pitch period nor any critical choice of parameters. Using the same MMF, we also developed a method for phonetic segmentation of speech signal. We showed that this method outperforms state of the art ones in term of accuracy and efficiency.

Pathological speech analysis and classification: we made a critical analysis of some widely used methodologies in pathological speech classification. We then introduced some novel methods for extracting some common features used in pathological speech analysis and proposed more robust techniques for classification.

Speech analysis of patients with Parkinsonism: with our collaborators from the Czech Republic, we started preliminary studies of some machine learning issues in the field essentially due the small amount of training data.

3.5. Excitable systems: analysis of physiological time series

The research described in this section is a collaboration effort of GEOSTAT, CNRS LOMA (Laboratoire Ondes et Matière d'Aquitaine) and Laboratory of Physical Foundation of Strength, Institute of Continuous Media Mechanics (Perm, Russia Federation).

AF is an arrhythmia originating in the rapid and irregular electrical activity of the atria (the heart's two upper chambers) that causes their pump function to fail, increasing up to fivefold the risk of embolic stroke. The prevailing electrophysiological concepts describing tachy-arrhythmias are more than a century old. They involve abnormal automaticity and conduction [52]. Initiation and maintenance are thought to arise from a vulnerable substrate prone to the emergence of multiple self-perpetuating reentry circuits, also called "multiple wavelets" [59], [60]. Reentries may be driven structurally, for instance because of locally high fibrous tissue content which badly conducts, or functionally because of high spatial dispersion of decreased refractoriness and APD [58]. The latter is coined the leading circle concept with the clinically more relevant notion of a critical "wavelength" (in fact the length) of the cardiac impulse [26], [65], [62], [30]. The related concept of vulnerability was originally introduced to uncover a physiological substrate evolving from normality to pathology. It was found in vulnerable patients that high rate frequency would invariably lead to functional disorder as cardiac cells would no longer properly adapt their refractoriness [29]. Mathematical models have managed to exhibit likewise phenomena, with the generation of breaking spiral waves in various conditions [49], [54]. The triggering role of abnormal ectopic activity of the pulmonary veins has been demonstrated on patients with paroxysmal AF resistant to drug therapy [48], but its origin still remains poorly understood. This region is highly innervated with sympathetic and parasympathetic stimulation from the ANS [68], [69], [28]. In particular, Coumel et al. [39], [38] have revealed the pathophysiological role of the vagal tone on a vulnerable substrate. It is frequently observed that rapid tachycardia of ectopic origin transits to AF. This is known to result from electrical remodeling. As described for the first time by Allessie et al. [25], remodeling is a transient and reversible process by which the impulse properties such as its refractory period are altered during the course of the arrhythmia, promoting its perpetuation: “AF begets AF” [71]. Under substantial beating rate increase, cells may undergo remodeling to overcome the toxicity of their excessive intercellular calcium loading, by a rapid down regulation (a few minutes) of their L-type calcium membrane current. Moreover, other ionic channel functions are also modified such as the potassium channel function, inducing a change in the conduction properties including the conduction velocity. The intercellular coupling at the gap junction level shows also alterations of their connexin expression and dispersion.

Wavelet-based methods (WTMM, log-cumulants, two point scale correlations), and confidence statistical methodology, have been applied to catheter recordings in the coronary sinus vein right next to the left atria of a small sample of patients with various conditions, and exhibit clear multifractal scaling without cross-scale correlation, which are coined ”multifractal white noise”, and that can be grouped according to two anatomical regions. One of our main result was to show that this is incompatible with the common lore for atrial fibrillation based on so-called circuit reentries. We used two declinations of a wavelet-based multiscale method, the moment (partition function) method and the magnitude cumulant method, as originally introduced in the field of fully developed turbulence. In the context of cardiac physiology, this methodology was shown to be valuable in assessing congestive heart failure from the monitoring of sinus heart rate variability [50]. We develop a model such that the substrate function is modulated by the kinetics of conduction. A simple reversible mechanism of short term remodeling under rapid pacing is demonstrated, by which ionic overload acts locally (dynamical feedback) on the kinetics of gap junction conductance. The whole process may propagate and pervade the myocardium via electronic currents, becoming desynchronized. In a new description, we propose that circuit reentries may well exist before the onset of fibrillation, favoring onset but not contributing directly to the onset and perpetuation. By contrast, cell-to-cell coupling is considered fundamentally dynamical. The rationale stems from the observation that multifractal scaling necessitates a high number of degrees of freedom (tending to infinity with system size), which can originate in excitable systems in hyperbolic spatial coupling.

3.6. Data-based identification of characteristic scales and automated modeling

Data are often acquired at the highest possible resolution, but that scale is not necessarily the best for modeling and understanding the system from which data was measured. The intrinsic properties of natural processes do not depend on the arbitrary scale at which data is acquired; yet, usual analysis techniques operate at the acquisition resolution. When several processes interact at different scales, the identification of their characteristic scales from empirical data becomes a necessary condition for properly modeling the system. A classical method for identifying characteristic scales is to look at the work done by the physical processes, the energy they dissipate over time. The assumption is that this work matches the most important action of each process on the studied natural system, which is usually a reasonable assumption. In the framework of time-frequency analysis [45], the power of the signal can be easily computed in each frequency band, itself matching a temporal scale.

However, in open and dissipating systems, energy dissipation is a prerequisite and thus not necessarily the most useful metric to investigate. In fact, most natural, physical and industrial systems we deal with fall in this category, while balanced quasi-static assumptions are practical approximation only for scales well below the characteristic scale of the involved processes. Open and dissipative systems are not locally constrained by the inevitable rise in entropy, thus allowing the maintaining through time of mesoscopic ordered structures. And, according to information theory [47], more order and less entropy means that these structures have a higher information content than the rest of the system, which usually gives them a high functional role.

We propose to identify characteristic scales not only with energy dissipation, as usual in signal processing analysis, but most importantly with information content. Information theory can be extended to look at which scales are most informative (e.g. multi-scale entropy [37], ε-entropy [36]). Complexity measures quantify the presence of structures in the signal (e.g. statistical complexity [42], MPR [56] and others [44]). With these notions, it is already possible to discriminate between random fluctuations and hidden order, such as in chaotic systems [41], [56]. The theory of how information and structures can be defined through scales is not complete yet, but the state of art is promising [43]. Current research in the team focuses on how informative scales can be found using collections of random paths, assumed to capture local structures as they reach out [35].

Building on these notions, it should also possible to fully automate the modeling of a natural system. Once characteristic scales are found, causal relationships can be established empirically. They are then clustered together in internal states of a special kind of Markov models called ϵ-machines [42]. These are known to be the optimal predictors of a system, with the drawback that it is currently quite complicated to build them properly, except for small system [64]. Recent extensions with advanced clustering techniques [34], [46], coupled with the physics of the studied system (e.g. fluid dynamics), have proved that ϵ-machines are applicable to large systems, such as global wind patterns in the atmosphere [51]. Current research in the team focuses on the use of reproducing kernels, coupled possibly with sparse operators, in order to design better algorithms for ϵ-machines reconstruction. In order to help with this long-term project, a collaboration is ongoing with J. Crutchfield lab at UC Davis.

4. Application Domains

4.1. Sparse signals & optimization

This research topic involves **Geostat** team and is used to set up an InnovationLab with I2S company

Sparsity can be used in many ways and there exist various sparse models in the literature; for instance minimizing the l_0 quasi-norm is known to be an NP-hard problem as one needs to try all the possible combinations of the signal's elements. The l_1 norm, which is the convex relation of the l_0 quasi-norm results in a tractable optimization problem. The l_p pseudo-norms with $0 < p < 1$ are particularly interesting as they give closer approximation of l_0 but result in a non-convex minimization problem. Thus, finding a global minimum for this kind of problem is not guaranteed. However, using a non-convex penalty instead of the l_1 norm has been shown to improve significantly various sparsity-based applications. Nonconvexity has a lot of statistical implications in signal and image processing. Indeed, natural images tend to have a heavy-tailed (kurtotic) distribution in certain domains such as wavelets and gradients. Using the l_1 norm comes to consider a Laplacian distribution. More generally, the hyper-Laplacian distribution is related to the l_p pseudo-norm ($0 < p < 1$) where the value of p controls how the distribution is heavy-tailed. As the hyper-Laplacian distribution for $0 < p < 1$ represents better the empirical distribution of the transformed images, it makes sense to use the l_p pseudo-norms instead of l_1. Other functions that better reflect heavy-tailed distributions of images have been used as well such as Student-t or Gaussian Scale Mixtures. The internal properties of natural images have helped researchers to push the sparsity principle further and develop highly efficient algorithms for restoration, representation and coding. Group sparsity is an extension of the sparsity principle where data is clustered into groups and each group is sparsified differently. More specifically, in many cases, it makes sense to follow a certain structure when sparsifying by forcing similar sets of points to be zeros or non-zeros simultaneously. This is typically true for natural images that represent coherent structures. The concept of group sparsity has been first used for simultaneously shrinking groups of wavelet coefficients because of the relations between wavelet basis elements. Lastly, there is a strong relationship between sparsity, nonpredictability and scale invariance.

We have shown that the two powerful concepts of sparsity and scale invariance can be exploited to design fast and efficient imaging algorithms. A general framework has been set up for using non-convex sparsity by applying a first-order approximation. When using a proximal solver to estimate a solution of a sparsity-based optimization problem, sparse terms are always separated in subproblems that take the form of a proximal operator. Estimating the proximal operator associated to a non-convex term is thus the key component to use efficient solvers for non-convex sparse optimization. Using this strategy, only the shrinkage operator changes and thus the solver has the same complexity for both the convex and non-convex cases. While few previous works have also proposed to use non-convex sparsity, their choice of the sparse penalty is rather limited to functions like the l_p pseudo-norm for certain values of $p \geq 0.5$ or the Minimax Concave (MC) penalty because they admit an analytical solution. Using a first-order approximation only requires calculating the (super)gradient of the function, which makes it possible to use a wide range of penalties for sparse regularization. This is important in various applications where we need a flexible shrinkage function such as in edge-aware processing. Apart from non-convexity, using a first-order approximation makes it easier to verify the optimality condition of proximal operator-based solvers via fixed-point interpretation. Another problem that arises in various imaging applications but has attracted less works is the problem of multi-sparsity, when the minimization problem includes various sparse terms that can be non-convex. This is typically the case when looking for a sparse solution in a certain domain while rejecting outliers in the data-fitting term. By using one intermediate variable per sparse term, we show that proximal-based solvers can be efficient. We give a detailed study of the Alternating Direction Method of Multipliers (ADMM) solver for multi-sparsity and study its properties. The following subjects are addressed and receive new solutions:

1. **Edge aware smoothing**: given an input image g, one seeks a smooth image u "close" to g by minimizing:

$$\underset{u}{\text{argmin}}\ \frac{\lambda}{2}\|u-g\|_2^2 + \psi(\nabla u)$$

   where ψ is a sparcity-inducing non-convex function and λ a positive parameter. Splitting and alternate minimization lead to the sub-problems:

$$\begin{aligned} (\text{sp1}) \quad &: \quad v^{(k+1)} \longleftarrow \underset{v}{\text{argmin}}\ \psi(v) + \frac{\beta}{2}\|\nabla u^{(k)} - v\|_2^2 \\ (\text{sp2}) \quad &: \quad u^{(k+1)} \longleftarrow \underset{u}{\text{argmin}}\ \lambda\|u-g\|_2^2 + \beta\|\nabla u - v^{(k+1)}\|_2^2. \end{aligned}$$

   We solve sub-problem (sp2) through deconvolution and efficient estimation via separable filters and warm-start initialization for fast GPU implementation, and sub-problem (sp1) through non-convex proximal form.

2. **Structure-texture separation**: gesign of an efficient algorithm using non-convex terms on both the data-fitting and the prior. The resulting problem is solved via a combination of Half-Quadratic (HQ) and Maximization-Minimization (MM) methods. We extract challenging texture layers outperforming existing techniques while maintaining a low computational cost. Using spectral sparsity in the framework of low-rank estimation, we propose to use robust Principal Component Analysis (RPCA) to perform robust separation on multi-channel images such as glare and artifacts removal of flash/no-flash photographs. As in this case, the matrix to decompose has much less columns than lines, we propose to use a QR decomposition trick instead of a direct singular value decomposition (SVD) which makes the decomposition faster.

3. **Robust integration**: in many applications, we need to reconstruct an image from corrupted gradient fields. The corruption can take the form of outliers only when the vector field is the result of transformed gradient fields (low-level vision), or mixed outliers and noise when the field is estimated from corrupted measurements (surface reconstruction, gradient camera, Magnetic Resonance Imaging (MRI) compressed sensing, etc.). We use non-convexity and multi-sparsity to build efficient integrability enforcement algorithms. We present two algorithms : 1) a local algorithm that uses sparsity in the gradient field as a prior together with a sparse data-fitting term, 2) a non-local algorithm that uses sparsity in the spectral domain of non-local patches as a prior together with a

sparse data-fitting term. Both methods make use of a multi-sparse version of the Half-Quadratic solver. The proposed methods were the first in the literature to propose a sparse regularization to improve integration. Results produced with these methods significantly outperform previous works that use no regularization or simple l_1 minimization. Exact or near-exact recovery of surfaces is possible with the proposed methods from highly corrupted gradient fields with outliers.

4. **Learning image denoising**: deep convolutional networks that consist in extracting features by repeated convolutions with high-pass filters and pooling/downsampling operators have shown to give near-human recognition rates. Training the filters of a multi-layer network is costly and requires powerful machines. However, visualizing the first layers of the filters shows that they resemble wavelet filters, leading to sparse representations in each layer. We propose to use the concept of scale invariance of multifractals to extract invariant features on each sparse representation. We build a bi-Lipschitz invariant descriptor based on the distribution of the singularities of the sparsified images in each layer. Combining the descriptors of each layer in one feature vector leads to a compact representation of a texture image that is invariant to various transformations. Using this descriptor that is efficient to calculate with learning techniques such as classifiers combination and artificially adding training data, we build a powerful texture recognition system that outperforms previous works on 3 challenging datasets. In fact, this system leads to quite close recognition rates compared to latest advanced deep nets while not requiring any filters training.

5. Highlights of the Year

5.1. Highlights of the Year

- Inria's exploratory action "TRACME" led by N. Brodu, starting October 2019.

6. New Software and Platforms

6.1. Fluex

KEYWORDS: Signal - Signal processing

SCIENTIFIC DESCRIPTION: Fluex is a package consisting of the Microcanonical Multiscale Formalism for 1D, 2D 3D and 3D+t general signals.

FUNCTIONAL DESCRIPTION: Fluex is a C++ library developed under Gforge. Fluex is a library in nonlinear signal processing. Fluex is able to analyze turbulent and natural complex signals, Fluex is able to determine low level features in these signals that cannot be determined using standard linear techniques.

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- URL: http://fluex.gforge.inria.fr/

6.2. FluidExponents

KEYWORDS: Signal processing - Wavelets - Fractal - Spectral method - Complexity

FUNCTIONAL DESCRIPTION: FluidExponents is a signal processing software dedicated to the analysis of complex signals displaying multiscale properties. It analyzes complex natural signals by use of nonlinear methods. It implements the multifractal formalism and allows various kinds of signal decomposition and reconstruction. One key aspect of the software lies in its ability to evaluate key concepts such as the degree of impredictability around a point in a signal, and provides different kinds of applications. The software can be used for times series or multidimensional signals.

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6.3. classifemo

KEYWORDS: Classification - Audio

FUNCTIONAL DESCRIPTION: Classifies vocal audio signals. Classifemo extracts characteristics from vocal audio signals. These characteristics are extracted from signals of different type: initially these were emotion databases, but it can also process signals recorded from patients with motor speach disorders. The software can train usual classifiers (SVM, random forests, etc) on these databases as well as classify new signals.

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6.4. superres

Super-Resolution of multi-spectral and multi-resolution images

KEYWORD: Multiscale

SCIENTIFIC DESCRIPTION: This resolution enhancement method is designed for multispectral and multiresolution images, such as these provided by the Sentinel-2 satellites (but not only). Starting from the highest resolution bands, band-dependent information (reflectance) is separated from information that is common to all bands (geometry of scene elements). This model is then applied to unmix low-resolution bands, preserving their reflectance, while propagating band-independent information to preserve the sub-pixel details.

FUNCTIONAL DESCRIPTION: This super-resolution software for multi-spectral images consists of: - A core C++ library, which can be used directly - A Python module interface to this library - A Java JNI interface to the library - An end-user Python script for super-resolving Sentinel-2 images - An end-user plugin for the widely used SNAP software of the ESA.

- Participant: Nicolas Brodu
- Contact: Nicolas Brodu
- URL: http://nicolas.brodu.net/recherche/superres/index.html

6.5. EdgeReconstruct

Edge Reconstruction With UPM Manifold

KEYWORDS: 2D - Fractal - Signal processing

FUNCTIONAL DESCRIPTION: EdgeReconstruct is a software that reconstructs a complex signal from the computation of most unpredictible points in the framework of the Microcanonical Multifractal Formalism. The quality of the reconstruction is also evaluated. The software is a companion of a paper published in 2013: https://hal.inria.fr/hal-00924137.

- Contact: Suman Kumar Maji
- URL: https://geostat.bordeaux.inria.fr/index.php/downloads.html

6.6. ProximalDenoising

KEYWORDS: 2D - Image filter - Filtering - Minimizing overall energy - Noise - Signal processing - Image reconstruction - Image processing

SCIENTIFIC DESCRIPTION: Image filtering is contemplated in the form of a sparse minimization problem in a non-convex setting. Given an input image I, one seeks to compute a denoised output image u such that u is close to I in the L2 norm. To do so, a minimization term is added which favors sparse gradients for output image u. Imposing sparse gradients lead to a non-convex minimization term: for instance a pseudo-norm Lp with $0 < p < 1$ or a Cauchy or Welsh function. Half-quadratic algorithm is used by adding a new variable in the minimization functionnal which leads to two sub-problems, the first sub-problem is non-convex and solved by use of proximal operators. The second sub-problem can be written in variational form, and is best solved in Fourier space: it takes the form of a deconvolution operator whose kernel can be approximated by a finite sum of separable filters. This solution method produces excellent computation times even on big images.

FUNCTIONAL DESCRIPTION: Use of proximal and non quadratic minimization. GPU implementation.

RELEASE FUNCTIONAL DESCRIPTION: This software implements H. Badri PhD thesis results.

- Authors: Marie Martin, Chiheb Sakka, Hussein Yahia, Nicolas Brodu, Gabriel Augusto Zebadua Garcia and Khalid Daoudi
- Partner: Innovative Imaging Solutions I2S
- Contact: Hussein Yahia
- URL: https://gitlab.inria.fr/marmarti/i2s_geostat_C

6.7. Amuencha

Musical analyzer and singing training

KEYWORDS: Audio - Real-time rendering

SCIENTIFIC DESCRIPTION: The typical audio analyzer uses Fast Fourier Transforms (FFT) in order to find the frequency content. The problem with this approach is that notes follow the logarithm of the frequencies... while the FFT is linear in frequency. This results in a loss of precision. Even worse, the window function used for localizing the frequencies in time is often non-optimal, which increases this precision loss. Generally, nearby frequencies « bleed on » the one being analyed. Amuencha does not uses FFT. I first create a bank of filters, each centered on one frequency to analyze. These filters are complex exponentials convoluted with a Kaiser window, which support is set according to the frequency to analyze. Once these filters are applied to the signal, I use a time-frequency reassignement technique in order to exploit the complex phase of the signal. This method combines the information from nearby filters, but with a different phase, in order to restore very precisely the frequency content with the smallest possible delay.

FUNCTIONAL DESCRIPTION: Amuencha gathers notes separated by an octave along the same directions of a spiral, so that chords clearly stand out, even reversed. You can also record yourself with a microphone (in red) while playing some recording (in blue), so you can work your tuning :-)

RELEASE FUNCTIONAL DESCRIPTION: Initial version

- Author: Nicolas Brodu
- Contact: Nicolas Brodu
- URL: https://nicolas.brodu.net/programmation/amuencha/

6.8. Manzana

KEYWORDS: 2D - Image processing - Filtering

SCIENTIFIC DESCRIPTION: Software library developed in the framework of I2S-GEOSTAT innovationlab and made of high-level image processing functionalities based on sparsity and non-convex optimization.

FUNCTIONAL DESCRIPTION: Library of software in image processing: filtering, hdr, inpainting etc.

- Partner: Innovative Imaging Solutions I2S
- Contact: Hussein Yahia

7. New Results

7.1. Excitable systems

Participants: G. Attuel , E. Gerasimova-Chechkina , F. Argoul , H. Yahia , A. Arnéodo .

In a companion paper (I. Multifractal analysis of clinical data), we used a wavelet-based multiscale analysis to reveal and quantify the multifractal intermittent nature of the cardiac impulse energy in the low frequency range 2Hz during atrial fibrillation (AF). It demarcated two distinct areas within the coronary sinus (CS) with regionally stable multifractal spectra likely corresponding to different anatomical substrates. The electrical activity also showed no sign of the kind of temporal correlations typical of cascading processes across scales, thereby indicating that the multifractal scaling is carried by variations in the large amplitude oscillations of the recorded bipolar electric potential. In the present study, to account for these observations, we explore the role of the kinetics of gap junction channels (GJCs), in dynamically creating a new kind of imbalance between depolarizing and repolarizing currents. We propose a one-dimensional (1D) spatial model of a denervated myocardium, where the coupling of cardiac cells fails to synchronize the network of cardiac cells because of abnormal transjunctional capacitive charging of GJCs. We show that this non-ohmic nonlinear conduction 1D modeling accounts quantitatively well for the "multifractal random noise" dynamics of the electrical activity experimentally recorded in the left atrial posterior wall area. We further demonstrate that the multifractal properties of the numerical impulse energy are robust to changes in the model parameters.

Publications: Frontiers in Physiology, Frontiers, 2019, 10, pp.480 (1-18), HAL

Second international Summer Institute on Network Physiology, Jul 2019 HAL

7.2. Differential diagnosis between atypical Parkinsonian syndromes

Participants: B. Das , K. Daoudi , J. Kemplir , J. Rusz .

In the early stage of disease, the symptoms of Parkinson's disease (PD) are similar to atypical Parkinsonian syndromes (APS). The early differential diagnosis between PD and APS and within APS is thus a very challenging task. It turns out that speech disorder is an early and common symptom to PD and APS. The goal of research is to develop a digital marker based on speech analysis in order to assist the neurologists in their diagnosis. We addressed the problem of differential diagnosis between two APS, Progressive Supranuclear Palsy (PSP) and Multiple System Atrophy (MSA). Using linear discriminant analysis we designed an hypokinetic and an ataxic dysarthria measure which yield a discrimination between PSP and MSA with a high accuracy (88%). This result indicates that hypokinetic and ataxic dysarthria convey valuable discriminative information when mutually considered.

Publication: ICASSP 2019 HAL

7.3. Turbulent dynamics of ocean upwelling

Participants: A. El Aouni , V. Garçon , J. Sudre , H. Yahia , K. Daoudi , K. Minaoui .

The region along the NorthWest African coast (20° N to 36° N and 4° W to 19° W) is characterized by a persistent and variable upwelling phenomenon almost all year round. In this article, the upwelling features are investigated using an algorithm dedicated to delimit the upwelling area from thermal and biological satellite observations. This method has been developed specifically for sea-surface temperature (SST) images, since they present a high latitudinal variation, which is not present in chlorophyll-a concentration images. Developing on the proposed approach, the spatial and temporal variations of the main physical and biological upwelling patterns are studied. Moreover, a study on the upwelling dynamics, which explores the interplay between the upwelling spatiotemporal extents and intensity, is presented, based on a 14-year time archive of weekly SST and chlorophyll-a concentration data.

Publication: IEEE Transactions on Geoscience and Remote Sensing, HAL

7.4. Fourier approach to Lagrangian vortex detection

Participants: A. El Aouni , H. Yahia , K. Daoudi , K. Minaoui .

We study the transport properties of coherent vortices over a finite time duration. Here we reveal that such vortices can be identified based on frequency-domain representation of Lagrangian trajectories. We use Fourier analysis to convert particles' trajectories from their time domain to a presentation in the frequency domain. We then identify and extract coherent vortices as material surfaces along which particles' trajectories share similar frequencies. Our method identifies all coherent vortices in an automatic manner, showing high vortices' monitoring capacity. We illustrate our new method by identifying and extracting Lagrangian coherent vortices in different two-and three-dimensional flows.

Publication: Chaos, American Institute of Physics, HAL

7.5. Surface mixing and biological activity

Participants: A. El Aouni , K. Daoudi , H. Yahia , K. Minaoui , A. Benazzouz .

Near-shore water along the NorthWest African margin is one of the world's major upwelling regions. It is associated with physical structures of oceanic fronts which influence the biological productivity. The study of these coherent structures in connection with chlorophyll concentration data is of fundamental importance for understanding the spatial distributions of the plankton. In this work, we study the horizontal stirring and mixing in different upwelling areas using Lagrangian coherent structures (LCSs). These LCSs are calculated using the recent geodesic theory of LCSs. We use these LCSs to study the link between the chlorophyll fronts concentrations and surface mixing, based on 10 years of satellite data. These LCSs move with the flow as material lines, thus the horizontal mixing is calculated from the intersection of these LCSs with the finite time Lyapunov exponents (FTLEs) maps. We compare our results with those of a recent study conducted over the same area, but based on Finite Size Lyapunov Exponents (FSLEs) whose output is a plot of scalar distributions. We discuss the differences between FSLE and geodesic theory of LCS. The latter yields analytical solutions of LCSs, while FSLEs can only provide LCSs for sharp enough ridges of nearly constant height.

Publication: Chaos, American Institute of Physics, HAL

7.6. Contribution and influence of coherent mesoscale eddies off the North-West African upwelling on the open ocean

Participants: A. El Aouni , K. Daoudi , H. Yahia , K. Minaoui .

Eastern Boundary Upwelling zones include some of the most productive ecosystems in the world, particularly the NorthWest (NW) African upwelling which presents one of the world's major upwelling regions. This latter is forced by the equator-ward trade winds which are known to exhibit mesoscale instabilities; thus, in addition to upwelled cold and nutrient-rich deep waters, significant energy is transferred into mesoscale fronts and eddies in the upper ocean. Oceanic structures of type eddies are well know to stir and mix surrounding water masses. However, they can also carry and transport organic matter and marine in a coherent manner. Here, we are interested in those that remain coherent. The Aim of this work, is to understand the impact and the contribution of the mesoscale eddies off the NW African margin on the open ocean. Our approach to analyze such coherent eddies is based upon the use of our recently developed technique from nonlinear dynamics theory, which is capable of identifying coherent vortices and their centers in an automatic manner. The role of these mesoscale eddies is investigated based on a statistical study of eddies properties off NW African margin (cyclone/anticyclone, their lifetimes, traveled distance, translational speeds, quantity of water masses transported to the open ocean...). This statistical study is carried out over a sets of 24 years (spans from January 1993 to December 2016) of sea surface velocity field derived from satellite surface altimetry under the geostrophic approximation.

Publication: SIAM Conference on Mathematics of Planet Earth, (MPE18) HAL

7.7. Defining coherent vortices from particles trajectories

Participants: A. El Aouni , H. Yahia , K. Daoudi , K. Minaoui .

Tracer patterns in the ocean, such as sea surface temperature, chlorophyll concentration and salinity suggest the emergence of coherence even in the ocean, typically with fluxes dominated by advective transport over diffusion. Mesoscale eddies are known to govern advective transport in the ocean, with typical horizontal scales $\mathcal{O}(100km)$ and timescales of $\mathcal{O}(weeks)$. These oceanic structures are omnipresent in the ocean and usually exhibit different properties to their surroundings. They are known to stir and mix surroundings water masses as well as by their ability to trap and carry fluid properties in a coherent manner. As the effect of these mesoscale eddies on the global circulation is remarkable, we focused on studying and understanding the dynamic transport properties of these coherent oceanic structures. For this reason, we have developed a Lagrangian method to identify and extract Lagrangian coherent vortices. The method analyzes particles' trajectories to identify vortices' boundaries and their attractor centers. Indeed, it is based on a decomposition of particle trajectory into two parts: closed curves which give information about uniformly rotating flow, and one that describes the mean displacement. The former part yields an objective measure of material rotation. We define Lagrangian coherent vortex as closed material lines in which fluid parcels complete the same polar rotation. This turns out to be filled with outward-increasing closed contours of the Lagrangian Averaged Closed Curve Length.

Publications: 3 articles submitted.

7.8. Soft hydrogel particle packings

Participants: J. Bares , N. Brodu , H. Zheng , J. A. Dijksman .

We provide the raw data from several years worth of effort on index matching experiments on soft hydrogel particle packings exposed to various loading conditions. Many of the data sets have not before been used, described explicitly in scientific publications or even analyzed. We will present a general overview of methods used to perform the imaging experiments. We provide particle-level information extracted from the 3D images, including contact forces and particle shapes, along with complementary boundary force measurements. We also provide a final working version of the code used to extract these microscopic features.

Publication: *Releasing data from mechanical tests on three dimensional hydrogel sphere packings*, Granular Matter, HAL

7.9. Feature based reconstruction model for fluorescence microscopy image denoising

Participants: S. K. Maji , H. Yahia .

: the advent of Fluorescence Microscopy over the last few years have dramatically improved the problem of visualization and tracking of specific cellular objects for biological inference. But like any other imaging system, fluorescence microscopy has its own limitations. The resultant images suffer from the effect of noise due to both signal dependent and signal independent factors, thereby limiting the possibility of biological inferencing. Denoising is a class of image processing algorithms that aim to remove noise from acquired images and has gained wide attention in the field of fluorescence microscopy image restoration. In this paper, we propose an image denoising algorithm based on the concept of feature extraction through multifractal decomposition and then estimate a noise free image from the gradients restricted to these features. Experimental results over simulated and real fluorescence microscopy data prove the merit of the proposed approach, both visually and quantitatively.

Publication: Scientific Reports, Nature Publishing Group, HAL

7.10. InnovationLab with I2S, sparse signals & optimisation

Participants: M. Martin, H. Yahia, A. Zebadua, S. Sakka, N. Brodu, K. Daoudi, A. Cherif [I2S], J. L. Vallancogne [I2S], A. Cailly [I2S], A. Billy [I2S], B. Lebouill [I2S].

During 2019:

Linear inverse problems in image processing, denoising, deconvolution, non-convex optimization, plug, and play algorithms.

HDR (High Dynamic Range) : C++ implementation with OpenCV library; code deposited on gitlab, sharing with I2S company, enhancement of the code architecture. GPU implementation.

Reflecting improvement: development and C++ implementation.

3D reconstruction: implementation and test with openMVG and openMVS libraries. Depth map enhancement through non-convex optimization.

Image smoothing implementation [57].

CPU and GPU patchmatch implementation [55].

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

InnovationLab with I2S company, starting scheduled after 1st 2019 COPIL in January 2019.

9. Partnerships and Cooperations

9.1. Regional Initiatives

Geostat is a member of the GPR ("Grand Projet de Recherche") **ORIGINS** ("Origine, évolution, matière primordiale, nucléosynthèse, complexification, étoiles, planètes, Terre, habitabilité, climat, biodiversité, homininés, big data, sociologie, médiation scientifique) carried by Laboratoire d'Astrophysique de Bordeaux (LAB) (M. Gargaud). Geostat is involved in the axis "Data Science pour les Sciences de Origins".

9.2. National Initiatives

- ANR project *Voice4PD-MSA*, led by K. Daoudi, which targets the differential diagnosis between Parkinson's disease and Multiple System Atrophy. The total amount of the grant is 468555 euros, from which GeoStat has 203078 euros. The duration of the project is 42 months. Partners: CHU Bordeaux (Bordeaux), CHU Toulouse, IRIT, IMT (Toulouse).
- Prolongation for A. El Aouni in 2019 (4 months) through the program "BOOSTE TON DOC" of the Toubkal PHC project PHC-Toubkal project "Caractérisation multi-capteurs et suivi spatio-temporel de l'Upwelling sur la côte atlantique marocaine par imagerie satellitaire", which finished December 2018.
- GEOSTAT is a member of ISIS (Information, Image & Vision), AMF (Multifractal Analysis) GDRs.
- GEOSTAT is participating in the CNRS IMECO project *Intermittence multi-échelles de champs océaniques : analyse comparative d'images satellitaires et de sorties de modèles numériques*. CNRS call AO INSU 2018. PI: F. Schmitt, DR CNRS, UMR LOG 8187. Duration: 2 years.

9.3. European Initiatives

9.3.1. Collaborations in European Programs, Except FP7 & H2020

GENESIS Program: supported by Deutsche Forschungsgemeinde (DFG) and the Agence national de recherche (ANR). *GENeration and Evolution of Structures in the ISm.* Duration: start 1.5. 2017, 3 years. Coordinator: N. Schneider (I. Physik, Cologne). Other partners: Cologne (R. Simon, N. Schneider, V. Ossenkopf, M. Roellig), LAB (S. Bontemps, A. Roy, L. Bonne, F. Herpin, J. Braine, N. Brouillet, T. Jacq), ATN Canberra (Australia), LERMA Paris (France), MPIfR Bonn (Germany), CEA Saclay (France), ITA/ZAH Heidelberg (Germany), Institute of Astronomy, Cardiff (UK), ESO (Germany, Chile), CfA Harvard (USA), IPAG Grenoble (France), Argelander Institut Bonn (Germany), CASS San Diego (USA), University of Sofia (Bulgaria). Web site: link.

9.4. International Initiatives

9.4.1. Inria exploratory action

TRACME This project focuses on modelling a physical system from measurements on that system. How, starting from observations, to build a reliable model of the system dynamics? When multiple processes interact at different scales, how to obtain a significant model at each of these scales? The goal is to provide a model simple enough to bring some understanding of the system studied, but also a model elaborated enough to allow precise predictions. In order to do so, this project proposes to identify causally equivalent classes of system states, then model their evolution with a stochastic process. Renormalizing these equations is necessary in order to relate the scale of the continuum to that, arbitrary, at which data are acquired. Applications primarily concern natural sciences. PI: N. Brodu.

9.4.2. Participation in Other International Programs

9.4.2.1. IFCAM: Generalization for land cover identification. Geostat and the Indo-French Centre For Applied Mathematics

Land cover classification from satellite imagery is an important application for agriculture, environmental monitoring, tracking changes for emergency, etc. The typical methodology is to train a machine learning algorithm to recognize specified classes (urban, forest, fields, etc...) over regions of interest and classify new images when they become available. This proposal investigates how to use local context and how to best sample the data in order to provide the best generalization ability. Data will be sampled on reference locations and used for training and validation.

PIs: N. Brodu (Geostat) and D. Singh (IIT Roorkee).

Duration: 3 years. Starting 2018.

9.5. Introduction

9.5.1. Visits of International Scientists

- D. Singh [IIT Rookee, June 2019]

9.5.1.1. Internships

- D. Nash, level L3, intern in June 2019. Supervisor: N. Brodu.

9.5.2. Visits to International Teams

- PhD student A. Rashidi met with Dr Francis Bach of Inria Paris on optimization methods. first meeting was on November 2019.
- A. Rashidi registered for "Inversion et imagerie haute resolution" lectures of Dr. Francois Giovannelli, starting from January 2020.
- A. Rashidi participated in PRAIRE artificial intelligence summer school in October 2019 at Paris.

10. Dissemination

10.1. Introduction

10.1.1. Member of the Editorial Boards

- H. Yahia is Review Editor for the journal Frontiers in Physiology (Fractal Physiology).

10.1.2. Invited Talks

- Journée des Systèmes et de la Matière Complexe 4ème édition, Paris-Saclay, October 2019: G. Attuel gave the presentation *Voir au coeur d'une turbulence forte sans cascade et mourir...*, link.

10.2. Introduction

10.2.1. Teaching

Master : K. Daoudi, Data mining, 20 hours, M2 MIAGE, University of Lorraine.

Master : A. Rashidi, Introduction to deep learning, 12 hours, M1, course given in the team during D. Singh's visit.

10.2.2. Supervision

PhD : A. El Aouni, Lagrangian coherent structures and physical processes of coastal upwelling, Bordeaux University, September 24, 2019, supervisors: H. Yahia, K. Minaoui.

Master : H. Belmajdoub, Upwelling dynamics along the Atlantic coast of Morocco, Rabat University, supervised by A. El Aouni.

PhD in progress : H. Belmajdoub, Upwelling dynamics along the Atlantic coast of Morocco, Rabat University, cosupervised by A. El Aouni.

PhD in progress : Z. El Abidi, caractérisation multicapteur de l'upwelling marocain, Rabat University, cosupervised by A. El Aouni.

11. Bibliography

Major publications by the team in recent years

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Project-Team HIEPACS

High-End Parallel Algorithms for Challenging Numerical Simulations

IN COLLABORATION WITH: Laboratoire Bordelais de Recherche en Informatique (LaBRI)

IN PARTNERSHIP WITH:
CNRS

Institut Polytechnique de Bordeaux

Université de Bordeaux

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Distributed and High Performance Computing

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Creation of the Team: 2009 January 01, updated into Project-Team: 2010 January 01

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2. Overall Objectives

2.1. Introduction

Over the last few decades, there have been innumerable science, engineering and societal breakthroughs enabled by the development of High Performance Computing (HPC) applications, algorithms and architectures. These powerful tools have provided researchers with the ability to computationally find efficient solutions for some of the most challenging scientific questions and problems in medicine and biology, climatology, nanotechnology, energy and environment. It is admitted today that *numerical simulation is the third pillar for the development of scientific discovery at the same level as theory and experimentation*. Numerous reports and papers also confirmed that very high performance simulation will open new opportunities not only for research but also for a large spectrum of industrial sectors

An important force which has continued to drive HPC has been to focus on frontier milestones which consist in technical goals that symbolize the next stage of progress in the field. In the 1990s, the HPC community sought to achieve computing at a teraflop rate and currently we are able to compute on the first leading architectures at a petaflop rate. Generalist petaflop supercomputers are available and exaflop computers are foreseen in early 2020.

For application codes to sustain petaflops and more in the next few years, hundreds of thousands of processor cores or more are needed, regardless of processor technology. Currently, a few HPC simulation codes easily scale to this regime and major algorithms and codes development efforts are critical to achieve the potential of these new systems. Scaling to a petaflop and more involves improving physical models, mathematical modeling, super scalable algorithms that will require paying particular attention to acquisition, management and visualization of huge amounts of scientific data.

In this context, the purpose of the HIEPACS project is to contribute performing efficiently frontier simulations arising from challenging academic and industrial research. The solution of these challenging problems require a multidisciplinary approach involving applied mathematics, computational and computer sciences. In applied mathematics, it essentially involves advanced numerical schemes. In computational science, it involves massively parallel computing and the design of highly scalable algorithms and codes to be executed on emerging hierarchical many-core, possibly heterogeneous, platforms. Through this approach, HIEPACS intends to contribute to all steps that go from the design of new high-performance more scalable, robust and more accurate numerical schemes to the optimized implementations of the associated algorithms and codes on very high performance supercomputers. This research will be conduced on close collaboration in particular with European and US initiatives and likely in the framework of EuroHPC collaborative projects.

The methodological part of HIEPACS covers several topics. First, we address generic studies concerning massively parallel computing, the design of high-end performance algorithms and software to be executed on future extreme scale platforms. Next, several research prospectives in scalable parallel linear algebra techniques are addressed, ranging from dense direct, sparse direct, iterative and hybrid approaches for large linear systems. We are also interested in the general problem of minimizing memory consumption and data movements, by changing algorithms and possibly performing extra computations, in particular in the context of Deep Neural Networks. Then we consider research on N-body interaction computations based on efficient parallel fast multipole methods and finally, we address research tracks related to the algorithmic challenges for complex code couplings in multiscale/multiphysic simulations.

Currently, we have one major multiscale application that is in *material physics*. We contribute to all steps of the design of the parallel simulation tool. More precisely, our applied mathematics skill will contribute to the modeling and our advanced numerical schemes will help in the design and efficient software implementation for very large parallel multiscale simulations. Moreover, the robustness and efficiency of our algorithmic research in linear algebra are validated through industrial and academic collaborations with different partners involved in various application fields. Finally, we are also involved in a few collaborative initiatives in various application domains in a co-design like framework. These research activities are conducted in a wider multi-disciplinary context with colleagues in other academic or industrial groups where our contribution is related to our expertises. Not only these collaborations enable our expertise to have a stronger impact in various application domains through the promotion of advanced algorithms, methodologies or tools, but in return they open new avenues for research in the continuity of our core research activities.

Thanks to the two Inria collaborative agreements such as with Airbus/Conseil Régional Grande Aquitaine and with CEA, we have joint research efforts in a co-design framework enabling efficient and effective technological transfer towards industrial R&D. Furthermore, thanks to the past associate team FASTLA we contribute with world leading groups at Berkeley National Lab and Stanford University to the design of fast numerical solvers and their parallel implementations.

Our high performance software packages are integrated in several academic or industrial complex codes and are validated on very large scale simulations. For all our software developments, we use first the experimental platform PLAFRIM, the various large parallel platforms available through GENCI in France (CCRT, CINES and IDRIS Computational Centers), and next the high-end parallel platforms that will be available via European and US initiatives or projects such that PRACE.

3. Research Program

3.1. Introduction

The methodological component of HIEPACS concerns the expertise for the design as well as the efficient and scalable implementation of highly parallel numerical algorithms to perform frontier simulations. In order to address these computational challenges a hierarchical organization of the research is considered. In this bottom-up approach, we first consider in Section 3.2 generic topics concerning high performance computational science. The activities described in this section are transversal to the overall project and their outcome will support all the other research activities at various levels in order to ensure the parallel scalability of the algorithms. The aim of this activity is not to study general purpose solution but rather to address these problems in close relation with specialists of the field in order to adapt and tune advanced approaches in our algorithmic designs. The next activity, described in Section 3.3, is related to the study of parallel linear algebra techniques that currently appear as promising approaches to tackle huge problems on extreme scale platforms. We highlight the linear problems (linear systems or eigenproblems) because they are in many large scale applications the main computational intensive numerical kernels and often the main performance bottleneck. These parallel numerical techniques will be the basis of both academic and industrial collaborations, some are described in Section 4.1, but will also be closely related to some functionalities developed in the parallel fast multipole activity described in Section 3.4. Finally, as the accuracy of the physical models increases, there is a real need to go for parallel efficient algorithm implementation for multiphysics and multiscale modeling in particular in the context of code coupling. The challenges associated with this activity will be addressed in the framework of the activity described in Section 3.5.

Currently, we have one major application (see Section 4.1) that is in material physics. We will collaborate to all steps of the design of the parallel simulation tool. More precisely, our applied mathematics skill will contribute to the modelling, our advanced numerical schemes will help in the design and efficient software implementation for very large parallel simulations. We also participate to a few co-design actions in close collaboration with some applicative groups. The objective of this activity is to instantiate our expertise in fields where they are critical for designing scalable simulation tools. We refer to Section 4.2 for a detailed description of these activities.

3.2. High-performance computing on next generation architectures

Participants: Emmanuel Agullo, Olivier Beaumont, Olivier Coulaud, Pierre Esterie, Lionel Eyraud-Dubois, Mathieu Faverge, Luc Giraud, Abdou Guermouche, Gilles Marait, Pierre Ramet, Jean Roman, Nick Schenkels, Alena Shilova, Mathieu Verite.

The research directions proposed in HiePACS are strongly influenced by both the applications we are studying and the architectures that we target (i.e., massively parallel heterogeneous many-core architectures, ...). Our main goal is to study the methodology needed to efficiently exploit the new generation of high-performance computers with all the constraints that it induces. To achieve this high-performance with complex applications we have to study both algorithmic problems and the impact of the architectures on the algorithm design.

From the application point of view, the project will be interested in multiresolution, multiscale and hierarchical approaches which lead to multi-level parallelism schemes. This hierarchical parallelism approach is necessary to achieve good performance and high-scalability on modern massively parallel platforms. In this context, more specific algorithmic problems are very important to obtain high performance. Indeed, the kind of applications we are interested in are often based on data redistribution for example (e.g., code coupling applications). This well-known issue becomes very challenging with the increase of both the number of computational nodes and the amount of data. Thus, we have both to study new algorithms and to adapt the existing ones. In addition, some issues like task scheduling have to be restudied in this new context. It is important to note that the work developed in this area will be applied for example in the context of code coupling (see Section 3.5).

Considering the complexity of modern architectures like massively parallel architectures or new generation heterogeneous multicore architectures, task scheduling becomes a challenging problem which is central to obtain a high efficiency. With the recent addition of colleagues from the scheduling community (O. Beaumont and L. Eyraud-Dubois), the team is better equipped than ever to design scheduling algorithms and models specifically tailored to our target problems. It is important to note that this topic is strongly linked to the underlying programming model. Indeed, considering multicore and heterogeneous architectures, it has appeared, in the last five years, that the best programming model is an approach mixing multi-threading within computational nodes and message passing between them. In the last five years, a lot of work has been developed in the high-performance computing community to understand what is critic to efficiently exploit massively multicore platforms that will appear in the near future. It appeared that the key for the performance is firstly the granularity of the computations. Indeed, in such platforms the granularity of the parallelism must be small so that we can feed all the computing units with a sufficient amount of work. It is thus very crucial for us to design new high performance tools for scientific computing in this new context. This will be developed in the context of our solvers, for example, to adapt to this new parallel scheme. Secondly, the larger the number of cores inside a node, the more complex the memory hierarchy. This remark impacts the behavior of the algorithms within the node. Indeed, on this kind of platforms, NUMA effects will be more and more problematic. Thus, it is very important to study and design data-aware algorithms which take into account the affinity between computational threads and the data they access. This is particularly important in the context of our high-performance tools. Note that this work has to be based on an intelligent cooperative underlying run-time (like the tools developed by the Inria STORM Project-Team) which allows a fine management of data distribution within a node.

Another very important issue concerns high-performance computing using "heterogeneous" resources within a computational node. Indeed, with the deployment of the GPU and the use of more specific co-processors, it is important for our algorithms to efficiently exploit these new type of architectures. To adapt our algorithms and tools to these accelerators, we need to identify what can be done on the GPU for example and what cannot. Note that recent results in the field have shown the interest of using both regular cores and GPU to perform computations. Note also that in opposition to the case of the parallelism granularity needed by regular multicore architectures, GPU requires coarser grain parallelism. Thus, making both GPU and regular cores work all together will lead to two types of tasks in terms of granularity. This represents a challenging problem especially in terms of scheduling. From this perspective, we investigate new approaches for composing parallel applications within a runtime system for heterogeneous platforms.

In the context of scaling up, and particularly in the context of minimizing energy consumption, it is generally acknowledged that the solution lies in the use of heterogeneous architectures, where each resource is particularly suited to specific types of tasks, and in a fine control at the algorithmic level of data movements and the trade-offs to be made between computation and communication. In this context, we are particularly interested in the optimization of the training phase of deep convolutional neural networks which consumes a lot of memory and for which it is possible to exchange computations for data movements and memory occupation. We are also interested in the complexity introduced by resource heterogeneity itself, both from a theoretical point of view on the complexity of scheduling problems and from a more practical point of view on the implementation of specific kernels in dense or sparse linear algebra.

In order to achieve an advanced knowledge concerning the design of efficient computational kernels to be used on our high performance algorithms and codes, we will develop research activities first on regular frameworks before extending them to more irregular and complex situations. In particular, we will work first on optimized dense linear algebra kernels and we will use them in our more complicated direct and hybrid solvers for sparse linear algebra and in our fast multipole algorithms for interaction computations. In this context, we will participate to the development of those kernels in collaboration with groups specialized in dense linear algebra. In particular, we intend develop a strong collaboration with the group of Jack Dongarra at the University of Tennessee and collaborating research groups. The objectives will be to develop dense linear algebra algorithms and libraries for multicore architectures in the context the PLASMA project and for GPU and hybrid multicore/GPU architectures in the context of the MAGMA project. A new solver has emerged from the associate team, Chameleon. While PLASMA and MAGMA focus on multicore and GPU architectures, respectively, Chameleon makes the most out of heterogeneous architectures thanks to task-based dynamic runtime systems.

A more prospective objective is to study the resiliency in the context of large-scale scientific applications for massively parallel architectures. Indeed, with the increase of the number of computational cores per node, the probability of a hardware crash on a core or of a memory corruption is dramatically increased. This represents a crucial problem that needs to be addressed. However, we will only study it at the algorithmic/application level even if it needed lower-level mechanisms (at OS level or even hardware level). Of course, this work can be performed at lower levels (at operating system) level for example but we do believe that handling faults at the application level provides more knowledge about what has to be done (at application level we know what is critical and what is not). The approach that we will follow will be based on the use of a combination of fault-tolerant implementations of the run-time environments we use (like for example ULFM) and an adaptation of our algorithms to try to manage this kind of faults. This topic represents a very long range objective which needs to be addressed to guaranty the robustness of our solvers and applications.

Finally, it is important to note that the main goal of HiePACS is to design tools and algorithms that will be used within complex simulation frameworks on next-generation parallel machines. Thus, we intend with our partners to use the proposed approach in complex scientific codes and to validate them within very large scale simulations as well as designing parallel solution in co-design collaborations.

3.3. High performance solvers for large linear algebra problems

Participants: Emmanuel Agullo, Olivier Coulaud, Tony Delarue, Mathieu Faverge, Aurélien Falco, Marek Felsoci, Luc Giraud, Abdou Guermouche, Esragul Korkmaz, Gilles Marait, Van Gia Thinh Nguyen, Jean Rene Poirier, Pierre Ramet, Jean Roman, Cristobal Samaniego Alvarado, Guillaume Sylvand, Nicolas Venkovic, Yanfei Xiang.

Starting with the developments of basic linear algebra kernels tuned for various classes of computers, a significant knowledge on the basic concepts for implementations on high-performance scientific computers has been accumulated. Further knowledge has been acquired through the design of more sophisticated linear algebra algorithms fully exploiting those basic intensive computational kernels. In that context, we still look at the development of new computing platforms and their associated programming tools. This enables us to identify the possible bottlenecks of new computer architectures (memory path, various level of caches, inter processor or node network) and to propose ways to overcome them in algorithmic design. With the goal of designing efficient scalable linear algebra solvers for large scale applications, various tracks will be followed in order to investigate different complementary approaches. Sparse direct solvers have been for years the methods of choice for solving linear systems of equations, it is nowadays admitted that classical approaches are not scalable neither from a computational complexity nor from a memory view point for large problems such as those arising from the discretization of large 3D PDE problems. We will continue to work on sparse direct solvers on the one hand to make sure they fully benefit from most advanced computing platforms and on the other hand to attempt to reduce their memory and computational costs for some classes of problems where data sparse ideas can be considered. Furthermore, sparse direct solvers are a key building boxes for the design of some of our parallel algorithms such as the hybrid solvers described in the sequel of this section. Our activities in that context will mainly address preconditioned Krylov subspace methods; both components, preconditioner and Krylov solvers, will be investigated. In this framework, and possibly in relation with the research activity on fast multipole, we intend to study how emerging $\mathcal{H}$-matrix arithmetic can benefit to our solver research efforts.

3.3.1. *Parallel sparse direct solvers*

For the solution of large sparse linear systems, we design numerical schemes and software packages for direct and hybrid parallel solvers. Sparse direct solvers are mandatory when the linear system is very ill-conditioned; such a situation is often encountered in structural mechanics codes, for example. Therefore, to obtain an industrial software tool that must be robust and versatile, high-performance sparse direct solvers are mandatory, and parallelism is then necessary for reasons of memory capability and acceptable solution time. Moreover, in order to solve efficiently 3D problems with more than 50 million unknowns, which is now a reachable challenge with new multicore supercomputers, we must achieve good scalability in time and control memory overhead. Solving a sparse linear system by a direct method is generally a highly irregular problem that induces some challenging algorithmic problems and requires a sophisticated implementation scheme in order to fully exploit the capabilities of modern supercomputers.

New supercomputers incorporate many microprocessors which are composed of one or many computational cores. These new architectures induce strongly hierarchical topologies. These are called NUMA architectures. In the context of distributed NUMA architectures, in collaboration with the Inria STORM team, we study optimization strategies to improve the scheduling of communications, threads and I/O. We have developed dynamic scheduling designed for NUMA architectures in the PaStiX solver. The data structures of the solver, as well as the patterns of communication have been modified to meet the needs of these architectures and dynamic scheduling. We are also interested in the dynamic adaptation of the computation grain to use efficiently multi-core architectures and shared memory. Experiments on several numerical test cases have been performed to prove the efficiency of the approach on different architectures. Sparse direct solvers such as PaStiX are currently limited by their memory requirements and computational cost. They are competitive for small matrices but are often less efficient than iterative methods for large matrices in terms of memory. We are currently accelerating the dense algebra components of direct solvers using block low-rank compression techniques.

In collaboration with the ICL team from the University of Tennessee, and the STORM team from Inria, we are evaluating the way to replace the embedded scheduling driver of the PaStiX solver by one of the generic frameworks, PaRSEC or StarPU, to execute the task graph corresponding to a sparse factorization. The aim is to design algorithms and parallel programming models for implementing direct methods for the solution of sparse linear systems on emerging computer equipped with GPU accelerators. More generally, this work will be performed in the context of the ANR SOLHARIS project which aims at designing high performance sparse direct solvers for modern heterogeneous systems. This ANR project involves several groups working either on the sparse linear solver aspects (HIEPACS and ROMA from Inria and APO from IRIT), on runtime systems (STORM from Inria) or scheduling algorithms (HIEPACS and ROMA from Inria). The results of these efforts will be validated in the applications provided by the industrial project members, namely CEA-CESTA and Airbus Central R & T.

3.3.2. Hybrid direct/iterative solvers based on algebraic domain decomposition techniques

One route to the parallel scalable solution of large sparse linear systems in parallel scientific computing is the use of hybrid methods that hierarchically combine direct and iterative methods. These techniques inherit the advantages of each approach, namely the limited amount of memory and natural parallelization for the iterative component and the numerical robustness of the direct part. The general underlying ideas are not new since they have been intensively used to design domain decomposition techniques; those approaches cover a fairly large range of computing techniques for the numerical solution of partial differential equations (PDEs) in time and space. Generally speaking, it refers to the splitting of the computational domain into sub-domains with or without overlap. The splitting strategy is generally governed by various constraints/objectives but the main one is to express parallelism. The numerical properties of the PDEs to be solved are usually intensively exploited at the continuous or discrete levels to design the numerical algorithms so that the resulting specialized technique will only work for the class of linear systems associated with the targeted PDE.

In that context, we continue our effort on the design of algebraic non-overlapping domain decomposition techniques that rely on the solution of a Schur complement system defined on the interface introduced by the partitioning of the adjacency graph of the sparse matrix associated with the linear system. Although it is better conditioned than the original system the Schur complement needs to be precondition to be amenable to a solution using a Krylov subspace method. Different hierarchical preconditioners will be considered, possibly multilevel, to improve the numerical behaviour of the current approaches implemented in our software library MaPHyS. This activity will be developed further developped in the H2020 EOCOE2 project. In addition to this numerical studies, advanced parallel implementation will be developed that will involve close collaborations between the hybrid and sparse direct activities.

3.3.3. Linear Krylov solvers

Preconditioning is the main focus of the two activities described above. They aim at speeding up the convergence of a Krylov subspace method that is the complementary component involved in the solvers of interest for us. In that framework, we believe that various aspects deserve to be investigated; we will consider the following ones:

- preconditioned block Krylov solvers for multiple right-hand sides. In many large scientific and industrial applications, one has to solve a sequence of linear systems with several right-hand sides given simultaneously or in sequence (radar cross section calculation in electromagnetism, various source locations in seismic, parametric studies in general, ...). For "simultaneous" right-hand sides, the solvers of choice have been for years based on matrix factorizations as the factorization is performed once and simple and cheap block forward/backward substitutions are then performed. In order to effectively propose alternative to such solvers, we need to have efficient preconditioned Krylov subspace solvers. In that framework, block Krylov approaches, where the Krylov spaces associated with each right-hand side are shared to enlarge the search space will be considered. They are not only attractive because of this numerical feature (larger search space), but also from an implementation point of view. Their block-structures exhibit nice features with respect to data locality and re-usability that comply with the memory constraint of multicore architectures. We will continue the numerical study and design of the block GMRES variant that combines inexact breakdown detection, deflation at restart and subspace recycling. Beyond new numerical investigations, a software implementation to be included in our linear solver libray `Fabulous` originately developed in the context of the DGA HiBox project and further developped in the LynCs (Linear Algebra, Krylov-subspace methods, and multi-grid solvers for the discovery of New Physics) sub-project of PRACE-6IP.
- Extension or modification of Krylov subspace algorithms for multicore architectures: finally to match as much as possible to the computer architecture evolution and get as much as possible performance out of the computer, a particular attention will be paid to adapt, extend or develop numerical schemes that comply with the efficiency constraints associated with the available computers. Nowadays, multicore architectures seem to become widely used, where memory latency and bandwidth are the main bottlenecks; investigations on communication avoiding techniques will be undertaken in the framework of preconditioned Krylov subspace solvers as a general guideline for all the items mentioned above.

3.3.4. Eigensolvers

Many eigensolvers also rely on Krylov subspace techniques. Naturally some links exist between the Krylov subspace linear solvers and the Krylov subspace eigensolvers. We plan to study the computation of eigenvalue problems with respect to the following two different axes:

- Exploiting the link between Krylov subspace methods for linear system solution and eigensolvers, we intend to develop advanced iterative linear methods based on Krylov subspace methods that use some spectral information to build part of a subspace to be recycled, either though space augmentation or through preconditioner update. This spectral information may correspond to a certain part of the spectrum of the original large matrix or to some approximations of the eigenvalues obtained by solving a reduced eigenproblem. This technique will also be investigated in the framework of block Krylov subspace methods.
- In the context of the calculation of the ground state of an atomistic system, eigenvalue computation is a critical step; more accurate and more efficient parallel and scalable eigensolvers are required.

3.3.5. Fast Solvers for FEM/BEM Coupling

In this research project, we are interested in the design of new advanced techniques to solve large mixed dense/sparse linear systems, the extensive comparison of these new approaches to the existing ones, and the application of these innovative ideas on realistic industrial test cases in the domain of aeroacoustics (in collaboration with Airbus Central R & T).

- The use of $\mathcal{H}$-matrix solvers on these problems has been investigated in the context of the PhD of A. Falco. Airbus CR&T, in collaboration with Inria Bordeaux Sud-Ouest, has developed a task-based $\mathcal{H}$-matrix solver on top of the runtime engine StarPU. Ideas coming from the field of sparse direct solvers (such as nested dissection or symbolic factorization) have been tested within $\mathcal{H}$-matrices.

- The question of parallel scalability of task-based tools is an active subject of research, using new communication engine such as NewMadeleine, that will be investigated during this project, in conjunction with new algorithmic ideas on the task-based writing of $\mathcal{H}$-matrix algorithms.
- Naturally, comparison with existing tools will be performed on large realistic test cases. Coupling schemes between these tools and the hierarchical methods used in $\mathcal{H}$-matrix will be developed and benched as well.

3.4. High performance Fast Multipole Method for N-body problems

Participants: Emmanuel Agullo, Olivier Coulaud, Pierre Esterie, Guillaume Sylvand.

In most scientific computing applications considered nowadays as computational challenges (like biological and material systems, astrophysics or electromagnetism), the introduction of hierarchical methods based on an octree structure has dramatically reduced the amount of computation needed to simulate those systems for a given accuracy. For instance, in the N-body problem arising from these application fields, we must compute all pairwise interactions among N objects (particles, lines, ...) at every timestep. Among these methods, the Fast Multipole Method (FMM) developed for gravitational potentials in astrophysics and for electrostatic (coulombic) potentials in molecular simulations solves this N-body problem for any given precision with $O(N)$ runtime complexity against $O(N^2)$ for the direct computation.

The potential field is decomposed in a near field part, directly computed, and a far field part approximated thanks to multipole and local expansions. We introduced a matrix formulation of the FMM that exploits the cache hierarchy on a processor through the Basic Linear Algebra Subprograms (BLAS). Moreover, we developed a parallel adaptive version of the FMM algorithm for heterogeneous particle distributions, which is very efficient on parallel clusters of SMP nodes. Finally on such computers, we developed the first hybrid MPI-thread algorithm, which enables to reach better parallel efficiency and better memory scalability. We plan to work on the following points in HIEPACS .

3.4.1. Improvement of calculation efficiency

Nowadays, the high performance computing community is examining alternative architectures that address the limitations of modern cache-based designs. GPU (Graphics Processing Units) and the Cell processor have thus already been used in astrophysics and in molecular dynamics. The Fast Mutipole Method has also been implemented on GPU. We intend to examine the potential of using these forthcoming processors as a building block for high-end parallel computing in N-body calculations. More precisely, we want to take advantage of our specific underlying BLAS routines to obtain an efficient and easily portable FMM for these new architectures. Algorithmic issues such as dynamic load balancing among heterogeneous cores will also have to be solved in order to gather all the available computation power. This research action will be conduced on close connection with the activity described in Section 3.2.

3.4.2. Non uniform distributions

In many applications arising from material physics or astrophysics, the distribution of the data is highly non uniform and the data can grow between two time steps. As mentioned previously, we have proposed a hybrid MPI-thread algorithm to exploit the data locality within each node. We plan to further improve the load balancing for highly non uniform particle distributions with small computation grain thanks to dynamic load balancing at the thread level and thanks to a load balancing correction over several simulation time steps at the process level.

3.4.3. Fast multipole method for dislocation operators

The engine that we develop will be extended to new potentials arising from material physics such as those used in dislocation simulations. The interaction between dislocations is long ranged ($O(1/r)$) and anisotropic, leading to severe computational challenges for large-scale simulations. Several approaches based on the FMM or based on spatial decomposition in boxes are proposed to speed-up the computation. In dislocation codes, the calculation of the interaction forces between dislocations is still the most CPU time consuming. This computation has to be improved to obtain faster and more accurate simulations. Moreover, in such simulations, the number of dislocations grows while the phenomenon occurs and these dislocations are not uniformly distributed in the domain. This means that strategies to dynamically balance the computational load are crucial to achieve high performance.

3.4.4. Fast multipole method for boundary element methods

The boundary element method (BEM) is a well known solution of boundary value problems appearing in various fields of physics. With this approach, we only have to solve an integral equation on the boundary. This implies an interaction that decreases in space, but results in the solution of a dense linear system with $O(N^3)$ complexity. The FMM calculation that performs the matrix-vector product enables the use of Krylov subspace methods. Based on the parallel data distribution of the underlying octree implemented to perform the FMM, parallel preconditioners can be designed that exploit the local interaction matrices computed at the finest level of the octree. This research action will be conduced on close connection with the activity described in Section 3.3. Following our earlier experience, we plan to first consider approximate inverse preconditionners that can efficiently exploit these data structures.

3.5. Load balancing algorithms for complex simulations

Participants: Cyril Bordage, Aurélien Esnard, Pierre Ramet.

Many important physical phenomena in material physics and climatology are inherently complex applications. They often use multi-physics or multi-scale approaches, which couple different models and codes. The key idea is to reuse available legacy codes through a coupling framework instead of merging them into a stand-alone application. There is typically one model per different scale or physics and each model is implemented by a parallel code.

For instance, to model a crack propagation, one uses a molecular dynamic code to represent the atomistic scale and an elasticity code using a finite element method to represent the continuum scale. Indeed, fully microscopic simulations of most domains of interest are not computationally feasible. Combining such different scales or physics is still a challenge to reach high performance and scalability.

Another prominent example is found in the field of aeronautic propulsion: the conjugate heat transfer simulation in complex geometries (as developed by the CFD team of CERFACS) requires to couple a fluid/convection solver (AVBP) with a solid/conduction solver (AVTP). As the AVBP code is much more CPU consuming than the AVTP code, there is an important computational imbalance between the two solvers.

In this context, one crucial issue is undoubtedly the load balancing of the whole coupled simulation that remains an open question. The goal here is to find the best data distribution for the whole coupled simulation and not only for each stand-alone code, as it is most usually done. Indeed, the naive balancing of each code on its own can lead to an important imbalance and to a communication bottleneck during the coupling phase, which can drastically decrease the overall performance. Therefore, we argue that it is required to model the coupling itself in order to ensure a good scalability, especially when running on massively parallel architectures (tens of thousands of processors/cores). In other words, one must develop new algorithms and software implementation to perform a *coupling-aware* partitioning of the whole application. Another related problem is the problem of resource allocation. This is particularly important for the global coupling efficiency and scalability, because each code involved in the coupling can be more or less computationally intensive, and there is a good trade-off to find between resources assigned to each code to avoid that one of them waits for the other(s). What does furthermore happen if the load of one code dynamically changes relatively to the other one? In such a case, it could be convenient to dynamically adapt the number of resources used during the execution.

There are several open algorithmic problems that we investigate in the HIEPACS project-team. All these problems uses a similar methodology based upon the graph model and are expressed as variants of the classic graph partitioning problem, using additional constraints or different objectives.

3.5.1. Dynamic load-balancing with variable number of processors

As a preliminary step related to the dynamic load balancing of coupled codes, we focus on the problem of dynamic load balancing of a single parallel code, with variable number of processors. Indeed, if the workload varies drastically during the simulation, the load must be redistributed regularly among the processors. Dynamic load balancing is a well studied subject but most studies are limited to an initially fixed number of processors. Adjusting the number of processors at runtime allows one to preserve the parallel code efficiency or keep running the simulation when the current memory resources are exceeded. We call this problem, *MxN graph repartitioning*.

We propose some methods based on graph repartitioning in order to re-balance the load while changing the number of processors. These methods are split in two main steps. Firstly, we study the migration phase and we build a “good” migration matrix minimizing several metrics like the migration volume or the number of exchanged messages. Secondly, we use graph partitioning heuristics to compute a new distribution optimizing the migration according to the previous step results.

3.5.2. Load balancing of coupled codes

As stated above, the load balancing of coupled code is a major issue, that determines the performance of the complex simulation, and reaching high performance can be a great challenge. In this context, we develop new graph partitioning techniques, called *co-partitioning*. They address the problem of load balancing for two coupled codes: the key idea is to perform a "coupling-aware" partitioning, instead of partitioning these codes independently, as it is classically done. More precisely, we propose to enrich the classic graph model with *inter-edges*, which represent the coupled code interactions. We describe two new algorithms, and compare them to the naive approach. In the preliminary experiments we perform on synthetically-generated graphs, we notice that our algorithms succeed to balance the computational load in the coupling phase and in some cases they succeed to reduce the coupling communications costs. Surprisingly, we notice that our algorithms do not degrade significantly the global graph edge-cut, despite the additional constraints that they impose.

Besides this, our co-partitioning technique requires to use graph partitioning with *fixed vertices*, that raises serious issues with state-of-the-art software, that are classically based on the well-known recursive bisection paradigm (RB). Indeed, the RB method often fails to produce partitions of good quality. To overcome this issue, we propose a *new* direct k-way greedy graph growing algorithm, called KGGGP, that overcomes this issue and succeeds to produce partition with better quality than RB while respecting the constraint of fixed vertices. Experimental results compare KGGGP against state-of-the-art methods, such as Scotch, for real-life graphs available from the popular *DIMACS'10* collection.

3.5.3. Load balancing strategies for hybrid sparse linear solvers

Graph handling and partitioning play a central role in the activity described here but also in other numerical techniques detailed in sparse linear algebra Section. The Nested Dissection is now a well-known heuristic for sparse matrix ordering to both reduce the fill-in during numerical factorization and to maximize the number of independent computation tasks. By using the block data structure induced by the partition of separators of the original graph, very efficient parallel block solvers have been designed and implemented according to super-nodal or multi-frontal approaches. Considering hybrid methods mixing both direct and iterative solvers such as MaPHyS, obtaining a domain decomposition leading to a good balancing of both the size of domain interiors and the size of interfaces is a key point for load balancing and efficiency in a parallel context.

We intend to revisit some well-known graph partitioning techniques in the light of the hybrid solvers and design new algorithms to be tested in the Scotch package.

4. Application Domains

4.1. Material physics

Participants: Olivier Coulaud, Pierre Esterie.

Due to the increase of available computer power, new applications in nano science and physics appear such as study of properties of new materials (photovoltaic materials, bio- and environmental sensors, ...), failure in materials, nano-indentation. Chemists, physicists now commonly perform simulations in these fields. These computations simulate systems up to billion of atoms in materials, for large time scales up to several nanoseconds. The larger the simulation, the smaller the computational cost of the potential driving the phenomena, resulting in low precision results. So, if we need to increase the precision, there are two ways to decrease the computational cost. In the first approach, we improve algorithms and their parallelization and in the second way, we will consider a multiscale approach.

A domain of interest is the material aging for the nuclear industry. The materials are exposed to complex conditions due to the combination of thermo-mechanical loading, the effects of irradiation and the harsh operating environment. This operating regime makes experimentation extremely difficult and we must rely on multi-physics and multi-scale modeling for our understanding of how these materials behave in service. This fundamental understanding helps not only to ensure the longevity of existing nuclear reactors, but also to guide the development of new materials for 4th generation reactor programs and dedicated fusion reactors. For the study of crystalline materials, an important tool is dislocation dynamics (DD) modeling. This multiscale simulation method predicts the plastic response of a material from the underlying physics of dislocation motion. DD serves as a crucial link between the scale of molecular dynamics and macroscopic methods based on finite elements; it can be used to accurately describe the interactions of a small handful of dislocations, or equally well to investigate the global behavior of a massive collection of interacting defects.

To explore i.e. to simulate these new areas, we need to develop and/or to improve significantly models, schemes and solvers used in the classical codes. In the project, we want to accelerate algorithms arising in those fields. We will focus on the following topics (in particular in the currently under definition OPTIDIS project in collaboration with CEA Saclay, CEA Ile-de-france and SIMaP Laboratory in Grenoble) in connection with research described at Sections 3.4 and 3.5.

- The interaction between dislocations is long ranged ($O(1/r)$) and anisotropic, leading to severe computational challenges for large-scale simulations. In dislocation codes, the computation of interaction forces between dislocations is still the most CPU time consuming and has to be improved to obtain faster and more accurate simulations.
- In such simulations, the number of dislocations grows while the phenomenon occurs and these dislocations are not uniformly distributed in the domain. This means that strategies to dynamically construct a good load balancing are crucial to acheive high performance.
- From a physical and a simulation point of view, it will be interesting to couple a molecular dynamics model (atomistic model) with a dislocation one (mesoscale model). In such three-dimensional coupling, the main difficulties are firstly to find and characterize a dislocation in the atomistic region, secondly to understand how we can transmit with consistency the information between the two micro and meso scales.

4.2. Co-design of algorithms in scientific applications

Participants: Emmanuel Agullo, Aurélien Falco, Olivier Beaumont, Lionel Eyraud-Dubois, Mathieu Faverge, Marek Felsoci, Luc Giraud, Gilles Marait, Van Gia Thinh Nguyen, Pierre Ramet, Guillaume Sylvand, Alena Shilova.

4.2.1. High performance simulation for ITER tokamak

Scientific simulation for ITER tokamak modeling provides a natural bridge between theory and experimentation and is also an essential tool for understanding and predicting plasma behavior. Recent progresses in numerical simulation of fine-scale turbulence and in large-scale dynamics of magnetically confined plasma have been enabled by access to petascale supercomputers. These progresses would have been unreachable without new computational methods and adapted reduced models. In particular, the plasma science community has developed codes for which computer runtime scales quite well with the number of processors up to thousands cores. The research activities of HIEPACS concerning the international ITER challenge have started in the Inria Project Lab C2S@EXA in collaboration with CEA-IRFM and were related to two complementary studies: a first one concerning the turbulence of plasma particles inside a tokamak (in the context of GYSELA code) and a second one concerning the MHD instability edge localized modes (in the context of JOREK code). The activity concerning GYSELA was completed at the end of 2018.

Other numerical simulation tools designed for the ITER challenge aim at making a significant progress in understanding active control methods of plasma edge MHD instability Edge Localized Modes (ELMs) which represent a particular danger with respect to heat and particle loads for Plasma Facing Components (PFC) in the tokamak. The goal is to improve the understanding of the related physics and to propose possible new strategies to improve effectiveness of ELM control techniques. The simulation tool used (JOREK code) is related to non linear MHD modeling and is based on a fully implicit time evolution scheme that leads to 3D large very badly conditioned sparse linear systems to be solved at every time step. In this context, the use of PaStiX library to solve efficiently these large sparse problems by a direct method is a challenging issue.

This activity continues within the context of the EoCoE2 project, in which the PaStiX solver is identified to allow the processing of very larger linear systems for the nuclear fusion code TOKAM3X from CEA-IRFM. Contrary to the JOREK code, the problem to be treated corresponds to the complete 3D volume of the plasma torus. The objective is to be competitive, for complex geometries, compared to an Algebraic MultiGrid approach designed by one partner of EoCoE2.

4.2.2. Numerical and parallel scalable hybrid solvers in large scale calculations

Parallel and numerically scalable hybrid solvers based on a fully algebraic coarse space correction have been theoretically studied and various advanced parallel implementations have been designed. Their parallel scalability has been initially investigated on large scale problems within the EoCoE project thanks to a close collaboration with the BSC and the integration of MaPHyS within the Alya software. This activity will further develop in the EoCoE2 project. The performance has also been assessed on PRACE Tier-0 machine within a PRACE Project Access through a collaboration with CERFACS and Laboratoire de Physique des Plasmas at Ecole Polytechnique for the calculation of plasma propulsion. A comparative parallel scalability study with the Algebraic MultiGrid from Petsc has been conducted in that framework.

4.2.3. Aeroacoustics Simulation

This domains is in the context of a long term collaboration with Airbus Research Centers. Wave propagation phenomena intervene in many different aspects of systems design at Airbus. They drive the level of acoustic vibrations that mechanical components have to sustain, a level that one may want to diminish for comfort reason (in the case of aircraft passengers, for instance) or for safety reason (to avoid damage in the case of a payload in a rocket fairing at take-off). Numerical simulations of these phenomena plays a central part in the upstream design phase of any such project. Airbus Central R & T has developed over the last decades an in-depth knowledge in the field of Boundary Element Method (BEM) for the simulation of wave propagation in homogeneous media and in frequency domain. To tackle heterogeneous media (such as the jet engine flows, in the case of acoustic simulation), these BEM approaches are coupled with volumic finite elements (FEM). We end up with the need to solve large (several millions unknowns) linear systems of equations composed of a dense part (coming for the BEM domain) and a sparse part (coming from the FEM domain). Various parallel solution techniques are available today, mixing tools created by the academic world (such as the Mumps and Pastix sparse solvers) as well as parallel software tools developed in-house at Airbus (dense solver SPIDO, multipole solver, $\mathcal{H}$-matrix solver with an open sequential version available online). In the current state of knowledge and technologies, these methods do not permit to tackle the simulation of aeroacoustics problems at the highest acoustic frequencies (between 5 and 20 kHz, upper limits of human audition) while considering the whole complexity of geometries and phenomena involved (higher acoustic frequency implies smaller mesh sizes that lead to larger unknowns number, a number that grows like f^2 for BEM and f^3 for FEM, where f is the studied frequency). The purpose of the study in this domain is to develop advanced solvers able to tackle this kind of mixed dense/sparse linear systems efficiently on parallel architectures.

4.2.4. Optimization for Deep Convolutional Neural Networks

The training phase of Deep Convolutional Neural Networks represents nowadays a significant share of the computations performed on HPC supercomputers. It introduces several new problems concerning resource allocation and scheduling issues, because of the specific pattern of task graphs induced by the stochastic gradient descent and because memory consumption is particularly critical when performing training. As of today, the most classical parallelization methods consists in partitioning mini-batches, images, filters,... but all these methods induce high synchronization and communication costs, and only very partially resolve memory issues. Within the framework of the Inria IPL on HPC Big Data and Learning convergence, we are working on re-materialization techniques and on the use of model parallelism, in particular to be able to build on the research that has been carried out in a more traditional HPC framework on the exploitation of resource heterogeneity and dynamic runtime scheduling.

5. Highlights of the Year

5.1. Highlights of the Year

- HIEPACS was extremely pleased to welcome two new permanent Inria members, namely O. Beaumont and L. Eyraud-Dubois, whose scientific expertises clearly strengthen the impact of the team on the HPC research.
- We are very delighted to report that seven new PhD students have joined the team this year on research topics covering the full range of those adressed by the team. These PhD students, with gender parity, come from different places in France (Bordeaux, Strasbourg) as well as other places worldwide (China, Italy and Russia). This cultural and scientific variety will surely lead to a nice and fruitful blend and will contribute to the stimulating research atmosphere within the team.
- In June 2019, we organized the 14th Scheduling for Large Scale Systems Workshop, in the campus of Victoire in Bordeaux. 48 participants from all over the world registered to the workshop and gave 36 presentations over 3 days, covering topics like Numerical Algorithms, Resilience, Performance Evaluation, Job and DAG Scheduling.
- Inria's Autumn school, November 4-8 2019, Inria Bordeaux Sud-Ouest co-organized by E. Agullo (HIEPACS), H. Beaugendre (CARDAMON) and J. Diaz (MAGIQUE3D)

  The school aimed at simulating a physical problem, from its modeling to its implementation in a high performance computing (HPC) framework. The school offered both plenary courses and hands-on sessions that involved many members of the three teams. The physical problem considered was the harmonic wave propagation.

  The first day was dedicated to the modeling of the problem and its discretization using a Discontinuous Galerkin scheme. The following two days were dedicated to linear algebra for solving large sparse systems. Background on direct, iterative and hybrid methods for sparse linear systems were discussed. Hands-on on related parallel solvers were then be proposed. Has followed a session dedicated to advanced parallel schemes using task-based paradigms, including a hands-on with the starpu runtime system. The ultimate hands-on session was devoted to the use of parallel profiling tools. The school was closed with plenary talks illustrating the usage of such a workflow in an industrial context.

  The hands-on session were conducted on the Federative Platform for Research in Computer Science and Mathematics (PlaFRIM) machine in a guix-hpc reproducible environment

  The school was attended by about 40 participants mostly PhDs and postdocs from Inria teams.

6. New Software and Platforms

6.1. AVCI

Adaptive vibrational configuration interaction

KEYWORDS: Vibrational spectra - Eigen value

FUNCTIONAL DESCRIPTION: A-VCI is a theoretical vibrational spectroscopy algorithm developed to effectively reduce the number of vibrational states used in the configuration-interaction (CI) process. It constructs a nested basis for the discretization of the Hamiltonian operator inside a large CI approximation space and uses an a-posteriori error estimator (residue) to select the most relevant directions to expand the discretization space.

The Hamiltonian operator consists of 3 operators: a harmonic oscillator sum, the potential energy surface operator and the Coriolis operators. In addition, the code can compute the intensity of eigenvectors.

The code can handle molecules up to 10 atoms, which corresponds to solving an eigenvalue problem in a 24-dimensional space.

- Partner: IPREM
- Contact: Olivier Coulaud

6.2. Chameleon

KEYWORDS: Runtime system - Task-based algorithm - Dense linear algebra - HPC - Task scheduling

SCIENTIFIC DESCRIPTION: Chameleon is part of the MORSE (Matrices Over Runtime Systems @ Exascale) project. The overall objective is to develop robust linear algebra libraries relying on innovative runtime systems that can fully benefit from the potential of those future large-scale complex machines.

We expect advances in three directions based first on strong and closed interactions between the runtime and numerical linear algebra communities. This initial activity will then naturally expand to more focused but still joint research in both fields.

1. Fine interaction between linear algebra and runtime systems. On parallel machines, HPC applications need to take care of data movement and consistency, which can be either explicitly managed at the level of the application itself or delegated to a runtime system. We adopt the latter approach in order to better keep up with hardware trends whose complexity is growing exponentially. One major task in this project is to define a proper interface between HPC applications and runtime systems in order to maximize productivity and expressivity. As mentioned in the next section, a widely used approach consists in abstracting the application as a DAG that the runtime system is in charge of scheduling. Scheduling such a DAG over a set of heterogeneous processing units introduces a lot of new challenges, such as predicting accurately the execution time of each type of task over each kind of unit, minimizing data transfers between memory banks, performing data prefetching, etc. Expected advances: In a nutshell, a new runtime system API will be designed to allow applications to provide scheduling hints to the runtime system and to get real-time feedback about the consequences of scheduling decisions.

2. Runtime systems. A runtime environment is an intermediate layer between the system and the application. It provides low-level functionality not provided by the system (such as scheduling or management of the heterogeneity) and high-level features (such as performance portability). In the framework of this proposal, we will work on the scalability of runtime environment. To achieve scalability it is required to avoid all centralization. Here, the main problem is the scheduling of the tasks. In many task-based runtime environments the scheduler is centralized and becomes a bottleneck as soon as too many cores are involved. It is therefore required to distribute the scheduling decision or to compute a data distribution that impose the mapping of task using, for instance the so-called “owner-compute” rule. Expected advances: We will design runtime systems that enable an efficient and scalable use of thousands of distributed multicore nodes enhanced with accelerators.

3. Linear algebra. Because of its central position in HPC and of the well understood structure of its algorithms, dense linear algebra has often pioneered new challenges that HPC had to face. Again, dense linear algebra has been in the vanguard of the new era of petascale computing with the design of new algorithms that can efficiently run on a multicore node with GPU accelerators. These algorithms are called "communication-avoiding" since they have been redesigned to limit the amount of communication between processing units (and between the different levels of memory hierarchy). They are expressed through Direct Acyclic Graphs (DAG) of fine-grained tasks that are dynamically scheduled. Expected advances: First, we plan to investigate the impact of these principles in the case of sparse applications (whose algorithms are slightly more complicated but often rely on dense kernels). Furthermore, both in the dense and sparse cases, the scalability on thousands of nodes is still limited, new numerical approaches need to be found. We will specifically design sparse hybrid direct/iterative methods that represent a promising approach.

Overall end point. The overall goal of the MORSE associate team is to enable advanced numerical algorithms to be executed on a scalable unified runtime system for exploiting the full potential of future exascale machines.

FUNCTIONAL DESCRIPTION: Chameleon is a dense linear algebra software relying on sequential task-based algorithms where sub-tasks of the overall algorithms are submitted to a Runtime system. A Runtime system such as StarPU is able to manage automatically data transfers between not shared memory area (CPUs-GPUs, distributed nodes). This kind of implementation paradigm allows to design high performing linear algebra algorithms on very different type of architecture: laptop, many-core nodes, CPUs-GPUs, multiple nodes. For example, Chameleon is able to perform a Cholesky factorization (double-precision) at 80 TFlop/s on a dense matrix of order 400 000 (i.e. 4 min 30 s).

RELEASE FUNCTIONAL DESCRIPTION: Chameleon includes the following features:

- BLAS 3, LAPACK one-sided and LAPACK norms tile algorithms - Support QUARK and StarPU runtime systems and PaRSEC since 2018 - Exploitation of homogeneous and heterogeneous platforms through the use of BLAS/LAPACK CPU kernels and cuBLAS/MAGMA CUDA kernels - Exploitation of clusters of interconnected nodes with distributed memory (using OpenMPI)

- Participants: Cédric Castagnede, Samuel Thibault, Emmanuel Agullo, Florent Pruvost and Mathieu Faverge
- Partners: Innovative Computing Laboratory (ICL) - King Abdullha University of Science and Technology - University of Colorado Denver
- Contact: Emmanuel Agullo
- URL: https://gitlab.inria.fr/solverstack/chameleon

6.3. Diodon

KEYWORDS: Dimensionality reduction - Data analysis

FUNCTIONAL DESCRIPTION: Most of dimension reduction methods inherited from Multivariate Data Analysis, and currently implemented as element in statistical learning for handling very large datasets (the dimension of spaces is the number of features) rely on a chain of pretreatments, a core with a SVD for low rank approximation of a given matrix, and a post-treatment for interpreting results. The costly part in computations is the SVD, which is in cubic complexity. Diodon is a list of functions and drivers which implement (i) pre-treatments, SVD and post-treatments on a large diversity of methods, (ii) random projection methods for running the SVD which permits to bypass the time limit in computing the SVD, and (iii) an implementation in C++ of the SVD with random projection at prescribed rank or precision, connected to MDS.

- Contact: Alain Franc

6.4. DPLASMA

Distributed Parallel Linear Algebra Software for Multicore Architectures

FUNCTIONAL DESCRIPTION: DPLASMA is the leading implementation of a dense linear algebra package for distributed heterogeneous systems. It is designed to deliver sustained performance for distributed systems where each node featuring multiple sockets of multicore processors, and if available, accelerators like GPUs or Intel Xeon Phi. DPLASMA achieves this objective through the state of the art PaRSEC runtime, porting the PLASMA algorithms to the distributed memory realm.

- Contact: Mathieu Faverge
- URL: http://icl.cs.utk.edu/parsec/index.html

6.5. Fabulous

Fast Accurate Block Linear krylOv Solver

KEYWORDS: Numerical algorithm - Block Krylov solver

SCIENTIFIC DESCRIPTION: Versatile and flexible numerical library that implements Block Krylov iterative schemes for the solution of linear systems of equations with multiple right-hand sides

FUNCTIONAL DESCRIPTION: Versatile and flexible numerical library that implements Block Krylov iterative schemes for the solution of linear systems of equations with multiple right-hand sides. The library implements block variants of minimal norm residual variants with partial convergence management and spectral information recycling. The package already implements regular block-GMRES (BGMRES), Inexact Breakdown BGMRES (IB-BMGRES), Inexact Breakdown BGMRES with Deflated Restarting (IB-BGMRES-DR), Block Generalized Conjugate Residual with partial convergence management. The C++ library relies on callback mechanisms to implement the calculations (matrix-vector, dot-product, ...) that depend on the parallel data distribution selected by the user.

- Participants: Emmanuel Agullo, Luc Giraud, Gilles Marait and Cyrille Piacibello
- Contact: Luc Giraud
- Publication: Block GMRES method with inexact breakdowns and deflated restarting
- URL: https://gitlab.inria.fr/solverstack/fabulous/

6.6. MAPHYS

Massively Parallel Hybrid Solver

KEYWORD: Parallel hybrid direct/iterative solution of large linear systems

FUNCTIONAL DESCRIPTION: MaPHyS is a software package that implements a parallel linear solver coupling direct and iterative approaches. The underlying idea is to apply to general unstructured linear systems domain decomposition ideas developed for the solution of linear systems arising from PDEs. The interface problem, associated with the so called Schur complement system, is solved using a block preconditioner with overlap between the blocks that is referred to as Algebraic Additive Schwarz. A fully algebraic coarse space is available for symmetric positive definite problems, that insures the numerical scalability of the preconditioner.

The parallel implementation is based on MPI+thread. Maphys relies on state-of-the art sparse and dense direct solvers.

MaPHyS is essentially a preconditioner that can be used to speed-up the convergence of any Krylov subspace method and is coupled with the ones implemented in the Fabulous package.

- Participants: Emmanuel Agullo, Luc Giraud, Matthieu Kuhn, Gilles Marait and Louis Poirel
- Contact: Emmanuel Agullo
- Publications: Hierarchical hybrid sparse linear solver for multicore platforms - Robust coarse spaces for Abstract Schwarz preconditioners via generalized eigenproblems
- URL: https://gitlab.inria.fr/solverstack/maphys

6.7. MetaPart

KEYWORDS: High performance computing - HPC - Parallel computing - Graph algorithmics - Graph - Hypergraph

FUNCTIONAL DESCRIPTION: MetaPart is a framework for graph or hypergraph manipulation that addresses different problems, like partitioning, repartitioning, or co-partitioning, ... MetaPart is made up of several projects, such as StarPart, LibGraph or CoPart. StarPart is the core of the MetaPart framework. It offers a wide variety of graph partitioning methods (Metis, Scotch, Zoltan, Patoh, ParMetis, Kahip, ...), which makes it easy to compare these different methods and to better adjust the parameters of these methods. It is built upon the LibGraph library, that provides basic graph and hypergraph routines. The Copart project is a library used on top of StarPart, that provides co-partitioning algorithms for the load-blancing of parallel coupled simulations.

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6.8. MPICPL

MPI CouPLing

KEYWORDS: MPI - Coupling software

FUNCTIONAL DESCRIPTION: MPICPL is a software library dedicated to the coupling of parallel legacy codes, that are based on the well-known MPI standard. It proposes a lightweight and comprehensive programing interface that simplifies the coupling of several MPI codes (2, 3 or more). MPICPL facilitates the deployment of these codes thanks to the mpicplrun tool and it interconnects them automatically through standard MPI intercommunicators. Moreover, it generates the universe communicator, that merges the world communicators of all coupled-codes. The coupling infrastructure is described by a simple XML file, that is just loaded by the mpicplrun tool.

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6.9. OptiDis

KEYWORDS: Dislocation dynamics simulation - Fast multipole method - Large scale - Collision

FUNCTIONAL DESCRIPTION: OptiDis is a new code for large scale dislocation dynamics simulations. Its purpose is to simulate real life dislocation densities (up to 5.1022 dislocations/m-2) in order to understand plastic deformation and study strain hardening. The main application is to observe and understand plastic deformation of irradiated zirconium. Zirconium alloys are the first containment barrier against the dissemination of radioactive elements. More precisely, with neutron irradiated zirconium alloys we are talking about channeling mechanism, which means to stick with the reality, more than tens of thousands of induced loops, i. e. 100 million degrees of freedom in the simulation. The code is based on Numodis code developed at CEA Saclay and the ScalFMM library developed in HiePACS project. The code is written in C++ language and using the last features of C++11/14. One of the main aspects is the hybrid parallelism MPI/OpenMP that gives the software the ability to scale on large cluster while the computation load rises. In order to achieve that, we use different levels of parallelism. First of all, the simulation box is distributed over MPI processes, then we use a thinner level for threads, dividing the domain by an Octree representation. All theses parts are controlled by the ScalFMM library. On the last level, our data are stored in an adaptive structure that absorbs the dynamics of this type of simulation and manages the parallelism of tasks..

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- URL: http://optidis.gforge.inria.fr/

6.10. PaStiX

Parallel Sparse matriX package

KEYWORDS: Linear algebra - High-performance calculation - Sparse Matrices - Linear Systems Solver - Low-Rank compression

SCIENTIFIC DESCRIPTION: PaStiX is based on an efficient static scheduling and memory manager, in order to solve 3D problems with more than 50 million of unknowns. The mapping and scheduling algorithm handle a combination of 1D and 2D block distributions. A dynamic scheduling can also be applied to take care of NUMA architectures while taking into account very precisely the computational costs of the BLAS 3 primitives, the communication costs and the cost of local aggregations.

FUNCTIONAL DESCRIPTION: PaStiX is a scientific library that provides a high performance parallel solver for very large sparse linear systems based on block direct and block ILU(k) methods. It can handle low-rank compression techniques to reduce the computation and the memory complexity. Numerical algorithms are implemented in single or double precision (real or complex) for LLt, LDLt and LU factorization with static pivoting (for non symmetric matrices having a symmetric pattern). The PaStiX library uses the graph partitioning and sparse matrix block ordering packages Scotch or Metis.

The PaStiX solver is suitable for any heterogeneous parallel/distributed architecture when its performance is predictable, such as clusters of multicore nodes with GPU accelerators or KNL processors. In particular, we provide a high-performance version with a low memory overhead for multicore node architectures, which fully exploits the advantage of shared memory by using an hybrid MPI-thread implementation.

The solver also provides some low-rank compression methods to reduce the memory footprint and/or the time-to-solution.

- Participants: Tony Delarue, Grégoire Pichon, Mathieu Faverge, EsragÜl Korkmaz and Pierre Ramet
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- Contact: Pierre Ramet
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6.11. pmtool

KEYWORDS: Scheduling - Task scheduling - StarPU - Heterogeneity - GPGPU - Performance analysis

FUNCTIONAL DESCRIPTION: Analyse post-mortem the behavior of StarPU applications. Provide lower bounds on makespan. Study the performance of different schedulers in a simple context. Provide implementations of many scheduling algorithms from the literature

NEWS OF THE YEAR: Included many new algorithms, in particular online algorithms Better integration with StarPU by accepting .rec files as input

- Participant: Lionel Eyraud-Dubois
- Contact: Lionel Eyraud-Dubois
- Publications: Approximation Proofs of a Fast and Efficient List Scheduling Algorithm for Task-Based Runtime Systems on Multicores and GPUs - Fast Approximation Algorithms for Task-Based Runtime Systems
- URL: https://gitlab.inria.fr/eyrauddu/pmtool

6.12. rotor

Re-materializing Optimally with pyTORch

KEYWORDS: Deep learning - Optimization - Python - GPU - Automatic differentiation

FUNCTIONAL DESCRIPTION: Allows to train very large convolutional networks on limited memory by optimally selecting which activations should be kept and which should be recomputed. This code is meant to replace the checkpoint.py utility available in pytorch, by providing more efficient rematerialization strategies. The algorithm is easier to tune: the only required parameter is the available memory, instead of the number of segments.

- Contact: Lionel Eyraud-Dubois

6.13. ScalFMM

Scalable Fast Multipole Method

KEYWORDS: N-body - Fast multipole method - Parallelism - MPI - OpenMP

SCIENTIFIC DESCRIPTION: ScalFMM is a software library to simulate N-body interactions using the Fast Multipole Method. The library offers two methods to compute interactions between bodies when the potential decays like 1/r. The first method is the classical FMM based on spherical harmonic expansions and the second is the Black-Box method which is an independent kernel formulation (introduced by E. Darve @ Stanford). With this method, we can now easily add new non oscillatory kernels in our library. For the classical method, two approaches are used to decrease the complexity of the operators. We consider either matrix formulation that allows us to use BLAS routines or rotation matrix to speed up the M2L operator.

ScalFMM intends to offer all the functionalities needed to perform large parallel simulations while enabling an easy customization of the simulation components: kernels, particles and cells. It works in parallel in a shared/distributed memory model using OpenMP and MPI. The software architecture has been designed with two major objectives: being easy to maintain and easy to understand. There is two main parts:

the management of the octree and the parallelization of the method the kernels. This new architecture allow us to easily add new FMM algorithm or kernels and new paradigm of parallelization.

FUNCTIONAL DESCRIPTION: Compute N-body interactions using the Fast Multipole Method for large number of objects

- Participants: Bramas Bérenger, Olivier Coulaud and Pierre Estérie
- Contact: Olivier Coulaud
- URL: https://gitlab.inria.fr/solverstack/ScalFMM

6.14. VITE

Visual Trace Explorer

KEYWORDS: Visualization - Execution trace

FUNCTIONAL DESCRIPTION: ViTE is a trace explorer. It is a tool made to visualize execution traces of large parallel programs. It supports Pajé, a trace format created by Inria Grenoble, and OTF and OTF2 formats, developed by the University of Dresden and allows the programmer a simpler way to analyse, debug and/or profile large parallel applications.

- Participant: Mathieu Faverge
- Contact: Mathieu Faverge
- URL: http://vite.gforge.inria.fr/

6.15. PlaFRIM

Plateforme Fédérative pour la Recherche en Informatique et Mathématiques

KEYWORDS: High-Performance Computing - Hardware platform

FUNCTIONAL DESCRIPTION: PlaFRIM is an experimental platform for research in modeling, simulations and high performance computing. This platform has been set up from 2009 under the leadership of Inria Bordeaux Sud-Ouest in collaboration with computer science and mathematics laboratories, respectively Labri and IMB with a strong support in the region Aquitaine.

It aggregates different kinds of computational resources for research and development purposes. The latest technologies in terms of processors, memories and architecture are added when they are available on the market. It is now more than 1,000 cores (excluding GPU and Xeon Phi) that are available for all research teams of Inria Bordeaux, Labri and IMB. This computer is in particular used by all the engineers who work in HiePACS and are advised by F. Rue from the SED.

- Contact: Olivier Coulaud
- URL: https://www.plafrim.fr/en/home/

7. New Results

7.1. High-performance computing on next generation architectures

7.1.1. Memory optimization for the training phase of deep convolutional networks

Training Deep Neural Networks is known to be an expensive operation, both in terms of computational cost and memory load. Indeed, during training, all intermediate layer outputs (called activations) computed during the forward phase must be stored until the corresponding gradient has been computedin the backward phase. These memory requirements sometimes prevent to consider larger batch sizes and deeper networks, so that they can limit both convergence speed and accuracy. Recent works have proposed to offload some of the computed forward activations from the memory of the GPU to the memory of the CPU. This requires to determine which activations should be offloaded and when these transfers from and to the memory of the GPU should take place. In [28], We prove that this problem is NP-hard in the strong sense, and we propose two heuristics based on relaxations of the problem. We perform extensive experimental evaluation on standard Deep Neural Networks. We compare the performance of our heuristics against previous approaches from the literature, showing that they achieve much better performance in a wide variety of situations.

In [23], we also introduce a new activation checkpointing method which allows to significantly decrease memory usage when training Deep Neural Networks with the back-propagation algorithm. Similarly to checkpointing techniques coming from the literature on Automatic Differentiation, it consists in dynamically selecting the forward activations that are saved during the training phase, and then automatically recomputing missing activations from those previously recorded. We propose an original computation model that combines two types of activation savings: either only storing the layer inputs, or recording the complete history of operations that produced the outputs (this uses more memory, but requires fewer recomputations in the backward phase), and we provide an algorithm to compute the optimal computation sequence for this model. This paper also describes a PyTorch implementation that processes the entire chain, dealing with any sequential DNN whose internal layers may be arbitrarily complex and automatically executing it according to the optimal checkpointing strategy computed given a memory limit. Through extensive experiments, we show that our implementation consistently outperforms existing checkpointing approaches for a large class of networks, image sizes and batch sizes.

In [4], [24], we consider the problem of optimally scheduling the backpropagation of Deep Join Networks. Deep Learning training memory needs can prevent the user to consider large models and large batch sizes. In this work, we propose to use techniques from memory-aware scheduling and Automatic Differentiation (AD) to execute a backpropagation graph with a bounded memory requirement at the cost of extra recomputations. The case of a single homogeneous chain, i.e. the case of a network whose all stages are identical and form a chain, is well understood and optimal solutions have been proposed in the AD literature. The networks encountered in practice in the context of Deep Learning are much more diverse, both in terms of shape and heterogeneity. In this work, we define the class of backpropagation graphs, and extend those on which one can compute in polynomial time a solution that minimizes the total number of recomputations. In particular we consider join graphs which correspond to models such as Siamese or Cross Modal Networks.

7.1.2. Sizing and Partitioning Strategies for Burst-Buffers to Reduce IO Contention

Burst-Buffers are high throughput and small size storage which are being used as an intermediate storage between the PFS (Parallel File System) and the computational nodes of modern HPC systems. They can allow to hinder to contention to the PFS, a shared resource whose read and write performance increase slower than processing power in HPC systems. A second usage is to accelerate data transfers and to hide the latency to the PFS. In this work, we concentrate on the first usage. We propose a model for Burst-Buffers and application transfers. We consider the problem of dimensioning and sharing the Burst-Buffers between several applications. This dimensioning can be done either dynamically or statically. The dynamic allocation considers that any application can use any available portion of the Burst-Buffers. The static allocation considers that when a new application enters the system, it is assigned some portion of the Burst-Buffers, which cannot be used by the other applications until that application leaves the system and its data is purged from it. We show that the general sharing problem to guarantee fair performance for all applications is an NP-Complete problem. We propose a polynomial time algorithms for the special case of finding the optimal buffer size such that no application is slowed down due to PFS contention, both in the static and dynamic cases. Finally, we provide evaluations of our algorithms in realistic settings. We use those to discuss how to minimize the overhead of the static allocation of buffers compared to the dynamic allocation. More information on these results can be found in [9].

7.1.3. Efficient Ordering of Kernel Submission on GPUs

In distributed memory systems, it is paramount to develop strategies to overlap the data transfers between memory nodes with the computations in order to exploit their full potential. In [11], we consider the problem of determining the order of data transfers between two memory nodes for a set of independent tasks with the objective of minimizing the makespan. We prove that, with limited memory capacity, the problem of obtaining the optimal data transfer order is NP-complete. We propose several heuristics to determine this order and discuss the conditions that might be favorable to different heuristics. We analyze our heuristics on traces obtained by running two molecular chemistry kernels, namely, Hartree–Fock (HF) and Coupled Cluster Singles Doubles (CCSD), on 10 nodes of an HPC system. Our results show that some of our heuristics achieve significant overlap for moderate memory capacities and resulting in makespans that are very close to the lower bound.

Concurrent kernel execution is a relatively new feature in modern GPUs, which was designed to improve hardware utilization and the overall system throughput. However, the decision on the simultaneous execution of tasks is performed by the hardware with a leftover policy, that assigns as many resources as possible for one task and then assigns the remaining resources to the next task. This can lead to unreasonable use of resources. In [30], we tackle the problem of co-scheduling for GPUs with and without preemption, with the focus on determining the kernels submission order to reduce the number of preemptions and the kernels makespan, respectively. We propose a graph-based theoretical model to build preemptive and non-preemptive schedules. We show that the optimal preemptive makespan can be computed by solving a Linear Program in polynomial time, and we propose an algorithm based on this solution which minimizes the number of preemptions. We also propose an algorithm that transforms a preemptive solution of optimal makespan into a non-preemptive solution with the smallest possible preemption overhead. We show, however, that finding the minimal amount of preemptions among all preemptive solutions of optimal makespan is a NP-hard problem, and computing the optimal non-preemptive schedule is also NP-hard. In addition, we study the non-preemptive problem, without searching first for a good preemptive solution, and present a Mixed Integer Linear Program solution to this problem. We performed experiments on real-world GPU applications and our approach can achieve optimal makespan by preempting 6 to 9% of the tasks. Our non-preemptive approach, on the other side, obtains makespan within 2.5% of the optimal preemptive schedules, while previous approaches exceed the preemptive makespan by 5 to 12%.

7.1.4. Scheduling Tasks on Two Types of Resources

We consider the problem of scheduling task graphs on two types of unrelated resources, which arises in the context of task-based runtime systems on modern platforms containing CPUs and GPUs. In [10], we focus on an algorithm named HeteroPrio, which was originally introduced as an efficient heuristic for a particular application. HeteroPrio is an adaptation of the well known list scheduling algorithm, in which the tasks are picked by the resources in the order of their acceleration factor. This algorithm is augmented with a spoliation mechanism: a task assigned by the list algorithm can later on be reassigned to a different resource if it allows to finish this task earlier. We propose here the first theoretical analysis of the HeteroPrio algorithm in the presence of dependencies. More specifically, if the platform contains m and n processors of each type, we show that the worst-case approximation ratio of HeteroPrio is between $1 + \max(m/n, n/m)$ and $2 + \max(m/n, n/m)$. Our proof structure allows to precisely identify the necessary conditions on the spoliation strategy to obtain such a guarantee. We also present an in-depth experimental analysis, comparing several such spoliation strategies, and comparing HeteroPrio with other algorithms from the literature. Although the worst case analysis shows the possibility of pathological behavior, HeteroPrio is able to produce, in very reasonable time, schedules of significantly better quality.

The evolution in the design of modern parallel platforms leads to revisit the scheduling jobs on distributed heterogeneous resources. We contribute to [31], a survey whose goal is to present the main existing algorithms, to classify them based on their underlying principles and to propose unified implementations to enable their fair comparison, both in terms of running time and quality of schedules, on a large set of common benchmarks that we made available for the community [27]. Beyond this comparison, our goal is also to understand the main difficulties that heterogeneity conveys and the shared principles that guide the design of efficient algorithms.

7.1.5. Data-Locality Aware Tasks Scheduling with Replicated Inputs

In [5], we consider the influence on data-locality of the replication of data files, as automatically performed by Distributed File Systems such as HDFS. Replication is known to have a crucial impact on data locality in addition to system fault tolerance. Indeed, intuitively, having more replicas of the same input file gives more opportunities for this task to be processed locally, i.e. without any input file transfer. Given the practical importance of this problem, a vast literature has been proposed to schedule tasks, based on a random placement of replicated input files. Our goal in this paper is to study the performance of these algorithms, both in terms of makespan minimization (minimize the completion time of the last task when non-local processing is forbidden) and communication minimization (minimize the number of non-local tasks when no idle time on resources is allowed). In the case of homogenous tasks, we are able to prove, using models based on "balls into bins" and "power of two choices" problems, that the well known good behavior of classical strategies can be theoretically grounded. Going further, we even establish that it is possible, using semi-matchings theory, to find the optimal solution in very small time. We also use known graph-orientation results to prove that this optimal solution is indeed near-perfect with strong probability. In the more general case of heterogeneous tasks, we propose heuristics solutions both in the clairvoyant and non-clairvoyant cases (i.e. task length is known in advance or not), and we evaluate them through simulations, using actual traces of a Hadoop cluster.

7.2. High performance solvers for large linear algebra problems

7.2.1. Deflation and preconditioning strategies for sequences of sampled stochastic elliptic equations

We are interested in the quantification of uncertainties in discretized elliptic partial differential equations with random coefficients. In sampling-based approaches, this relies on solving large numbers of symmetric positive definite linear systems with different matrices. In this work, we investigate recycling Krylov subspace strategies for the iterative solution of sequences of such systems. The linear systems are solved using deflated conjugate gradient (CG) methods, where the Krylov subspace is augmented with approximate eigenvectors of the previously sampled operator. These operators are sampled by Markov chain Monte Carlo, which leads to sequences of correlated matrices. First, the following aspects of eigenvector approximation, and their effect on deflation, are investigated: (i) projection technique, and (ii) restarting strategy of the eigen-search space. Our numerical experiments show that these aspects only impact convergence behaviors of deflated CG at the early stages of the sampling sequence. Second, unlike sequences with multiple right-hand sides and a constant operator, our experiments with multiple matrices show the necessity to orthogonalize the iterated residual of the linear system with respect to the deflation subspace, throughout the sampling sequence. Finally, we observe a synergistic effect of deflation and block-Jacobi (bJ) preconditioning. While the action of bJ preconditioners leaves a trail of isolated eigenvalues in the spectrum of the preconditioned operator, for 1D problems, the corresponding eigenvectors are well approximated by the recycling strategy. Then, up to a certain number of blocks, deflated CG methods with bJ preconditioners achieve similar convergence behaviors to those observed with CG when using algebraic multigrid (AMG) as a preconditioner.

This work, developed in the framework of the PhD thesis of Nicolas Venkovic in collaboration with P. Mycek (Cerfacs) and O. Le Maitre (CMAP, Ecole Polytechnique), will be presented at the next Copper Mountain conference on iterative methods.

7.2.2. Robust preconditionners via generalized eigenproblems for hybrid sparse linear solvers

The solution of large sparse linear systems is one of the most time consuming kernels in many numerical simulations. The domain decomposition community has developed many efficient and robust methods in the last decades. While many of these solvers fall into the abstract Schwarz (aS) framework, their robustness has originally been demonstrated on a case-by-case basis. In this work, we propose a bound for the condition number of all deflated aS methods provided that the coarse grid consists of the assembly of local components that contain the kernel of some local operators. We show that classical results from the literature on particular instances of aS methods can be retrieved from this bound. We then show that such a coarse grid correction can be explicitly obtained algebraically via generalized eigenproblems, leading to a condition number independent of the number of domains. This result can be readily applied to retrieve or improve the bounds previously obtained via generalized eigenproblems in the particular cases of Neumann-Neumann (NN), Additive Schwarz (AS) and optimized Robin but also generalizes them when applied with approximate local solvers. Interestingly, the proposed methodology turns out to be a comparison of the considered particular aS method with generalized versions of both NN and AS for tackling the lower and upper part of the spectrum, respectively. We furthermore show that the application of the considered grid corrections in an additive fashion is robust in the AS case although it is not robust for aS methods in general. In particular, the proposed framework allows for ensuring the robustness of the AS method applied on the Schur complement (AS/S), either with deflation or additively, and with the freedom of relying on an approximate local Schur complement. Numerical experiments illustrate these statements.

More information on these results can be found in [3]

7.2.3. Rank Revealing QR Methods for Sparse Block Low Rank Solvers

In the context of the ANR Sashimi project and the Phd of Esragul Korkmaz, we have investigated several compression methods of dense blocks appearing inside sparse matrix solvers to reduce the memory consumption, as well as the time to solution.

Solving linear equations of type Ax=b for large sparse systems frequently emerges in science and engineering applications, which creates the main bottleneck. In spite that the direct methods are costly in time and memory consumption, they are still the most robust way to solve these systems. Nowadays, increasing the amount of computational units for the supercomputers became trendy, while the memory available per core is reduced. Therefore, when solving these linear equations, memory reduction becomes as important as time reduction. While looking for the lowest possible compression rank, Singular Value Decomposition (SVD) gives the best result. It is however too costly as the whole factorization is computed to find the resulting rank. In this respect, rank revealing QR decomposition variants are less costly, but can introduce larger ranks. Among these variants, column pivoting or matrix rotation can be applied on the matrix A, such that the most important information in the matrix is gathered to the leftmost columns and the remaining unnecessary information can be omitted. For reducing the communication cost of the classical QR decomposition with column pivoting, blocking versions with randomization are suggested as an alternative solution to find the pivots. In these randomized variants, the matrix A is projected on a much lower dimensional matrix by using an independent and identically distributed Gaussian matrix so that the pivoting/rotational matrix can be computed on the lower dimensional matrix. In addition, to avoid unnecessary updates of the trailing matrix at each iteration, a truncated randomized method is suggested and shown to be more efficient for larger matrix sizes. Thanks to these methods, closer results to SVD can be obtained and the cost of compression can be reduced.

A comparison of all these methods in terms of complexity, numerical stability and performance have been presented at the national conference COMPAS'2019 [18], and at the international workshop SparseDay'2019 [19].

7.2.4. Accelerating Krylov linear solvers with agnostic lossy data compression

In the context of the Inria International Lab JLESC we have an ongoing collaboration with Argonne National Laboratory on the use of agnostic compression techniques to reduce the memory footprint of iterative linear solvers. Krylov methods are among the most efficient and widely used algorithms for the solution of large linear systems. Some of these methods can, however, have large memory requirements. Despite the fact that modern high-performance computing systems have more and more memory available, the memory used by applications remains a major concern when solving large scale problems. This is one of the reasons why interest in lossy data compression techniques has grown tremendously in the last two decades: it can reduce the amount of information that needs to be stored and communicated. Recently, it has also been shown that Krylov methods allow for some inexactness in the matrix-vector product that is typically required in each iteration. We showed that the loss of accuracy caused by compressing and decompressing the solution of the preconditioning step in the flexible generalized minimal residual method can be interpreted as an inexact matrix-vector product. This allowed us to find a bound on the maximum compression error in each iteration based on the theory of inexact Krylov methods. We performed a series of numerical experiment in order to validate our results. A number of "relaxed compression strategies" was also considered in order to achieve higher compression ratios.

The results of this joint effort will be presented to the next SIAM conférence on Parallel processing SIAM-PP'20.

7.2.5. Energy Analysis of a Solver Stack for Frequency-Domain Electromagnetics

High-performance computing aims at developing models and simulations for applications in numerous scientific fields. Yet, the energy consumption of these HPC facilities currently limits their size and performance, and consequently the size of the tackled problems. The complexity of the HPC software stacks and their various optimizations makes it difficult to finely understand the energy consumption of scientific applications. To highlight this difficulty on a concrete use-case, we perform in [8] an energy and power analysis of a software stack for the simulation of frequency-domain electromagnetic wave propagation. This solver stack combines a high order finite element discretization framework of the system of three-dimensional frequency-domain Maxwell equations with an algebraic hybrid iterative-direct sparse linear solver. This analysis is conducted on the KNL-based PRACE-PCP system. Our results illustrate the difficulty in predicting how to trade energy and runtime.

7.2.6. Exploiting Parameterized Task-graph in Sparse Direct Solvers

Task-based programming models have been widely studied in the context of dense linear algebra, but remains less studied for the more complex sparse solvers. In this talk [17], we have presented the use of two different programming models: Sequential Task Flow from StarPU, and Parameterized Task Graph from PaRSEC to parallelize the factorization step of the `PaStiX` sparse direct solver. We have presented how those programming models have been used to integrate more complex and finer parallelism to take into account new architectures with many computational units. Efficiency of such solutions on homogeneous and heterogeneous architectures with a spectrum of matrices from different applications have been shown. We also have presented how such solutions enable, without extra cost to the programmer, better performance on irregular computations such as in the block low-rank implementation of the solver.

7.2.7. Block Low-rank Algebraic Clustering for Sparse Direct Solvers

In these talks [20], [21], we adressed the Block Low-Rank (BLR) clustering problem, to cluster unknowns within separators appearing during the factorization of sparse matrices. We have shown that methods considering only intra-separators connectivity (i.e., k-way or recursive bissection) as well as methods managing only interaction between separators have some limitations. The new strategy we proposed consider interactions between a separator and its children to pre-select some interactions while reducing the number of off-diagonal blocks. We demonstrated how this method enhance the BLR strategies in the sparse direct supernodal solver PaStiX, and discuss how it can be extended to low-rank formats with more than one level of hierarchy.

7.2.8. Leveraging Task-Based Polar Decomposition Using PARSEC on Massively Parallel Systems

In paper [13], we describe how to leverage a task-based implementation of the polar decomposition on massively parallel systems using the PARSEC dynamic runtime system. Based on a formulation of the iterative QR Dynamically-Weighted Halley (QDWH) algorithm, our novel implementation reduces data traffic while exploiting high concurrency from the underlying hardware architecture. First, we replace the most time-consuming classical QR factorization phase with a new hierarchical variant, customized for the specific structure of the matrix during the QDWH iterations. The newly developed hierarchical QR for QDWH exploits not only the matrix structure, but also shortens the length of the critical path to maximize hardware occupancy. We then deploy PARSEC to seamlessly orchestrate, pipeline, and track the data dependencies of the various linear algebra building blocks involved during the iterative QDWH algorithm. PARSEC enables to overlap communications with computations thanks to its asynchronous scheduling of fine-grained computational tasks. It employs look-ahead techniques to further expose parallelism, while actively pursuing the critical path. In addition, we identify synergistic opportunities between the task-based QDWH algorithm and the PARSEC framework. We exploit them during the hierarchical QR factorization to enforce a locality-aware task execution. The latter feature permits to minimize the expensive inter-node communication, which represents one of the main bottlenecks for scaling up applications on challenging distributed-memory systems. We report numerical accuracy and performance results using well and ill-conditioned matrices. The benchmarking campaign reveals up to 2X performance speedup against the existing state-of-the-art implementation for the polar decomposition on 36,864 cores.

7.3. Parallel Low-Rank Linear System and Eigenvalue Solvers Using Tensor Decompositions

It is common to accelerate the boundary element method by compression techniques (FMM, $\mathcal{H}$-matrix/ACA) that enable a more accurate solution or a solution in higher frequency. In this article, we present a compression method based on a transformation of the linear system into the tensor-train format by the quantization technique. The method is applied to a scattering problem on a canonical object with a regular mesh and improves the performance obtained from existing methods. This method has been presented at the 22nd International Conference on the Computation of Electromagnetic Field, (COMPUMAG 2019) [12] and an extented version is accepted in IEEE TRANSACTIONS ON MAGNETICS.

7.4. Efficient algorithmic for load balancing and code coupling in complex simulations

7.4.1. StarPart Redesign

In the context of the french ICARUS project (FUI), which focuses the development of high-fidelity calculation tools for the design of hot engine parts (aeronautics & automotive), we are looking to develop new load-balancing algorithms to optimize the complex numerical simulations of our industrial and academic partners (Turbomeca, Siemens, Cerfacs, Onera, ...). Indeed, the efficient execution of large-scale coupled simulations on powerful computers is a real challenge, which requires revisiting traditional load-balancing algorithms based on graph partitioning. A thesis on this subject has already been conducted in the Inria HiePACS team in 2016, which has successfully developed a co-partitioning algorithm that balances the load of two coupled codes by taking into account the coupling interactions between these codes. This work was initially integrated into the StarPart platform. The necessary extension of our algorithms to parallel & distributed (increasingly dynamic) versions has led to a complete redesign of StarPart, which has been the focus of our efforts this year (as in the previous year). The StarPart framework provides the necessary building blocks to develop new graph algorithms in the context of HPC, such as those we are targeting. The strength of StarPart lies in the fact that it is a light runtime system applied to the issue of "graph computing". It provides a unified data model and a uniform programming interface that allows easy access to a dozen partitioning libraries, including Metis, Scotch, Zoltan, etc. Thus, it is possible, for example, to load a mesh from an industrial test case provided by our partners (or an academic graph collection as DIMACS'10) and to easily compare the results for the different partitioners integrated in StarPart.

Alongside this work, we are beginning to work on the application of learning techniques to the problem of graph partitioning. Recent work on GCNs (Graph Convolutional Networks) is an interesting approach that we will explore.

7.5. Application Domains

7.5.1. Material physics

7.5.1.1. EigenSolver

The adaptive vibrational configuration interaction algorithm has been introduced as a new eigennvalues method for large dimension problem. It is based on the construction of nested bases for the discretization of the Hamiltonian operator according to a theoretical criterion that ensures the convergence of the method. It efficiently reduce the dimension of the set of basis functions used and then we are able solve vibrationnal eigenvalue problem up to the dimension 15 (7 atoms). Beyond this molecule size, two major issues appear. First, the size of the approximation domain increases exponentially with the number of atoms and the density of eigenvalues in the target area.

This year we have worked on two main areas. First of all, not all the eigenvalues that are calculated are determined by spectroscopy and therefore do not interest chemists. Only eigenvalues with an intensity are relevant. Also, we have set up a selection of interesting eigenvalues using the intensity operator. This requires calculating the scalar product between the smallest eigenvalues and the dipole moment applied to an eigenvector to evaluate its intensity. In addition, to get closer to the experimental values, we introduced the Coriolis operator into the Hamiltonian. A document is being written on these last two points showing that we can reach for a molecule 10 atoms the area of interest (i.e. more than 2 400 eigenvalues). Moreover, we continue to extend our shared memory parallelization to distributed memory using the message exchange paradigm to speedup the eigensolver time.

7.5.2. Co-design for scalable numerical algorithms in scientific applications

7.5.2.1. Numerical and parallel scalable hybrid solvers in large scale calculations

We have been working with the NACHOS team on the treatment of the system of three-dimensional frequency-domain (or time-harmonic) Maxwell equations using a high order hybridizable discontinuous Galerkin (HDG) approximation method combined to domain decomposition (DD) based hybrid iterative-direct parallel solution strategies. The proposed HDG method preserves the advantages of classical DG methods previously introduced for the time-domain Maxwell equations, in particular in terms of accuracy and flexibility with regards to the discretization of complex geometrical features, while keeping the computational efficiency at the level of the reference edge element based finite element formulation widely adopted for the considered PDE system. We study in details the computational performances of the resulting DD solvers in particular in terms of scalability metrics by considering both a model test problem and more realistic large-scale simulations performed on high performance computing systems consisting of networked multicore nodes. More information on these results can be found in [2].

In the context of a parallel plasma physics simulation code, we perform a qualitative performance study between two natural candidates for the parallel solution of 3D Poisson problems that are multigrid and domain decomposition. We selected one representative of each of these numerical techniques implemented in state of the art parallel packages and show that depending on the regime used in terms of number of unknowns per computing cores the best alternative in terms of time to solution varies. Those results show the interest of having both types of numerical solvers integrated in a simulation code that can be used in very different configurations in terms of problem sizes and parallel computing platforms. More information on these results will be shortly available in an Inria scientific report.

7.5.2.2. Efficient Parallel Solution of the 3D Stationary Boltzmann Transport Equation for Diffusive Problems

In the context of a collaboration with EDF-Lab with the Phd of Salli Moustafa, we present an efficient parallel method for the deterministic solution of the 3D stationary Boltzmann transport equation applied to diffusive problems such as nuclear core criticality computations. Based on standard MultiGroup-Sn-DD discretization schemes, our approach combines a highly efficient nested parallelization strategy with the PDSA parallel acceleration technique applied for the first time to 3D transport problems. These two key ingredients enable us to solve extremely large neutronic problems involving up to 10^{12} degrees of freedom in less than an hour using 64 super-computer nodes.

These contributions have been published in Journal of Computational Physics (JCP) [7].

7.5.2.3. Bridging the Gap Between $\mathcal{H}$-Matrices and Sparse Direct Methods for the Solution of Large Linear Systems

For the sake of numerical robustness in aeroacoustics simulations, the solution techniques based on the factorization of the matrix associated with the linear system are the methods of choice when affordable. In that respect, hierarchical methods based on low-rank compression have allowed a drastic reduction of the computational requirements for the solution of dense linear systems over the last two decades. For sparse linear systems, their application remains a challenge which has been studied by both the community of hierarchical matrices and the community of sparse matrices. On the one hand, the first step taken by the community of hierarchical matrices most often takes advantage of the sparsity of the problem through the use of nested dissection. While this approach benefits from the hierarchical structure, it is not, however, as efficient as sparse solvers regarding the exploitation of zeros and the structural separation of zeros from non-zeros. On the other hand, sparse factorization is organized so as to lead to a sequence of smaller dense operations, enticing sparse solvers to use this property and exploit compression techniques from hierarchical methods in order to reduce the computational cost of these elementary operations. Nonetheless, the globally hierarchical structure may be lost if the compression of hierarchical methods is used only locally on dense submatrices. In [1], we have reviewed the main techniques that have been employed by both those communities, trying to highlight their common properties and their respective limits with a special emphasis on studies that have aimed to bridge the gap between them. With these observations in mind, we have proposed a class of hierarchical algorithms based on the symbolic analysis of the structure of the factors of a sparse matrix. These algorithms rely on a symbolic information to cluster and construct a hierarchical structure coherent with the non-zero pattern of the matrix. Moreover, the resulting hierarchical matrix relies on low-rank compression for the reduction of the memory consumption of large submatrices as well as the time to solution of the solver. We have also compared multiple ordering techniques based on geometrical or topological properties. Finally, we have opened the discussion to a coupling between the Finite Element Method and the Boundary Element Method in a unified computational framework.

7.5.2.4. Design of a coupled MUMPS - $\mathcal{H}$-Matrix solver for FEM-BEM applications

In that approach, the FEM matrix is eliminated by computing a Schur complement using MUMPS. Given the size of the BEM matrix, this can not be done in one operation, so it is done block by block, and added in the $\mathcal{H}$-matrix, which is then factorized to complete the process. The overall process yields an interesting boost in performance when compared to the previously existing approach that coupled MUMPS with a classical dense solver. However, a full comparison with all the other existing methods must still be performed (full $\mathcal{H}$-matrix solver with [22] or without nested dissection, iterative approaches, etc.).

7.5.2.5. Metabarcoding

Distance Geometry Problem (DGP) and Nonlinear Mapping (NLM) are two well established questions: DGP is about finding a Euclidean realization of an incomplete set of distances in a Euclidean space, whereas Nonlinear Mapping is a weighted Least Square Scaling (LSS) method. We show how all these methods (LSS, NLM, DGP) can be assembled in a common framework, being each identified as an instance of an optimization problem with a choice of a weight matrix. In [6], we studied the continuity between the solutions (which are point clouds) when the weight matrix varies, and the compactness of the set of solutions (after centering). We finally studied a numerical example, showing that solving the optimization problem is far from being simple and that the numerical solution for a given procedure may be trapped in a local minimum.

We are involved in the ADT Gordon ((partners: TADAAM (coordinator), STORM, HIEPACS, PLEIADE). The objectives of this ADT is to scale our slolver stack on a PLEIADE dimensioning metabarcoding application (multidimensional scaling method). Our goal is to be able to handle a problem leading to a distance matrix around 100 million individuals. Our contribution concerns the the scalability of the multidimensional scaling method and more particulary the random projection methods to speed up the SVD solver. Experiments son PlaFRIM and MCIA CURTA plateforms have allowed us to show that the solver stack was able to solve efficiently a large problem up to 300,000 individuals in less than 10 minutes on 25 nodes. This has highlighted that for these problem sizes the management of I/O, inputs and outputs with the disks, becomes critical and dominates calculation times.

8. Partnerships and Cooperations

8.1. Regional Initiatives

8.1.1. HPC-Ecosystem

Participants: Emmanuel Agullo, Olivier Beaumont, Olivier Coulaud, Aurélien Esnard, Lionel Eyraud-Dubois, Mathieu Faverge, Luc Giraud, Abdou Guermouche, Pierre Ramet, Guillaume Sylvand.

Grant: Regional council
Dates: 2018 – 2020
Partners: EPIs STORM, TADAAM from Inria Bordeaux Sud-Ouest, Airbus, CEA-CESTA, INRA
Overview:

Numerical simulation is today integrated in all cycles of scientific design and studies, whether academic or industrial, to predict or understand the behavior of complex phenomena often coupled or multi-physical. The quality of the prediction requires having precise and adapted models, but also to have computation algorithms efficiently implemented on computers with architectures in permanent evolution. Given the ever increasing size and sophistication of simulations implemented, the use of parallel computing on computers with up to several hundred thousand computing cores and consuming / generating massive volumes of data becomes unavoidable; this domain corresponds to what is now called High Performance Computing (HPC). On the other hand, the digitization of many processes and the proliferation of connected objects of all kinds generate ever-increasing volumes of data that contain multiple valuable information; these can only be highlighted through sophisticated treatments; we are talking about Big Data. The intrinsic complexity of these digital treatments requires a holistic approach with collaborations of multidisciplinary teams capable of mastering all the scientific skills required for each component of this chain of expertise.

To have a real impact on scientific progress and advances, these skills must include the efficient management of the massive number of compute nodes using programming paradigms with a high level of expressiveness, exploiting high-performance communications layers, effective management for intensive I / O, efficient scheduling mechanisms on platforms with a large number of computing units and massive I / O volumes, innovative and powerful numerical methods for analyzing volumes of data produced and efficient algorithms that can be integrated into applications representing recognized scientific challenges with high societal and economic impacts. The project we propose aims to consider each of these links in a consistent, coherent and consolidated way.

For this purpose, we propose to develop a unified Execution Support (SE) for large-scale numerical simulation and the processing of large volumes of data. We identified four Application Challenges (DA) identified by the Nouvelle-Aquitaine region that we propose to carry over this unified support. We will finally develop four Methodological Challenges (CM) to evaluate the impact of the project. This project will make a significant contribution to the emerging synergy on the convergence between two yet relatively distinct domains, namely High Performance Computing (HPC) and the processing, management of large masses of data (Big Data); this project is therefore clearly part of the emerging field of High Performance Data Analytics (HPDA).

8.2. National Initiatives

8.2.1. ANR

8.2.1.1. SASHIMI: Sparse Direct Solver using Hierarchical Matrices

Participants: Aurélien Esnard, Mathieu Faverge, Pierre Ramet.

Grant: ANR-18-CE46-0006
Dates: 2018 – 2022
Overview: Nowadays, the number of computational cores in supercomputers has grown largely to a few millions. However, the amount of memory available has not followed this trend, and the memory per core ratio is decreasing quickly with the advent of accelerators. To face this problem, the SaSHiMi project wants to tackle the memory consumption of linear solver libraries used by many major simulation applications by using low-rank compression techniques. In particular, the direct solvers which offer the most robust solution to strategy but suffer from their memory cost. The project will especially investigate the super-nodal approaches for which low-rank compression techniques have been less studied despite the attraction of their large parallelism and their lower memory cost than for the multi-frontal approaches. The results will be integrated in the PaStiX solver that supports distributed and heterogeneous architectures.

8.2.1.2. SOLHARIS: SOLvers for Heterogeneous Architectures over Runtime systems, Investigating Scalability

Participants: Emmanuel Agullo, Olivier Beaumont, Mathieu Faverge, Lionel Eyraud-Dubois, Abdou Guermouche, Pierre Ramet, Guillaume Sylvand.

Grant: ANR-19-CE46-0009
Dates: 2019 – 2023
Overview: The SOLHARIS project aims at addressing the issues related to the development of fast and scalable linear solvers for large-scale, heterogeneous supercomputers. Because of the complexity and heterogeneity of the targeted algorithms and platforms, this project intends to rely on modern runtime systems to achieve high performance, programmability and portability. By gathering experts in computational linear algebra, scheduling algorithms and runtimes, SOLHARIS intends to tackle these issues through a considerable research effort for the development of numerical algorithms and scheduling methods that are better suited to the characteristics of large scale, heterogeneous systems and for the improvement and extension of runtime systems with novel features that more accurately fulfill the requirements of these methods. This is expected to lead to fundamental research results and software of great interest for researchers of the scientific computing community.

8.2.2. FUI

8.2.2.1. ICARUS: Intensive Calculation for AeRo and automotive engines Unsteady Simulations

Participants: Cyril Bordage, Aurélien Esnard.

Grant: FUI-22
Dates: 2016-2020
Partners: SAFRAN, SIEMENS, IFPEN, ONERA, DISTENE, CENAERO, GDTECH, Inria, CORIA, CERFACS.

Overview: Large Eddy Simulation (LES) is an increasingly attractive unsteady modelling approach for modelling reactive turbulent flows due to the constant development of massively parallel supercomputers. It can provide open and robust design tools that allow access to new concepts (technological breakthroughs) or a global consideration of a structure (currently processed locally). The mastery of this method is therefore a major competitive lever for industry. However, it is currently constrained by its access and implementation costs in an industrial context. The ICARUS project aims to significantly reduce them (costs and deadlines) by bringing together major industrial and research players to work on the entire high-fidelity LES computing process by:

- increasing the performance of existing reference tools (for 3D codes: AVBP, Yales2, ARGO) both in the field of code coupling and code/machine matching;
- developing methodologies and networking tools for the LES;
- adapting the ergonomics of these tools to the industrial world: interfaces, data management, code interoperability and integrated chains;
- validating this work on existing demonstrators, representative of the aeronautics and automotive industries.

8.2.3. Inria Project Labs

8.2.3.1. IPL HPC BigData

The goal of the HPC-BigData IPL is to gather teams from the HPC, Big Data and Machine Learning (ML) areas to work at the intersection between these domains. HPC and Big Data evolved with their own infrastructures (supercomputers versus clouds), applications (scientific simulations versus data analytics) and software tools (MPI and OpenMP versus Map/Reduce or Deep Learning frameworks). But Big Data analytics is becoming more compute-intensive (thanks to deep learning), while data handling is becoming a major concern for scientific computing. Within the IPL, we are in particular involved in a tight collaboration with Zenith Team (Montpellier) on how to parallelize and how to deal with memory issues in the context of the training phase of Pl@ntnet (https://www.plantnet.org). Alexis Joly (Zenith) co supervises with Olivier Beaumont the PhD Thesis of Alena Shilova.

8.3. European Initiatives

8.3.1. FP7 & H2020 Projects

8.3.1.1. EoCoE-II

Title: Energy oriented Centre of Excellence for computer applications

Program: H2020

Duration: January 2019 - December 2021

Coordinator: CEA

Partners:

Barcelona Supercomputing Center - Centro Nacional de Supercomputacion (Spain)

Commissariat A L Energie Atomique et Aux Energies Alternatives (France)

Centre Europeen de Recherche et de Formation Avancee en Calcul Scientifique (France)

Consiglio Nazionale Delle Ricerche (Italy)

The Cyprus Institute (Cyprus)

Agenzia Nazionale Per le Nuove Tecnologie, l'energia E Lo Sviluppo Economico Sostenibile (Italy)

Fraunhofer Gesellschaft Zur Forderung Der Angewandten Forschung Ev (Germany)

Instytut Chemii Bioorganicznej Polskiej Akademii Nauk (Poland)

Forschungszentrum Julich (Germany)

Max Planck Gesellschaft Zur Foerderung Der Wissenschaften E.V. (Germany)

University of Bath (United Kingdom)

Universite Libre de Bruxelles (Belgium)

Universita Degli Studi di Trento (Italy)

Inria contact: Bruno Raffin

The Energy-oriented Centre of Excellence (EoCoE) applies cutting-edge computational methods in its mission to accelerate the transition to the production, storage and management of clean, decarbonized energy. EoCoE is anchored in the High Performance Computing (HPC) community and targets research institutes, key commercial players and SMEs who develop and enable energy-relevant numerical models to be run on exascale supercomputers, demonstrating their benefits for low carbon energy technology. The present project will draw on a successful proof-of-principle phase of EoCoE-I, where a large set of diverse computer applications from four such energy domains achieved significant efficiency gains thanks to its multidisciplinary expertise in applied mathematics and supercomputing. During this 2nd round, EoCoE-II will channel its efforts into 5 scientific Exascale challenges in the low-carbon sectors of Energy Meteorology, Materials, Water, Wind and Fusion. This multidisciplinary effort will harness innovations in computer science and mathematical algorithms within a tightly integrated co-design approach to overcome performance bottlenecks and to anticipate future HPC hardware developments. A world-class consortium of 18 complementary partners from 7 countries will form a unique network of expertise in energy science, scientific computing and HPC, including 3 leading European supercomputing centres. New modeling capabilities in selected energy sectors will be created at unprecedented scale, demonstrating the potential benefits to the energy industry, such as accelerated design of storage devices, high-resolution probabilistic wind and solar forecasting for the power grid and quantitative understanding of plasma core-edge interactions in ITER-scale tokamaks. These flagship applications will provide a high-visibility platform for high-performance computational energy science, cross-fertilized through close working connections to the EERA and EUROfusion consortia.

8.3.1.2. PRACE 6IP

Title: PRACE Sixth Implementation Phase (PRACE-6IP) project

Duration: May 2019 - December 2021

Partners: see the following url

Inria contact: Luc Giraud

PRACE, the Partnership for Advanced Computing is the permanent pan-European High Performance Computing service providing world-class systems for world-class science. Systems at the highest performance level (Tier-0) are deployed by Germany, France, Italy, Spain and Switzerland, providing researchers with more than 17 billion core hours of compute time. HPC experts from 25 member states enabled users from academia and industry to ascertain leadership and remain competitive in the Global Race. Currently PRACE is finalizing the transition to PRACE 2, the successor of the initial five year period. The objectives of PRACE-6IP are to build on and seamlessly continue the successes of PRACE and start new innovative and collaborative activities proposed by the consortium. These include: assisting the development of PRACE 2; strengthening the internationally recognised PRACE brand; continuing and extend advanced training which so far provided more than 36 400 person·training days; preparing strategies and best practices towards Exascale computing, work on forward-looking SW solutions; coordinating and enhancing the operation of the multi-tier HPC systems and services; and supporting users to exploit massively parallel systems and novel architectures. A high level Service Catalogue is provided. The proven project structure will be used to achieve each of the objectives in 7 dedicated work packages. The activities are designed to increase Europe's research and innovation potential especially through: seamless and efficient Tier-0 services and a pan-European HPC ecosystem including national capabilities; promoting take-up by industry and new communities and special offers to SMEs; assistance to PRACE 2 development; proposing strategies for deployment of leadership systems; collaborating with the ETP4HPC, CoEs and other European and international organisations on future architectures, training, application support and policies. This will be monitored through a set of KPIs.

8.3.1.3. EOSC-Pillar

Title: Coordination and Harmonisation of National and Thematic Initiatives to support EOSC

Duration: 2019 - 2023

Partners: see the following url

Inria contact: Stefano Zacchiroli

The project aims to support the coordination and harmonization of national initiatives relevant to EOSC in Europe and investigate the option for them to interfederate at a later stage, help integrating initiatives and data/cloud providers through the development of common policies and tools, and facilitate user communities in adopting and using these services and propose new ones born from their scientific domain. To this end, the project will integrate a bottom-up approach (by voicing the requirements and needs expressed by the different scientific communities operating at the national level) and a top-down one (by harmonising the national strategies and translating them in a viable work plan). In the longer term, this is expected to facilitate the design and adoption of common policies and streamline the process of joining EOSC for service providers and user communities while helping populating the EOSC with useful services of wider European interest, based on the real needs and interests of the European scientific communities. In order to maximise this simplification process, the project will collaborate with related regional and thematic initiatives.

8.3.1.4. EXDCI-2

Title: European Extreme Data & Computing Initiative

Duration: 2010 - 2020

Partners: see the following url

Inria contact: Olivier Beaumont

Through the joint action of PRACE and ETP4HPC, EXDCI-2 mobilises the European HPC stakeholders. The project participates in the support of the European HPC Ecosystem with two main goals. First, the development and advocacy of a competitive European HPC Exascale Strategy by supporting the implementation of a common European HPC strategy, open to synergistic areas including High Performance Data Analytics (HPDA) and Artificial Intelligence (AI). Secondly, the coordination of the stakeholder community for European HPC at the Exascale through joint community structuring and synchronisation, such as (i) the development of relationships with other ecosystems including upstream technologies as Big Data (BDVA) (ii) in the context of the upcoming European Data Infrastructure (EDI) a road mapping activity toward future converged HPC, HPDA and AI needs and new services from PRACE users communities and CoE and (iii) the continuation of BDEC activities, for international participation of European stakeholders on the integration from edge computing to HPC, including Data Analytics and AI.

8.4. International Initiatives

8.4.1. Inria International Labs

There is an ongoing reasearch activity with Argonne National Laboratory in the framework of the JLESC International Lab, through a postdoc funded by the DPI, namely Nick Schenkels, who work on data compression techniques in Krylov methods for the solution of large linear systems. The objective is to use agnostic compressor developped at Argonne to compress the basis involved in Krylov methods that have a large memory footprint. The challange is to design algorithm that reduce the memory consumption, hence the energy, while preserving the numerical convergence of the numerical technique.

9. Dissemination

9.1. Promoting Scientific Activities

9.1.1. Scientific Events: Organisation

9.1.1.1. Member of the Organizing Committees

SIAM PP'20, Seattle (O. Beaumont).

9.1.1.2. Chair of Conference Program Committees

COMPAS'19 Algorithm Track (E. Agullo) ICPP'19 Algorithm Track vice-chair (E. Agullo)

9.1.1.3. Member of the Conference Program Committees

AlgoCloud'19 (O. Beaumont), COMPAS'19 (O. Beaumont), EuroPar'20 (O. Beaumont), HiPC'19 (L. Giraud), HPML'19 (O. Beaumont), ICPP'19 (A. Guermouche), IPDPS'19 (L. Eyraud-Dubois, O. Beaumont), IPDPS Workshops'19 (O. Beaumont), ISC'20 Workshops (E. Agullo), PDSEC'19 (O. Coulaud, M. Faverge, L. Giraud), IEEE PDP'19 (J. Roman), SC'19 (E. Agullo), SPAA'19 (O. Beaumont).

9.1.2. Journal

9.1.2.1. Member of the Editorial Boards

- O. Beaumont is Associate Editor in Chief for the Journal of Parallel and Distributed Computing (Elsevier).
- L. Giraud is member of the editorial board of the SIAM Journal on Scientific Computing (SISC) and SIAM Journal on Matrix Analysis and Applications (SIMAX).

9.1.2.2. Reviewer - Reviewing Activities

The members of the HIEPACS project have performed reviewing for the following list of journals: Computing and Fluid, International Journal of Antennas and Propagation, Parallel Computing, SIAM J. Matrix Analysis and Applications, SIAM J. Scientific Computing, Journal of Parallel and Distributed Computing, IEEE Transactions on Parallel and Distributed Systems, IEEE Access, Concurrency and Computation: Practice and Experience, ACM Transactions on Mathematical Software, ACM Computational and Mathematical Methods, International Journal of High Performance Computing Applications, Journal Of Computational Science.

The members of the HIEPACS project have performed reviewing for the following list of conferences (additionally to PC): Europar'19, IPDPS'19, SC'18, STACS'20, SPAA'19, SC'19.

9.1.3. Invited Talks

- L. Giraud, "Dealing with unreliable computing platforms at extreme scale" invited MOX Seminars (Laboratory for Modeling and Scientific Computing MOX), Politecnico di Milano, January 23, in conjunction with the ESCAPE2 workshop on fault tolerant algorithms and resilient approaches.

9.1.4. Scientific Expertise

- Olivier Beaumont acted as expert for 2019 FET Open Evaluation Committee
- Luc Giraud is member of the board on Modelization, Simulation and data analysis of the Competitiveness Cluster for Aeronautics, Space and Embedded Systems.
- Pierre Ramet is Scientific Advisor at the CEA-DAM CESTA.
- Jean Roman is member of the Scientific Board of the CEA-DAM. As representative of Inria, he is member of the board of ETP4HPC (European Technology Platform for High Performance Computing), of the French Information Group for PRACE, of the French Working Group for EuroHPC, and of the Technical Group of GENCI.

9.1.5. Research Administration

- Emmanuel Agullo and Luc Giraud are the scientific correspondents of the European and International partnership for Inria Bordeaux Sud-Ouest.
- Olivier Coulaud is the scientific manager of the PLAFRIM platform for Inria Bordeaux Sud-Ouest.
- Jean Roman is a member of the Direction for Science at Inria : he was until the end of December 2019 the Deputy Scientific Director of the Inria research domain entitled *Applied Mathematics, Computation and Simulation* and was in charge at the national level of the Inria activities concerning High Performance Computing.
- Until July 2019, Olivier Beaumont was the vice-head of Inria Evaluation Commission.

9.2. Teaching - Supervision - Juries

9.2.1. Teaching

Undergraduate level/Licence

- A. Esnard: System programming 36h, Computer architecture 40h, Network 23h, C programming 35h at Bordeaux University. He is also responsible for the second year of the computer science degree (L2 Informatique), which involves managing about 200 students each year.
- M. Faverge: Programming environment 26h, Numerical algorithmic 40h, C projects 25h at Bordeaux INP (ENSEIRB-MatMeca).
- A. Guermouche: System programming 36h at Bordeaux University.
- P. Ramet: System programming 24h, Databases 32h, Object programming 48h, Distributed programming 32h, Cryptography 32h, Introduction to AI Deep Learning and Data Analytics 16h at Bordeaux University.

Post graduate level/Master

- E. Agullo: Operating systems 24h at Bordeaux University ; Dense linear algebra kernels 8h, Numerical algorithms 30h at Bordeaux INP (ENSEIRB-MatMeca).
- O. Coulaud: Paradigms for parallel computing 8h, Introduction to Tensor methods 4h at Bordeaux INP (ENSEIRB-MatMeca).
- A. Esnard: Network management 27h, Network security 27h at Bordeaux University; Programming distributed applications 35h at Bordeaux INP (ENSEIRB-MatMeca).
- L. Eyraud-Dubois and Olivier Beaumont: Approximation and BigData 24h at Bordeaux University.
- M. Faverge: System programming 72h, Linear Algebra for high Performance Computing 13h at Bordeaux INP (ENSEIRB-MatMeca).
  He is also in charge of the master 2 internship for the Computer Science department at Bordeaux INP (ENSEIRB-MatMeca). Starting in September, he is in charge with Raymond Namyst of the High Performance Computing - High Performance Data Analytics option at ENSEIRB-MatMeca. This is a common training curriculum between the Computer Science and MatMeca departments at Bordeaux INP and with Bordeaux University in the context of the Computer Science Research Master.
- Alena Shilova and Olivier Beaumont: Deep Learning Frameworks, at Bordeaux INP (ENSEIRB-MatMeca), 20h.
- Olivier Beaumont, Sketching and Streaming Algorithms, ENS Lyon, 8h
- L. Giraud: Introduction to intensive computing and related programming tools 30h, INSA Toulouse; On mathematical tools for numerical simulations 10h, ENSEEIHT Toulouse.
- A. Guermouche: Network management 92h, Network security 64h, Operating system 24h at Bordeaux University.

- P. Ramet: Load balancing and scheduling 13h and Numerical algorithmic 40h at Bordeaux INP (ENSEIRB-Matmeca).

High School teachers

- A. Esnard, M. Faverge, and A. Guermouche participated to the training of the High School teachers (DIU Enseigner l'Informatique au Lycée) in computer science for the new computer science program starting in September 2019.

9.2.2. Supervision

- PhD Aurélien Falco; Data sparse calculation in Bridging the gap between $\mathcal{H}$-matrices and sparse direct methods for the solution of large linear systems; E. Agullo, L. Girau, G. Sylvand; defended on June 24, 2019; jury members: E. Ng (Lawrence Berkeley National Laboratory), S. Le Borne (Technische Universitat Hamburg), D. LLvadoux (ONERA) F. Alouges (Ecole Polytechnique), G. Pont (Airbus Group).
- PhD in progress: Tobias Castanet; Replication algorithms for multi-player virtual worlds; started Sep. 2019; O. Beaumont, N. Hanusse (LaBRI), C. Travers (Bordeaux INP - LaBRI).
- PhD in progress: Marek Felsoci; Fast solvers for high-frequency aeroacoustics; G. Sylvand, E. Agullo.
- PhD in progress: Martina Iannacito; Linear solvers in tensorial format for high dimensional problems; started Oct 2019; O. Coulaud, L. Giraud.
- PhD in progress: Esragul Korkmaz; Sparse linear solver and hierachical matrices; started Nov. 2018; M. Faverge, P. Ramet.
- PhD in progress: Romain Peressoni; Fast multidimensional scaling method for the study of biodiversity; started Oct 2019; E. Agullo, O. Coulaud, A. Franc (PLEIADE)
- PhD in progress: Alena Shilova; Scheduling for deep learning applications; started Oct. 2018; L. Eyraud-Dubois, O. Beaumont.
- PhD in progress: Nicolas Venkovic; Domain decomposition techniques for the solution of stochastics elliptic PDEs; started Nov. 2018; L. Giraud, P. Mycek (CERFACS).
- PhD in progress: Mathieu Vérité; Static allocation algorithms for scheduling High-Performance applications; started Sept. 2019; L. Eyraud-Dubois, O. Beaumont.
- PhD in progress: Yanfei Xiang; Solution of large linear systems with massive numbers of right-hand sides. Started Nov. 2019; L. Giraud, P. Mycek (CERFACS).

9.2.3. Juries

- Mohammad Issa, “Modélisation asymptotique et discrétisation des composants magnétiques dans les problèmes de courant de Foucault.", referees: R. V. Sabariego, S. Clénet, members: O. Coulaud, Y. Kefevren, R. Perrussel, J-R. Poirier, L. Krähenbül. Université Toulouse 3 Paul Sabatier, spécialité: électromagnétisme et Systèmes Haute Fréquence, 30 November 2019.
- Raphaël Prat, “Equilibrage dynamique de charge sur supercalculateur exaflopique appliqué à la dynamique moléculaire", referees: C. Calvin, J.F. Mehaut, reviewers: M. Baader, L. Colombet, P. Fortin, R. Namyst, J. Roman, CEA - Maison de la Simulation et Université de Bordeaux, spécialité: informatique, 9 October 2019.
- Mohamad El Sayah, "Random Generation for the Performance Evaluation of Scheduling Algorithms," referees: Olivier Beaumont and Arnaud Legrand, reviewers: Jean-Marc Nicod, Fany Dufosse, Pierre-Cyrille Heam, University of Besancon, 20 November 2019.

9.3. Popularization

9.3.1. Interventions

- Olivier Beaumont spoke to a class of high school students on algorithms (routing algorithms in particular) as part of the digital week organized by the BIJ (Bureau Information Jeunesse) of the City of La Teste de Buch.

10. Bibliography

Publications of the year

Doctoral Dissertations and Habilitation Theses

[1] A. FALCO.*Combler l'écart entre H-Matrices et méthodes directes creuses pour la résolution de systèmes linéaires de grandes tailles*, Université de Bordeaux, June 2019, https://tel.archives-ouvertes.fr/tel-02183902

Articles in International Peer-Reviewed Journal

[2] E. AGULLO, L. GIRAUD, A. GOBÉ, M. KUHN, S. LANTERI, L. MOYA.*High order HDG method and domain decomposition solvers for frequency-domain electromagnetics*, in "International Journal of Numerical Modelling: Electronic Networks, Devices and Fields", October 2019 [*DOI :* 10.1002/JNM.2678], https://hal.inria.fr/hal-02327982

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[6] A. A. FRANC, P. BLANCHARD, O. COULAUD.*Nonlinear mapping and distance geometry*, in "Optimization Letters", May 2019 [*DOI :* 10.1007/S11590-019-01431-Y], https://hal.inria.fr/hal-02124882

[7] S. MOUSTAFA, F. FÉVOTTE, M. FAVERGE, L. PLAGNE, P. RAMET.*Efficient Parallel Solution of the 3D Stationary Boltzmann Transport Equation for Diffusive Problems*, in "Journal of Computational Physics", March 2019 [*DOI :* 10.1016/J.JCP.2019.03.019], https://hal.inria.fr/hal-02080624

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[11] S. KUMAR, L. EYRAUD-DUBOIS, S. KRISHNAMOORTHY.*Performance Models for Data Transfers: A Case Study with Molecular Chemistry Kernels*, in "ICPP 2019 - 48th International Conference on Parallel Processing", Kyoto, Japan, August 2019 [*DOI :* 10.1145/3337821.3337921], https://hal.inria.fr/hal-02431877

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Project-Team LFANT

Lithe and fast algorithmic number theory

IN COLLABORATION WITH: Institut de Mathématiques de Bordeaux (IMB)

IN PARTNERSHIP WITH:
CNRS

Université de Bordeaux

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Algorithmics, Computer Algebra and Cryptology

Table of contents

Project-Team LFANT

Creation of the Team: 2009 March 01, updated into Project-Team: 2010 January 01

Keywords:

Computer Science and Digital Science:

A4.3.1. - Public key cryptography
A8.4. - Computer Algebra
A8.5. - Number theory
A8.10. - Computer arithmetic

Other Research Topics and Application Domains:

B6. - IT and telecom
B9.5.2. - Mathematics

1. Team, Visitors, External Collaborators

Research Scientists

Andreas Enge [Team leader, Inria, Senior Researcher, HDR]
Razvan Barbulescu [CNRS, Researcher, from Sep 2019]
Xavier Caruso [CNRS, Senior Researcher, HDR]
Fredrik Johansson [Inria, Researcher]
Aurel Page [Inria, Researcher]
Damien Robert [Inria, Researcher]

Faculty Members

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Jean-Paul Cerri [Univ de Bordeaux, Associate Professor]
Henri Cohen [Univ de Bordeaux, Professor emeritus, HDR]
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Technical Staff

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Amaury Durand [Univ de Bordeaux, PhD Student, from Sep 2019]
Elie Eid [Univ de Rennes I, PhD Student]
Jean Kieffer [École Normale Supérieure de Paris, PhD Student]
Abdoulaye Maiga [Senegal, PhD student]
Pavel Solomatin [Leiden University, PhD Student]
Ida Tucker [École Normale Supérieure de Lyon, PhD Student]
Anne Edgar Wilke [Inria, PhD Student, from Sep 2019]

Administrative Assistant

Sabrina Duthil [Inria, Administrative Assistant]

2. Overall Objectives

2.1. Presentation

Algorithmic number theory dates back to the dawn of mathematics itself, *cf.* Eratosthenes's sieve to enumerate consecutive prime numbers. With the arrival of computers, previously unsolvable problems have come into reach, which has boosted the development of more or less practical algorithms for essentially all number theoretic problems. The field is now mature enough for a more computer science driven approach, taking into account the theoretical complexities and practical running times of the algorithms.

Concerning the lower level multiprecision arithmetic, folklore has asserted for a long time that asymptotically fast algorithms such as SchÃ¶nhage–Strassen multiplication are impractical; nowadays, however, they are used routinely. On a higher level, symbolic computation provides numerous asymptotically fast algorithms (such as for the simultaneous evaluation of a polynomial in many arguments or linear algebra on sparse matrices), which have only partially been exploited in computational number theory. Moreover, precise complexity analyses do not always exist, nor do sound studies to choose between different algorithms (an exponential algorithm may be preferable to a polynomial one for a large range of inputs); folklore cannot be trusted in a fast moving area such as computer science.

Another problem is the reliability of the computations; many number theoretic algorithms err with a small probability, depend on unknown constants or rely on a Riemann hypothesis. The correctness of their output can either be ensured by a special design of the algorithm itself (slowing it down) or by an *a posteriori* verification. Ideally, the algorithm outputs a certificate, providing an independent *fast* correctness proof. An example is integer factorisation, where factors are hard to obtain but trivial to check; primality proofs have initiated sophisticated generalisations.

One of the long term goals of the LFANT project team is to make an inventory of the major number theoretic algorithms, with an emphasis on algebraic number theory and arithmetic geometry, and to carry out complexity analyses. So far, most of these algorithms have been designed and tested over number fields of small degree and scale badly. A complexity analysis should naturally lead to improvements by identifying bottlenecks, systematically redesigning and incorporating modern asymptotically fast methods.

Reliability of the developed algorithms is a second long term goal of our project team. Short of proving the Riemann hypothesis, this could be achieved through the design of specialised, slower algorithms not relying on any unproven assumptions. We would prefer, however, to augment the fastest unproven algorithms with the creation of independently verifiable certificates. Ideally, it should not take longer to check the certificate than to generate it.

All theoretical results are complemented by concrete reference implementations in PARI/GP, which allow to determine and tune the thresholds where the asymptotic complexity kicks in and help to evaluate practical performances on problem instances provided by the research community. Another important source for algorithmic problems treated by the LFANT project team is modern cryptology. Indeed, the security of all practically relevant public key cryptosystems relies on the difficulty of some number theoretic problem; on the other hand, implementing the systems and finding secure parameters require efficient algorithmic solutions to number theoretic problems.

3. Research Program

3.1. Number fields, class groups and other invariants

Participants: Bill Allombert, Jared Guissmo Asuncion, Karim Belabas, Jean-Paul Cerri, Henri Cohen, Jean-Marc Couveignes, Andreas Enge, Fredrik Johansson, Aurel Page.

Modern number theory has been introduced in the second half of the 19th century by Dedekind, Kummer, Kronecker, Weber and others, motivated by Fermat's conjecture: There is no non-trivial solution in integers to the equation $x^n + y^n = z^n$ for $n \geqslant 3$. Kummer's idea for solving Fermat's problem was to rewrite the equation as $(x+y)(x+\zeta y)(x+\zeta^2 y)\cdots(x+\zeta^{n-1}y) = z^n$ for a primitive n-th root of unity ζ, which seems to imply that each factor on the left hand side is an n-th power, from which a contradiction can be derived.

The solution requires to augment the integers by *algebraic numbers*, that are roots of polynomials in $\mathbb{Z}[X]$. For instance, ζ is a root of $X^n - 1$, $\sqrt[3]{2}$ is a root of $X^3 - 2$ and $\frac{\sqrt{3}}{5}$ is a root of $25X^2 - 3$. A *number field* consists of the rationals to which have been added finitely many algebraic numbers together with their sums, differences, products and quotients. It turns out that actually one generator suffices, and any number field K is isomorphic to $\mathbb{Q}[X]/(f(X))$, where $f(X)$ is the minimal polynomial of the generator. Of special interest are *algebraic integers*, "numbers without denominators", that are roots of a monic polynomial. For instance, ζ and $\sqrt[3]{2}$ are integers, while $\frac{\sqrt{3}}{5}$ is not. The *ring of integers* of K is denoted by $\mathcal{O}_K$; it plays the same role in K as $\mathbb{Z}$ in $\mathbb{Q}$.

Unfortunately, elements in $\mathcal{O}_K$ may factor in different ways, which invalidates Kummer's argumentation. Unique factorisation may be recovered by switching to *ideals*, subsets of $\mathcal{O}_K$ that are closed under addition and under multiplication by elements of $\mathcal{O}_K$. In $\mathbb{Z}$, for instance, any ideal is *principal*, that is, generated by one element, so that ideals and numbers are essentially the same. In particular, the unique factorisation of ideals then implies the unique factorisation of numbers. In general, this is not the case, and the *class group*Cl_K of ideals of $\mathcal{O}_K$ modulo principal ideals and its *class number*$h_K = |\,\mathrm{Cl}_K\,|$ measure how far $\mathcal{O}_K$ is from behaving like $\mathbb{Z}$.

Using ideals introduces the additional difficulty of having to deal with $units$, the invertible elements of $\mathcal{O}_K$: Even when $h_K = 1$, a factorisation of ideals does not immediately yield a factorisation of numbers, since ideal generators are only defined up to units. For instance, the ideal factorisation $(6) = (2) \cdot (3)$ corresponds to the two factorisations $6 = 2 \cdot 3$ and $6 = (-2) \cdot (-3)$. While in $\mathbb{Z}$, the only units are 1 and -1, the unit structure in general is that of a finitely generated $\mathbb{Z}$-module, whose generators are the *fundamental units*. The *regulator*R_K measures the "size" of the fundamental units as the volume of an associated lattice.

One of the main concerns of algorithmic algebraic number theory is to explicitly compute these invariants (Cl_K and h_K, fundamental units and R_K), as well as to provide the data allowing to efficiently compute with numbers and ideals of $\mathcal{O}_K$; see [36] for a recent account.

The *analytic class number formula* links the invariants h_K and R_K (unfortunately, only their product) to the ζ-function of K, $\zeta_K(s) := \prod_{\mathfrak{p} \text{ prime ideal of } \mathcal{O}_K} \left(1 - \mathrm{N}\,\mathfrak{p}^{-s}\right)^{-1}$, which is meaningful when $\Re(s) > 1$, but which may be extended to arbitrary complex $s \neq 1$. Introducing characters on the class group yields a generalisation of ζ- to L-functions. The *generalised Riemann hypothesis (GRH)*, which remains unproved even over the rationals, states that any such L-function does not vanish in the right half-plane $\Re(s) > 1/2$. The validity of the GRH has a dramatic impact on the performance of number theoretic algorithms. For instance, under GRH, the class group admits a system of generators of polynomial size; without GRH, only exponential bounds are known. Consequently, an algorithm to compute Cl_K via generators and relations (currently the only viable practical approach) either has to assume that GRH is true or immediately becomes exponential.

When $h_K = 1$ the number field K may be norm-Euclidean, endowing $\mathcal{O}_K$ with a Euclidean division algorithm. This question leads to the notions of the Euclidean minimum and spectrum of K, and another task in algorithmic number theory is to compute explicitly this minimum and the upper part of this spectrum, yielding for instance generalised Euclidean gcd algorithms.

3.2. Function fields, algebraic curves and cryptology

Participants: Karim Belabas, Guilhem Castagnos, Jean-Marc Couveignes, Andreas Enge, Damien Robert, Jean Kieffer, Razvan Barbulescu.

Algebraic curves over finite fields are used to build the currently most competitive public key cryptosystems. Such a curve is given by a bivariate equation $\mathcal{C}(X,Y) = 0$ with coefficients in a finite field $\mathbb{F}_q$. The main classes of curves that are interesting from a cryptographic perspective are *elliptic curves* of equation $\mathcal{C} = Y^2 - (X^3 + aX + b)$ and *hyperelliptic curves* of equation $\mathcal{C} = Y^2 - (X^{2g+1} + \cdots)$ with $g \geqslant 2$.

The cryptosystem is implemented in an associated finite abelian group, the *Jacobian*$\mathrm{Jac}_{\mathcal{C}}$. Using the language of function fields exhibits a close analogy to the number fields discussed in the previous section. Let $\mathbb{F}_q(X)$ (the analogue of $\mathbb{Q}$) be the *rational function field* with subring $\mathbb{F}_q[X]$ (which is principal just as $\mathbb{Z}$). The *function field* of $\mathcal{C}$ is $K_{\mathcal{C}} = \mathbb{F}_q(X)[Y]/(\mathcal{C})$; it contains the *coordinate ring*$\mathcal{O}_{\mathcal{C}} = \mathbb{F}_q[X, Y]/(\mathcal{C})$. Definitions and properties carry over from the number field case $K/\mathbb{Q}$ to the function field extension $K_{\mathcal{C}}/\mathbb{F}_q(X)$. The Jacobian $\mathrm{Jac}_{\mathcal{C}}$ is the divisor class group of $K_{\mathcal{C}}$, which is an extension of (and for the curves used in cryptography usually equals) the ideal class group of $\mathcal{O}_{\mathcal{C}}$.

The size of the Jacobian group, the main security parameter of the cryptosystem, is given by an L-function. The GRH for function fields, which has been proved by Weil, yields the Hasse–Weil bound $(\sqrt{q}-1)^{2g} \leqslant |\,\mathrm{Jac}_{\mathcal{C}}\,| \leqslant (\sqrt{q}+1)^{2g}$, or $|\,\mathrm{Jac}_{\mathcal{C}}\,| \approx q^g$, where the *genus*$g$ is an invariant of the curve that correlates with the degree of its equation. For instance, the genus of an elliptic curve is 1, that of a hyperelliptic one is $\frac{\deg_X \mathcal{C}-1}{2}$. An important algorithmic question is to compute the exact cardinality of the Jacobian.

The security of the cryptosystem requires more precisely that the *discrete logarithm problem* (DLP) be difficult in the underlying group; that is, given elements D_1 and $D_2 = xD_1$ of $\mathrm{Jac}_{\mathcal{C}}$, it must be difficult to determine x. Computing x corresponds in fact to computing $\mathrm{Jac}_{\mathcal{C}}$ explicitly with an isomorphism to an abstract product of finite cyclic groups; in this sense, the DLP amounts to computing the class group in the function field setting.

For any integer n, the *Weil pairing*e_n on $\mathcal{C}$ is a function that takes as input two elements of order n of $\mathrm{Jac}_{\mathcal{C}}$ and maps them into the multiplicative group of a finite field extension $\mathbb{F}_{q^k}$ with $k = k(n)$ depending on n. It is bilinear in both its arguments, which allows to transport the DLP from a curve into a finite field, where it is potentially easier to solve. The *Tate-Lichtenbaum pairing*, that is more difficult to define, but more efficient to implement, has similar properties. From a constructive point of view, the last few years have seen a wealth of cryptosystems with attractive novel properties relying on pairings.

For a random curve, the parameter k usually becomes so big that the result of a pairing cannot even be output any more. One of the major algorithmic problems related to pairings is thus the construction of curves with a given, smallish k.

3.3. Complex multiplication

Participants: Jared Guissmo Asuncion, Karim Belabas, Henri Cohen, Jean-Marc Couveignes, Andreas Enge, Fredrik Johansson, Chloe Martindale, Damien Robert.

Complex multiplication provides a link between number fields and algebraic curves; for a concise introduction in the elliptic curve case, see [38], for more background material, [37]. In fact, for most curves $\mathcal{C}$ over a finite field, the endomorphism ring of $\mathrm{Jac}_{\mathcal{C}}$, which determines its L-function and thus its cardinality, is an order in a special kind of number field K, called *CM field*. The CM field of an elliptic curve is an imaginary-quadratic field $\mathbb{Q}(\sqrt{D})$ with $D < 0$, that of a hyperelliptic curve of genus g is an imaginary-quadratic extension of a totally real number field of degree g. Deuring's lifting theorem ensures that $\mathcal{C}$ is the reduction modulo some prime of a curve with the same endomorphism ring, but defined over the *Hilbert class field*H_K of K.

Algebraically, H_K is defined as the maximal unramified abelian extension of K; the Galois group of H_K/K is then precisely the class group Cl_K. A number field extension H/K is called *Galois* if $H \simeq K[X]/(f)$ and H contains all complex roots of f. For instance, $\mathbb{Q}(\sqrt{2})$ is Galois since it contains not only $\sqrt{2}$, but also the second root $-\sqrt{2}$ of $X^2 - 2$, whereas $\mathbb{Q}(\sqrt[3]{2})$ is not Galois, since it does not contain the root $e^{2\pi i/3}\sqrt[3]{2}$ of $X^3 - 2$. The *Galois group*$\mathrm{Gal}_{H/K}$ is the group of automorphisms of H that fix K; it permutes the roots of f. Finally, an *abelian* extension is a Galois extension with abelian Galois group.

Analytically, in the elliptic case H_K may be obtained by adjoining to K the *singular value*$j(\tau)$ for a complex valued, so-called *modular* function j in some $\tau \in \mathcal{O}_K$; the correspondence between $\mathrm{Gal}_{H/K}$ and Cl_K allows to obtain the different roots of the minimal polynomial f of $j(\tau)$ and finally f itself. A similar, more involved construction can be used for hyperelliptic curves. This direct application of complex multiplication yields algebraic curves whose L-functions are known beforehand; in particular, it is the only possible way of obtaining ordinary curves for pairing-based cryptosystems.

The same theory can be used to develop algorithms that, given an arbitrary curve over a finite field, compute its L-function.

A generalisation is provided by *ray class fields*; these are still abelian, but allow for some well-controlled ramification. The tools for explicitly constructing such class fields are similar to those used for Hilbert class fields.

4. Highlights of the Year

4.1. Highlights of the Year

Guilhem Castagnos defended his professorial degree (“habilitation à diriger des recherches”) on the topic of *Cryptography based on quadratic fields: cryptanalyses, primitives and protocols*[11].

4.1.1. Awards

Fredrik Johansson won the best paper award at the conference ARITH26 — 26th IEEE Symposium on Computer Arithmetic in Kyoto for his contribution on dot products and matrix multiplication in arbitrary precision .
BEST PAPERS AWARDS :
[21]
F. JOHANSSON.*Faster arbitrary-precision dot product and matrix multiplication*, in "26th IEEE Symposium on Computer Arithmetic (ARITH26)", Kyoto, Japan, June 2019, https://arxiv.org/abs/1901.04289 , https://hal.inria.fr/hal-01980399

5. New Software and Platforms

5.1. APIP

Another Pairing Implementation in PARI

KEYWORDS: Cryptography - Computational number theory

SCIENTIFIC DESCRIPTION: Apip , Another Pairing Implementation in PARI, is a library for computing standard and optimised variants of most cryptographic pairings.

The following pairings are available: Weil, Tate, ate and twisted ate, optimised versions (à la Vercauteren–Hess) of ate and twisted ate for selected curve families.

The following methods to compute the Miller part are implemented: standard Miller double-and-add method, standard Miller using a non-adjacent form, Boxall et al. version, Boxall et al. version using a non-adjacent form.

The final exponentiation part can be computed using one of the following variants: naive exponentiation, interleaved method, Avanzi–Mihailescu’s method, Kato et al.’s method, Scott et al.’s method.

Part of the library has been included into Pari/Gp proper.

FUNCTIONAL DESCRIPTION: APIP is a library for computing standard and optimised variants of most cryptographic pairings.

- Participant: Jérôme Milan
- Contact: Andreas Enge
- URL: http://www.lix.polytechnique.fr/~milanj/apip/apip.xhtml

5.2. AVIsogenies

Abelian Varieties and Isogenies

KEYWORDS: Computational number theory - Cryptography

FUNCTIONAL DESCRIPTION: AVIsogenies is a Magma package for working with abelian varieties, with a particular emphasis on explicit isogeny computation.

Its prominent feature is the computation of (l,l)-isogenies between Jacobian varieties of genus-two hyperelliptic curves over finite fields of characteristic coprime to l, practical runs have used values of l in the hundreds.

It can also be used to compute endomorphism rings of abelian surfaces, and find complete addition laws on them.

- Participants: Damien Robert, Gaëtan Bisson and Romain Cosset
- Contact: Damien Robert
- URL: http://avisogenies.gforge.inria.fr/

5.3. CM

KEYWORD: Arithmetic

FUNCTIONAL DESCRIPTION: The Cm software implements the construction of ring class fields of imaginary quadratic number fields and of elliptic curves with complex multiplication via floating point approximations. It consists of libraries that can be called from within a C program and of executable command line applications.

RELEASE FUNCTIONAL DESCRIPTION: Features - Precisions beyond 300000 bits are now supported by an addition chain of variable length for the -function. Dependencies - The minimal version number of Mpfr has been increased to 3.0.0, that of Mpc to 1.0.0 and that of Pari to 2.7.0.

- Participant: Andreas Enge
- Contact: Andreas Enge
- URL: http://www.multiprecision.org/cm/home.html

5.4. CMH

Computation of Igusa Class Polynomials

KEYWORDS: Mathematics - Cryptography - Number theory

FUNCTIONAL DESCRIPTION: Cmh computes Igusa class polynomials, parameterising two-dimensional abelian varieties (or, equivalently, Jacobians of hyperelliptic curves of genus 2) with given complex multiplication.

- Participants: Andreas Enge, Emmanuel Thomé and Regis Dupont
- Contact: Emmanuel Thomé
- URL: http://cmh.gforge.inria.fr

5.5. CUBIC

KEYWORD: Number theory

FUNCTIONAL DESCRIPTION: Cubic is a stand-alone program that prints out generating equations for cubic fields of either signature and bounded discriminant. It depends on the Pari library. The algorithm has quasi-linear time complexity in the size of the output.

- Participant: Karim Belabas
- Contact: Karim Belabas
- URL: http://www.math.u-bordeaux.fr/~belabas/research/software/cubic-1.2.tgz

5.6. Euclid

KEYWORD: Number theory

FUNCTIONAL DESCRIPTION: Euclid is a program to compute the Euclidean minimum of a number field. It is the practical implementation of the algorithm described in [38] . Some corresponding tables built with the algorithm are also available. Euclid is a stand-alone program depending on the PARI library.

- Participants: Jean-Paul Cerri and Pierre Lezowski
- Contact: Jean-Paul Cerri
- URL: http://www.math.u-bordeaux1.fr/~plezowsk/euclid/index.php

5.7. KleinianGroups

KEYWORDS: Computational geometry - Computational number theory

FUNCTIONAL DESCRIPTION: KleinianGroups is a Magma package that computes fundamental domains of arithmetic Kleinian groups.

- Participant: Aurel Page
- Contact: Aurel Page
- URL: http://www.normalesup.org/~page/Recherche/Logiciels/logiciels-en.html

5.8. GNU MPC

KEYWORD: Arithmetic

FUNCTIONAL DESCRIPTION: Mpc is a C library for the arithmetic of complex numbers with arbitrarily high precision and correct rounding of the result. It is built upon and follows the same principles as Mpfr. The library is written by Andreas Enge, Philippe Théveny and Paul Zimmermann.

RELEASE FUNCTIONAL DESCRIPTION: Fixed `mpc_pow`, see http://lists.gforge.inria.fr/pipermail/mpc-discuss/2014-October/001315.html - `#18257`: Switched to libtool 2.4.5.

- Participants: Andreas Enge, Mickaël Gastineau, Paul Zimmermann and Philippe Théveny
- Contact: Andreas Enge
- URL: http://www.multiprecision.org/

5.9. MPFRCX

KEYWORD: Arithmetic

FUNCTIONAL DESCRIPTION: Mpfrcx is a library for the arithmetic of univariate polynomials over arbitrary precision real (Mpfr) or complex (Mpc) numbers, without control on the rounding. For the time being, only the few functions needed to implement the floating point approach to complex multiplication are implemented. On the other hand, these comprise asymptotically fast multiplication routines such as Toom-Cook and the FFT.

RELEASE FUNCTIONAL DESCRIPTION: - new function `product_and_hecke` - improved memory consumption for unbalanced FFT multiplications

- Participant: Andreas Enge
- Contact: Andreas Enge
- URL: http://www.multiprecision.org/mpfrcx/home.html

5.10. PARI/GP

KEYWORD: Computational number theory

FUNCTIONAL DESCRIPTION: Pari/Gp is a widely used computer algebra system designed for fast computations in number theory (factorisation, algebraic number theory, elliptic curves, modular forms ...), but it also contains a large number of other useful functions to compute with mathematical entities such as matrices, polynomials, power series, algebraic numbers, etc., and many transcendental functions.

- Participants: Andreas Enge, Hamish Ivey-Law, Henri Cohen and Karim Belabas
- Partner: CNRS
- Contact: Karim Belabas
- URL: http://pari.math.u-bordeaux.fr/

5.11. Platforms

5.11.1. SageMath

Following the article [19], Xavier Caruso and Thibaut Verron proposed an implementation of Tate algebras and ideals in Tate algebras (including an implementation of Buchberger algorithm) for SageMath; their implementation is now part of the standard distribution.

Xavier Caruso implemented a new unified framework for dealing with ring extensions and field extensions in SageMath. This code will be integrated soon in the standard distribution.

5.11.2. ARB

Fredrik Johansson released a new version, 2.17, of ARB.

6. New Results

6.1. Cryptographic Protocols

Participants: Guilhem Castagnos, Ida Tucker.

In [20], G. Castagnos, D. Catalano, F. Laguillaumie, F. Savasta and I. Tucker propose a new cryptographic protocol to compute ECDSA signatures with two parties.

ECDSA (Elliptic Curves Digital Signature Algorithm) is a widely adopted standard for electronic signatures. For instance, it is used in the TLS (Transport Layer Security) protocol and in many cryptocurrencies such as Bitcoin. For cryptocurrencies, ECDSA is used in order to sign the transactions: if Alice wants to give n bitcoins to Bob, she uses her secret key to sign with ECDSA a bit string encoding this information.

As a result, if the secret key of Alice is stolen, for example if her computer is compromised, an attacker can stole all her bitcoins. A common solution to this problem is to share the key on multiple devices, for example a laptop and a mobile phone. Both devices must collaborate in order to issue a signature, and if only one device is compromised, no information on the key is leaked. This setting belongs to the area of secure multiparty computation.

There have been recent proposals to construct 2 party variants of ECDSA signatures but constructing efficient protocols proved to be much harder than for other signature schemes. The main reason comes from the fact that the ECDSA signing protocol involves a complex equation compared to other signatures schemes. Lindell recently managed to get an efficient solution using the linearly homomorphic cryptosystem of Paillier. However his solution has some drawbacks, for example the security proof resorts to a non-standard interactive assumption.

By using another approach based on hash proofs systems we obtain a proof that relies on standard assumptions. Moving to concrete constructions, we show how to instantiate our framework using class groups of imaginary quadratic fields. Our implementations show that the practical impact of dropping such interactive assumptions is minimal. Indeed, while for 128-bit security our scheme is marginally slower than Lindell's, for 256-bit security it turns out to be better both in key generation and signing time. Moreover, in terms of communication cost, our implementation significantly reduces both the number of rounds and the transmitted bits without exception.

This paper was presented at the CRYPTO Conference 2019, and is part of the ALAMBIC project.

6.2. Coding Theory

Participants: Xavier Caruso, Aurel Page.

In [29], Xavier Caruso developed a theory of residues for skew rational functions (which are, by definition, the quotients of two skew polynomials), proving in particular a skew analogue of the residue formula and a skew analogue of the classical formula of change of variables for residues. He then used his theory to define and study a linearized version of Goppa codes. He showed that these codes meet the Singleton bound (for the sum-rank metric) and are the duals of the linearized Reed–Solomon codes defined recently by Martínez-Peñas. Efficient encoding and decoding algorithms are also designed.

C. Maire and A. Page updated the preprint *Error-correcting codes based on non-commutative algebras* [33] according to the comments of referees.

6.3. Number fields

Participants: Razvan Barbulescu, Jean-Marc Couveignes, Jean-Paul Cerri, Pierre Lezowski.

In [30], Jean-Marc Couveignes constructs small models of number fields and deduces a better bound for the number of number fields of given degree n and discriminant bounded by H. This work improves on previous results by Schmidt and Ellenberg-Venkatesh. Schmidt obtains a bound $H^{\frac{n+2}{4}}$ times a function of n. Ellenberg and Venkatesh obtain a bound $H^{\exp(O(\sqrt{\log n}))}$ times a function of n. The new idea is to combine geometry of numbers and interpolation theory to produces small projective models and lower the exponent of H down to $O(\log^3 n)$. A key point is to look for local equations rather than a full set of generators of the ideal of these models.

In [12], Razvan Barbulescu in a joint work with Jishnu Ray (University of British Columbia, Vancouver) brings elements to support Greenberg's p-rationality conjecture. On the theoretical side, they propose a new family proven to be p-rational. On the algorithmic side, the compare the tools to enumerate number fields of given abelian Galois group and of computing class numbers, and extend the experiments on the Cohen-Lenstra-Martinet conjectures.

In collaboration with Pierre Lezowski, Jean-Paul Cerri has studied in [15] norm-Euclidean properties of totally definite quaternion fields over number fields. Building on their previous work about number fields, they have proved that the Euclidean minimum and the inhomogeneous minimum of orders in such quaternion fields are always equal. Additionally, they are rational under the hypothesis that the base number field is not quadratic. This single remaning open case corresponds to the similar open case remaining for real number fields.

They also have extended Cerri's algorithm for the computation of the upper part of the norm-Euclidean spectrum of a number field to this non-commutative context. This algorithm has allowed to compute the exact value of the norm-Euclidean minimum of orders in totally definite quaternion fields over a quadratic number field. This has provided the first known values of this minimum when the base number field has degree strictly greater than 1.

6.4. Modular forms and L-functions

Participant: Henri Cohen.

Members of the team have taken part in an international autumn school on computational number theory at the Izmir Institute of Technology (IZTECH) in 2017. Henri Cohen has transformed his two lectures in book chapters. The text on modular forms [23] presents the (of course extremely condensed) view of the book [6] he has coauthored. The chapter on L-functions [24] is closely related to new developments in PARI/GP.

In [25] the same author explains how to compute Fourier expansions at all cusps of any modular form of integral or half-integral weight thanks to a theorem of Borisov–Gunnells and explicit expansions of Eisenstein series at all cusps. Using this, he gives a number of methods for computing arbitrary Petersson products. Implementations in our PARI/GP software are also described.

A complementary approach using modular symbols is used in [14] by Karim Belabas, Dominique Bernardi and Bernadette Perrin-Riou to compute Manin's constant and the modular degree of elliptic curves defined over $\mathbb{Q}$.

6.5. p-adic rings and geometry

Participant: Xavier Caruso.

In [19], Xavier Caruso, Tristan Vaccon and Thibaut Verron laid the foundations of an algorithmic treatment of rigid p-adic geometry by introducting and studing Gröbner bases over Tate algebras. In addition, they designed a Buchberger-like and a F4-like algorithm for computing such Gröbner bases.

In [22], Xavier Caruso presents a survey on Fontaine's theory of p-adic period rings. These notes are based on a course given jointly by Laurent Berger and Xavier Caruso in Rennes in 2014; their aim is to detail the construction of the rings B_{crys} and B_{dR} (and some of their variants) and state several comparison theorems between étale and crystalline or de Rham cohomologies for p-adic algebraic varieties.

6.6. Geometry

Participant: Aurel Page.

The paper [13], *Can you hear the homology of 3-dimensional drums?* by A. Bartel and A. Page was published in Commentarii Mathematici Helvetici.

6.7. Complex multiplication of abelian varieties and elliptic curves

Participants: Razvan Barbulescu, Sorina Ionica, Chloe Martindale, Enea Milio, Damien Robert.

In [16], Sorina Ionica, former postdoc of the team, and Emmanuel Thomé look at the structure of isogeny graphs of genus 2 Jacobians with maximal real multiplication. They generalise a result of Kohel's describing the structure of the endomorphism rings of the isogeny graph of elliptic curves. Their setting considers genus 2 jacobians with complex multiplication, with the assumptions that the real multiplication subring is maximal and has class number 1. Over finite fields, they derive a depth first search algorithm for computing endomorphism rings locally at prime numbers, if the real multiplication is maximal.

Antonin Riffaut examines in [18] whether there are relations defined over $\mathbb{Q}$ that link (additively or multiplicatively) different singular moduli $j(\tau)$, invariants of elliptic curves with complex multiplication by different quadratic rings.

In [34], Chloe Martindale presents an algorithm to compute higher dimensional Hilbert modular polynomials. She also explains applications of this algorithm to point counting, walking on isogeny graphs, and computing class polynomials.

In [28], Razvan Barbulescu and Sudarshan Shinde (Sorbonne Université) make a complete list of the 1525 infinite families of elliptic curves without CM which have a particular behaviour in the ECM factoring algorithm, the 20 previously known families having been found by ad-hoc methods. The new idea was to use the characterisation of ECM-friendly families in terms of their Galois image and to use the recent progress in the topic of Mazur's program. In particular, for some of the families mentioned theoretical in the literature the article offers the first publication of explicite equations.

E. Milio and D. Robert updated their paper [35] on computing cyclic modular polynomials.

6.8. Pairings

Participant: Razvan Barbulescu.

In [27], Razvan Barbulescu in a joint work with Nadia El Mrabet (École des Mines de Saint-Étienne) et Loubna Ghammam (Bosch) makes a review of the families of elliptic curves for pairing-based cryptology. This was necessary after the invention of a new variant of the NFS algorithm in 2016 by Barbulescu and Taechan Kim, which showed that the previously used key sizes for pairings were insecure. The novelty of this review article is double : first they consider a large number of families, some of which were never analysed in the literature because they were not likely to be the best and secondly they combine in the same article the security analysis of each family with a non-optimized implementation. This allows the industry to select a different family for each type of utilisation of pairings.

6.9. Multiprecision arithmetic

Participant: Fredrik Johansson.

In [17], F. Johansson and I. Blagouchine devise an efficient algorithm to compute the generalized Stieltjes constants $\gamma_n(a)$ to arbitrary precision with rigorous error bounds, for the first time achieving this with low complexity with respect to the order n. The algorithm consists of locating an approximate steepest descent contour and then evaluating the integral numerically in ball arithmetic using the Petras algorithm with a Taylor expansion for bounds near the saddle point. An implementation is provided in the Arb library.

In [26], F. Johansson describes algorithms to compute elliptic functions and their relatives (Jacobi theta functions, modular forms, elliptic integrals, and the arithmetic-geometric mean) numerically to arbitrary precision with rigorous error bounds for arbitrary complex variables. Implementations in ball arithmetic are available in the Arb library. This overview article discusses the standard algorithms from a concrete implementation point of view, and also presents some improvements.

In [21], Fredrik Johansson develops algorithms for real and complex dot product and matrix multiplication in arbitrary-precision floating-point and ball arithmetic. The new methods are implemented in Arb and significantly speed up polynomial operations and linear algebra in high precision.

7. Partnerships and Cooperations

7.1. National Initiatives

7.1.1. ANR Alambic – AppLicAtions of MalleaBIlity in Cryptography

Participant: Guilhem Castagnos.

https://crypto.di.ens.fr/projects:alambic:main

The ALAMBIC project is a research project formed by members of the Inria Project-Team CASCADE of ENS Paris, members of the AriC Inria project-team of ENS Lyon, and members of the CRYPTIS of the university of Limoges. G. Castagnos is an external member of the team of Lyon for this project.

Non-malleability is a security notion for public key cryptographic encryption schemes that ensures that it is infeasible for an adversary to modify ciphertexts into other ciphertexts of messages which are related to the decryption of the first ones. On the other hand, it has been realized that, in specific settings, malleability in cryptographic protocols can actually be a very useful feature. For example, the notion of homomorphic encryption allows specific types of computations to be carried out on ciphertexts and generate an encrypted result which, when decrypted, matches the result of operations performed on the plaintexts. The homomorphic property can be used to create secure voting systems, collision-resistant hash functions, private information retrieval schemes, and for fully homomorphic encryption enables widespread use of cloud computing by ensuring the confidentiality of processed data.

The aim of the ALAMBIC project to investigate further theoretical and practical applications of malleability in cryptography. More precisely, this project focuses on three different aspects: secure computation outsourcing and server-aided cryptography, homomorphic encryption and applications and << paradoxical >> applications of malleability.

7.1.2. ANR CLap–CLap – The p-adic Langlands correspondence: a constructive and algorithmical approach

Participants: Xavier Caruso, Jean-Marc Couveignes.

The p-adic Langlands correspondence has become nowadays one of the deepest and the most stimulating research programs in number theory. It was initiated in France in the early 2000's by Breuil and aims at understanding the relationships between the p-adic representations of p-adic absolute Galois groups on the one hand and the p-adic representations of p-adic reductive groups on the other hand. Beyond the case of $\mathrm{GL}_2(\mathbb{Q}_p)$ which is now well established, the p-adic Langlands correspondence remains quite obscure and mysterious new phenomena enter the scene; for instance, on the $\mathrm{GL}_n(F)$-side one encounters a vast zoology of representations which seems extremely difficult to organize.

The CLap–CLap ANR project aims at accelerating the expansion of the p-adic Langlands program beyond the well-established case of $\mathrm{GL}_2(\mathbb{Q}_p)$. Its main originality consists in its very constructive approach mostly based on algorithmics and calculations with computers at all stages of the research process. We shall pursue three different objectives closely related to our general aim:

1. draw a conjectural picture of the (still hypothetical) p-adic Langlands correspondence in the case of GL_n,
2. compute many deformation spaces of Galois representations and make the bridge with deformation spaces of representations of reductive groups,
3. design new algorithms for computations with Hilbert and Siegel modular forms and their associated Galois representations.

This project will also be the opportunity to contribute to the development of the mathematical software SAGEMATH and to the expansion of computational methodologies.

7.1.3. ANR Ciao – Cryptography, Isogenies and Abelian varieties Overwhelming

Participants: Jean-Marc Couveignes, Jean Kieffer, Aurel Page, Damien Robert.

The CIAO ANR project is a young researcher ANR project led by Damien Robert October 2019.

The aim of the CIAO project is to study the security and improve the efficiency of the SIDH (supersingular isogenies Diffie Helmann) protocol, which is one of the post-quantum cryptographic project submitted to NIST, which passed the first round selection.

The project include all aspects of SIDH, from theoretical ones (computing the endomorphism ring of supersingular elliptic curves, generalisation of SIDH to abelian surfaces) to more practical aspects like arithmetic efficiency and fast implementations, and also extending SIDH to more protocols than just key exchange.

Applications of this project is to improve the security of communications in a context where the currently used cryptosystems are vulnerable to quantum computers. Beyond post-quantum cryptography, isogeny based cryptosystems also allow to construct new interesting cryptographic tools, like Verifiable Delay Functions, used in block chains.

7.2. European Initiatives

7.2.1. FP7 & H2020 Projects

Title: OpenDreamKit

Program: H2020

Duration: January 2016 - December 2019

Coordinator: Nicolas Thiéry

Inria contact: Karim Belabas

Description http://cordis.europa.eu/project/rcn/198334_en.html, http://opendreamkit.org

OpenDreamKit was a Horizon 2020 European Research Infrastructure project (#676541) that ran for four years, starting from September 2015. It provided substantial funding to the open source computational mathematics ecosystem, and in particular popular tools such as LinBox, MPIR, SageMath, GAP, Pari/GP, LMFDB, Singular, MathHub, and the IPython/Jupyter interactive computing environment.

7.3. International Initiatives

7.3.1. Inria International Labs

International Laboratory for Research in Computer Science and Applied Mathematics
Associate Team involved in the International Lab:

7.3.1.1. FAST

Title: (Harder Better) FAster STronger cryptography

International Partner (Institution - Laboratory - Researcher): and the PRMAIS project

Université des Sciences et Techniques de Masuku (Gabon) - Tony Ezome

Start year: 2017

See also: http://fast.gforge.inria.fr/

The project aims to develop better algorithms for elliptic curve cryptography with prospect of the two challenges ahead: - securing the internet of things - preparing towards quantum computers.

Elliptic curves are currently the fastest public-key cryptosystem (with a key size that can fit on embeded devices) while still through a different mode of operation beeing (possibly) able to resist quantum based computers.

This was the last year of the Fast projet, which was represented at the Journees du Lirimia in Yaounde by Emmanuel Fouotsa.

In total the project funded one EMA and two CIMPA schools, had 14 publications in journals and conferences (with three upcoming preprints), two PhD defense with two upcoming.

7.3.2. Inria International Partners

7.3.2.1. Informal International Partners

The team is used to collaborating with Leiden University through the ALGANT programme for joint PhD supervision.

Eduardo Friedman (U. of Chile), long term collaborator of K. Belabas's and H. Cohen's, is a regular visitor in Bordeaux (about 1 month every year).

7.4. International Research Visitors

7.4.1. Visits of International Scientists

Researchers visiting the team to give a talk to the team seminar include David Lubicz (DGA Rennes), Hartmut Monien (Bethe Center for Theoretical Physics, Bonn), Francesco Battestoni (University of Milan), David Roe (MIT, Boston), Maria Dostert (EPFL, Lausanne), and Alice Pellet-Mary (KU Leuven).

Abdoulaye Maiga visited the team for one month in December 2019, and Tony Ezome visited for two weeks in November 2019.

8. Dissemination

8.1. Promoting Scientific Activities

8.1.1. Journal

8.1.1.1. Member of the Editorial Boards

X. Caruso is an editor and one of the founders of the journal *Annales Henri Lebesgue*.

J.-M. Couveignes is a member of the editorial board (scientific committee) of the *Publications mathématiques de Besançon* since 2010.

K. Belabas acts on the editorial board of *Journal de Théorie des Nombres de Bordeaux* since 2005 and of *Archiv der Mathematik* since 2006.

H. Cohen is an editor for the Springer book series *Algorithms and Computations in Mathematics (ACM)*.

A. Enge is an editor of *Designs, Codes and Cryptography* since 2004.

8.1.2. Invited Talks

F. Johansson, *Computing with precision*, Tech Talk, Google X, Mountain View, CA, USA (January 2019)

8.1.3. Scientific Expertise

K. Belabas is a member of the “conseil scientifique” of the Société Mathématique de France.

8.1.4. Research Administration

Since January 2015, K. Belabas is vice-head of the Math Institute (IMB). He also leads the computer science support service (“cellule informatique”) of IMB and coordinates the participation of the institute in the regional computation cluster PlaFRIM.

He is an elected member of “commission de la recherche” in the academic senate of Bordeaux University.

He was a member of the “Conseil National des Universités” (25th section, pure mathematics) since 2015 until november 2019.

Since January 2017, A. Enge is “délégué scientifique” of the Inria research centre Bordeaux–Sud-Ouest. As such, he is also a designated member of the “commission d’évaluation” of Inria.

He is a member of the administrative council of the Société Arithmétique de Bordeaux, qui édite le *Journal de théorie des nombres de Bordeaux* et qui soutient des congrès en théorie des nombres.

J.-P. Cerri is an elected member of the scientific council of the Mathematics Institute of Bordeaux (IMB) and responsible for the bachelor programme in mathematics and informatics.

8.2. Teaching - Supervision - Juries

8.2.1. Teaching

Master: G. Castagnos, *Cryptanalyse*, 60h, M2, University of Bordeaux, France;

Master: G. Castagnos, *Cryptologie avancée*, 30h, M2, University of Bordeaux, France;

Master: G. Castagnos, *Courbes elliptiques*, 30h, M2, University of Bordeaux, France;

Licence: G. Castagnos, *Arithmétique et Cryptologie*, 24h, L3, Université de Bordeaux, France

Master : D. Robert, *Courbes elliptiques*, 60h, M2, University of Bordeaux, France;

Master: X. Caruso and J.-M. Couveignes, *Algorithmique arithmétique, introduction à l’algorithmique quantique*, 60h, M2, University of Bordeaux, France;

Master : K. Belabas, *Computer Algebra*, 91h, M2, University of Bordeaux, France;

Master: J.-M. Couveignes, *Modules, espaces quadratiques*, 30h, M1, University of Bordeaux, France;

Licence : J.-P. Cerri, *Arithmétique et Cryptologie*, TD, 36h, L3, Université de Bordeaux, France

Licence : J.-P. Cerri, *Algèbre linéaire*, TD, 51h, L2, Université de Bordeaux, France

Licence : J.-P. Cerri, *Topologie*, TD, 35h, L3, Université de Bordeaux, France

Master : J.-P. Cerri, *Cryptologie*, Cours-TD, 60h, M1, Université de Bordeaux, France

Licence: J. Kieffer, *Algorithmique Mathématique 2*, 32h, L3, Université de Bordeaux, France

Master: R. Barbulescu, *Arithmetic algorithms for cryptology*, M2, Master Parisien de Recherche Informatique.

Licence, Master : J.-P. Cerri, 2 TER (L3, M1), 1 Projet (M2), Université de Bordeaux, France

Master : J. Asuncion, *Elliptic curves*, TD, 16h, M1, Universiteit Utrecht (Mastermath), Pays-Bas

8.2.2. Supervision

Master thesis: Jean-Raphaël Biehler, *Functional encryption*, supervised by Guilhem Castagnos

Master thesis: Béranger Seguin, *Deformations of Galois representations*, supervised by Xavier Caruso

Master thesis: William Dallaporta, *Parametrization of ideals and other algebraic structures by quadratic forms*, supervised by Karim Belabas

PhD in progress: Ida Tucker, *Design of new advanced cryptosystems from homomorphic building blocks*, since October 2017, supervised by Guilhem Castagnos and Fabien Laguillaumie

PhD in progress: Abdoulaye Maiga, *Computing canonical lift of genus 2 hyperelliptic curves*, University Dakar, supervised by Djiby Sow, Abdoul Aziz Ciss and D. Robert.

PhD in progress: Jared Asuncion, *Class fields of complex multiplication fields*, since September 2017, supervised by A. Enge and Marco Streng (Universiteit Leiden).

PhD in progress: Elie Eid, *Computing isogenies between elliptic curves and curves of higher genus*, since September 2018, supervised by Xavier Caruso and Reynald Lercier

PhD in progress: Amaury Durand, *Geometric Gabidulin codes*, since September 2019, supervised by Xavier Caruso

PhD in progress: Jean Kieffer, *Computing isogenies between abelian surfaces*, since September 2018, supervised by Damien Robert and Aurel Page

PhD in progress: Pavel Solomatin *Topics on L-functions*, since October 2014, supervised by B. de Smit and K. Belabas.

PhD in progress: Anne-Edgar Wilke *Enumerating integral orbits of prehomogeneous representations*, since September 2019, supervised by K. Belabas.

PhD in progress: Sudarshan Shinde *Cryptographic applications of modular curves* since October 2016, supervised by R. Barbulescu with Pierre-Vincent Koseleff (Sorbonne Université).

8.2.3. Juries

X. Caruso has written a report for the doctoral dissertation by Léo Poyeton, ÉNS de Lyon: *Extensions de Lie p-adiques et (φ, Γ)-modules*.

X. Caruso has written a report for the doctoral dissertation by Christopher Doris, University of Bristol: *Aspects of p-adic computation*.

X. Caruso has written a report for the doctoral dissertation by Joelle Saade, Université de Limoges: *Méthodes symboliques pour les systèmes différentiels linéaires à singularité irrégulière*.

R. Barbulescu was part of the three members jury of the oral examination in mathematics for math-info the admission examination for ENS de Lyon

D. Robert is a member of the jury of Agregations de Mathematiques. He is also the director of the option “calcul formel” of the Modelisation part of the oral examination.

8.3. Popularization

8.3.1. Education

Alkindi : R. Barbulescu is one of the three organizers of the Alkindi contest, a contest for 13-to-15 year old students which gathers more than 60000 participants from France and Switzerland. D. Robert and the other members invite the winners of the Bordeaux region for a 2 hour visit each year.

8.3.2. Interventions

- from 27/05/2019 to 31/05/2019, X. Caruso supervised a stage at the fablab Coh@bit (at IUT Gradignan) to build some educational material
- 30/06/2019, X. Caruso: *Ramène pas ta science* on a physical experiment demonstrating that the fastest path between two points is an arc of cycloid
- 8-10/10/2019, A. Page: *Fête de la Science* at Inria Bordeaux, activity on cryptography (8 groups of students).
- 17/10/2019, X. Caruso and A. Page: *Village des 80 ans du CNRS*, discussion stand "Quizz des idées reçues" on research in mathematics.
- 19/10/2019, X. Caruso and M.-L. Chabanol: *Village des 80 ans du CNRS* on physical experiment demonstrating that the fastest path between two points is an arc of cycloid
- from 07/04/2019 to 14/04/2019, R. Barbulescu was one of two teachers for a math camp in Kinshasa of 150 students https://www.cnrs.fr/insmi/spip.php?article3190.
- from 06/07/2019 to 13/07/2019, R. Barbulescu was the main organiser for a math training camp which gathered the national teams for the International Olympiad of Mathematics of France, Romania and Bulgaria.
- 5/12/2019, D. Robert: small presentations of cryptography for the student of Ecole Normale Superieure de Lyon.

9. Bibliography

Major publications by the team in recent years

[1] E. BAYER-FLUCKIGER, J.-P. CERRI, J. CHAUBERT.*Euclidean minima and central division algebras*, in "International Journal of Number Theory", 2009, vol. 5, n^{o} 7, p. 1155–1168, http://www.worldscinet.com/ijnt/05/0507/S1793042109002614.html

[2] K. BELABAS, M. BHARGAVA, C. POMERANCE.*Error estimates for the Davenport-Heilbronn theorems*, in "Duke Mathematical Journal", 2010, vol. 153, n^{o} 1, p. 173–210, http://projecteuclid.org/euclid.dmj/1272480934

[3] X. CARUSO, J. L. BORGNE.*A new faster algorithm for factoring skew polynomials over finite fields*, in "J. Symbolic Comput.", 2018, vol. 79, p. 411–443

[4] X. CARUSO, D. ROE, T. VACCON.*Tracking p-adic precision*, in "LMS J. Comput. Math.", 2014, vol. 17, p. 274–294

[5] G. CASTAGNOS, F. LAGUILLAUMIE, I. TUCKER.*Practical Fully Secure Unrestricted Inner Product Functional Encryption modulo p*, in "Advances in Cryptology – ASIACRYPT 2018, Part II", T. PEYRIN, S. GALBRAITH (editors), Lecture Notes in Computer Science, International Association for Cryptologic Research, 2018, vol. 11273, p. 733–764

[6] H. COHEN, F. STRÖMBERG.*Modular Forms: A Classical Approach*, Graduate Studies in Mathematics, American Mathematical Society, 2017, vol. 179, http://bookstore.ams.org/gsm-179/

[7] J.-M. COUVEIGNES, B. EDIXHOVEN.*Computational aspects of modular forms and Galois representations*, Princeton University Press, 2011

[8] A. ENGE, P. GAUDRY, E. THOMÉ.*An L(1/3) Discrete Logarithm Algorithm for Low Degree Curves*, in "Journal of Cryptology", 2011, vol. 24, n^o 1, p. 24–41

[9] A. ENGE, W. HART, F. JOHANSSON.*Short addition sequences for theta functions*, in "Journal of Integer Sequences", 2018, vol. 18, n^o 2, p. 1–34

[10] D. LUBICZ, D. ROBERT.*Computing isogenies between abelian varieties*, in "Compositio Mathematica", 09 2012, vol. 148, n^o 05, p. 1483–1515, http://dx.doi.org/10.1112/S0010437X12000243

Publications of the year

Doctoral Dissertations and Habilitation Theses

[11] G. CASTAGNOS.*Cryptography based on quadratic fields: cryptanalyses, primitives and protocols*, Université de Bordeaux, November 2019, Habilitation à diriger des recherches, https://tel.archives-ouvertes.fr/tel-02403707

Articles in International Peer-Reviewed Journal

[12] R. BARBULESCU, J. RAY.*Numerical verification of the Cohen-Lenstra-Martinet heuristics and of Greenberg's p-rationality conjecture*, in "Journal de Théorie des Nombres de Bordeaux", 2019, forthcoming, https://hal.archives-ouvertes.fr/hal-01534050

[13] A. BARTEL, A. PAGE.*Group representations in the homology of 3-manifolds*, in "Commentarii Mathematici Helvetici", March 2019, https://arxiv.org/abs/1605.04866 [*DOI :* 10.4171/CMH/455], https://hal.inria.fr/hal-01671748

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[16] S. IONICA, E. THOMÉ.*Isogeny graphs with maximal real multiplication*, in "Journal of Number Theory", February 2020, vol. 207, p. 385-422, https://arxiv.org/abs/1407.6672 [*DOI :* 10.1016/J.JNT.2019.06.019], https://hal.archives-ouvertes.fr/hal-00967742

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[19] X. CARUSO, T. VACCON, T. VERRON.*Gröbner bases over Tate algebras*, in "ISSAC", Beijing, China, July 2019, https://arxiv.org/abs/1901.09574 [*DOI :* 10.1145/3326229.3326257], https://hal.archives-ouvertes.fr/hal-01995881

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F. JOHANSSON.*Faster arbitrary-precision dot product and matrix multiplication*, in "26th IEEE Symposium on Computer Arithmetic (ARITH26)", Kyoto, Japan, June 2019, https://arxiv.org/abs/1901.04289 , https://hal.inria.fr/hal-01980399.

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[22] X. CARUSO.*An introduction to p-adic period rings*, in "An introduction to p-adic Hodge theory", 2019, https://arxiv.org/abs/1908.08424 , forthcoming, https://hal.archives-ouvertes.fr/hal-02268787

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Project-Team MAGIQUE-3D

Advanced 3D Numerical Modeling in Geophysics

IN COLLABORATION WITH: Laboratoire de mathématiques et de leurs applications (LMAP)

IN PARTNERSHIP WITH:
CNRS

Université de Pau et des Pays de l'Adour

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Earth, Environmental and Energy Sciences

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Project-Team MAGIQUE-3D

Creation of the Project-Team: 2007 July 01

Keywords:

Computer Science and Digital Science:

A6. - Modeling, simulation and control
A6.1. - Methods in mathematical modeling
A6.1.1. - Continuous Modeling (PDE, ODE)
A6.1.4. - Multiscale modeling
A6.1.5. - Multiphysics modeling
A6.2. - Scientific computing, Numerical Analysis & Optimization
A6.2.1. - Numerical analysis of PDE and ODE
A6.2.7. - High performance computing
A6.3.1. - Inverse problems
A6.5. - Mathematical modeling for physical sciences
A6.5.1. - Solid mechanics
A6.5.4. - Waves

Other Research Topics and Application Domains:

B3. - Environment and planet
B3.3. - Geosciences
B3.3.1. - Earth and subsoil
B4. - Energy
B4.1. - Fossile energy production (oil, gas)
B5.2. - Design and manufacturing
B5.5. - Materials
B5.7. - 3D printing
B9.2.1. - Music, sound
B9.5.2. - Mathematics
B9.5.3. - Physics

1. Team, Visitors, External Collaborators

Research Scientists

Hélène Barucq [Team leader, Inria, Senior Researcher, HDR]
Juliette Chabassier [Inria, Researcher]
Julien Diaz [Inria, Senior Researcher, HDR]
Ha Howard Faucher [Inria, Researcher]
Yder Masson [Inria, Starting Research Position]

Faculty Members

Marc Duruflé [Institut National Polytechnique de Bordeaux, Associate Professor]
Victor Péron [Univ de Pau et des pays de l'Adour, Associate Professor, HDR]
Sébastien Tordeux [Univ de Pau et des pays de l'Adour, Associate Professor, HDR]

Technical Staff

Aurelien Citrain [Inria, Engineer, from Nov 2019]
Florian Faucher [Inria, Engineer, until Sep 2019]
Robin Tournemenne [Inria, Engineer, from Jul 2019 until Aug 2019]

PhD Students

Aurelien Citrain [INSA Rouen, PhD Student, until Oct 2019]
Stefano Frambati [Total, PhD Student]
Alexandre Gras [Institut d'optique graduate school, PhD Student]
Pierre Jacquet [Inria, PhD Student]
Justine Labat [Univ de Pau et des pays de l'Adour, PhD Student]
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Chengyi Shen [Univ de Pau et des pays de l'Adour, PhD Student]
Margot Sirdey [Univ de Pau et des pays de l'Adour, PhD Student]
Vinduja Vasanthan [Inria, PhD Student, from Oct 2019]

Post-Doctoral Fellows

Augustin Ernoult [Inria, Post-Doctoral Fellow, from Mar 2019]
Titly Farhana Faisal [Inria, Post-Doctoral Fellow]
Papa Mangane [Inria, Post-Doctoral Fellow]
Robin Tournemenne [Inria, Post-Doctoral Fellow, until Jun 2019]

2. Overall Objectives

2.1. General setting

MAGIQUE-3D is a joint project-team between Inria and the Department of Applied Mathematics of the University of Pau (LMAP), in partnership with CNRS. The main mission of MAGIQUE-3D is to develop and validate efficient solution methodologies for solving complex three-dimensional geophysical problems, with a particular emphasis on problems arising in seismic imaging, in response to the local industrial and community needs. Indeed, as it is well known, the region of Pau has long-standing tradition in the Geosciences activities. However, in spite of the recent significant advances in algorithmic considerations as well as in computing platforms, the solution of most real-world problems in this field remains intractable. Hence, there is a scientific need of pressing importance to design new numerical methods for solving efficiently and accurately wave propagation problems defined in strongly heterogeneous domains. More recently, MAGIQUE-3D has launched a research program in computational helioseismology. The idea is to apply seismic imaging techniques for understanding the interior of the Sun. This new research area will lead the team to develop new full waveform simulations of vector wave problems including new physical parameters like the gravity. Still in the spirit of widening its scope of applications from its skills in seismic imaging, MAGIQUE-3D has also developed a strong research partnership for the design of wind instruments based upon the solution of inverse problems.

MAGIQUE-3D program possesses an exceptional combination that is a prerequisite for accomplishing its mission: the investigator backgrounds, research interests, and technical skills complement to form a research team with a potential for significant impact on the computational infrastructure of geophysical, acoustical and astrophysical sciences. The research record of MAGIQUE-3D group covers a large spectrum of accomplishments in the field of wave propagation including (a) the design, validation, and performance assessment of a class of DG-methods for solving efficiently high frequency wave problems, (b) the construction, convergence analysis, and performance assessment of various absorbing-type boundary conditions that are key ingredients for solving problems in infinite domains, (c) the development of asymptotic models that are the primary candidate in the presence of heterogeneities that are small compared to the wave length, and (d) the development and analysis of high-order time schemes for solving time-dependent wave problems. Very recently, the team has also opened its research activities to laboratory experiments which help to improve wave modelling by giving a straightforward access to measurements that can be used for calibration. MAGIQUE-3D has built strong collaborations and partnerships with various institutions including (a) local industry (TOTAL), (b) national research centers (ONERA and CEA), and (c) international academic partnerships (e.g. Interdisciplinary Research Institute for the Sciences (IRIS) at California State University, Northridge, USA; University of Pays Basque and Basque Center of Applied Mathematics at Bilbao, Spain; University of California at Berkeley, Lawrence Berkeley National Laboratory, Max Planck Institute at Göttingen).

3. Research Program

3.1. Introduction

Probing the invisible is a quest that is shared by a wide variety of scientists such as archaeologists, geologists, astrophysicists, physicists, etc... Magique-3D is mainly involved in Geophysical imaging which aims at understanding the internal structure of the Earth from the propagation of waves. Both qualitative and quantitative information are required and two geophysical techniques can be used: **seismic reflection** and **seismic inversion**. Seismic reflection provides a qualitative description of the subsurface from reflected seismic waves by indicating the position of the reflectors while seismic inversion transforms seismic reflection data into a quantitative description of the subsurface. Both techniques are inverse problems based upon the numerical solution of wave equations. Oil and Gas explorations have been pioneering application domains for seismic reflection and inversion and even if numerical seismic imaging is computationally intensive, oil companies clearly promote the use of numerical simulations to provide synthetic maps of the subsurface. This is due to the tremendous progresses of scientific computing which have pushed the limits of existing numerical methods and it is now conceivable to tackle realistic 3D problems. However, mathematical wave modeling has to be well-adapted to the region of interest and the numerical schemes which are employed to solve wave equations have to be both accurate and scalable enough to take full advantage of parallel computing. Today, geophysical imaging tackles more and more realistic problems and we contribute to this task by improving the modeling and by deriving advanced numerical methods for solving wave problems.
MAGIQUE-3D research program is divided into four axes that are: (1) Imaging the Earth; (2) Exploring the Sun; (3) Detecting defaults in complex media; (4) Designing objects with a variety of shapes. Those applications stand out from the collaborations that we have established with interested end-user groups. It is worth noting that they share basic common methodologies which imparts consistency to our program despite they may appear quite distant. MAGIQUE-3D keep modeling and simulating geophysical phenomena for understanding the Earth interior and developing its resources sustainably, and our xperience with numerical geophysics may help us to address other challenging applications. We mainly used DG finite elements and spectral elements and both have demonstrated very good performance. However, in particular for reducing the computational costs and/or for better capturing the propagation characteristics, we are working on the development of hybrid solvers based on the coupling of different finite element methods. Other open questions deserve attention like the problem of numerical pollution or the poor scalability of decomposition domain techniques which are both significantly hampering computations in very large domains. For those purposes, we focus ourselves on the development of Trefftz-like approximations that are based on a particular computation of the fluxes by making a judicious use of an auxiliary numerical method (e.g. boundary integral equations, spectral elements, etc...). Those problems cannot be ignored and can be found in all of our research axes. In addressing those issues, we participate in the construction of new numerical schemes and for that purpose, we continuously need to improve our understanding of the underlying physics. By this way, we make our mathematical models evolve to more realistic representations of the wave propagation phenomenon. This motivated us to introduce experimental studies in our activities and to collaborate with geophysicists of the UPPA who own experimental devices adapted to our concerns. Moreover, we have hired recently Yder Masson who is an experienced researcher developing modeling and imaging methods to investigate the Earth's internal structure. This creates all the conditions for improving our mathematical representation of waves in complex media. It is worth noting that modeling is a concern for both geophysicists and mathematicians. Indeed, the

Physics must be reproduced accurately and the underlying mathematical properties should be clarified. By this way, we can develop a numerical scheme respecting the main properties of the continuous problem of interest (energy conservation or attenuation, stability, well-posedness, etc...). Magique-3D proposes to define its research program from in-house accurate solution methodologies for simulating wave propagation in realistic scenarios to various applications involving trans-disciplinary efforts. The development of high-order numerical methods for wave simulations is serving as a basis for our contributions regarding applications. In particular, we pursue and strengthen our collaboration with HPC teams, in order to improve the scalability of our codes and to run them on very large heterogeneous architectures (using task based programming libraries as StarPU developed by Inria project-team Storm, improving the I/O by collaborating with UFRGS at Porto Alegre, using the metaprogramming framework Boast developed by Inria project-team Corse to produce portable and efficient computing kernels). We are also continuing our collaboration with Inria project team Hiepacs on the use of hybrid linear solvers, by considering the multiple Right-Hand Sides feature and by integrating appropriate transmission conditions between the various domains. During 2019, we have worked a lot on: (a) High-order numerical methods for modeling wave propagation in porous media: development and implementation; (b) Understanding the interior of the Earth and the Sun by solving inverse problems; (c) Full waveform inversion for the optimal design of wind musical instruments.

3.2. High-order numerical methods for modeling wave propagation in porous media: development and implementation

We aim at achieving the characterization of conducting porous media which are media favoring the conversion of seismic waves into electromagnetic waves.. This project is identified as a ”New scientific challenge” which is a set of research projects funded by the E2S project of UPPA. The shape and form of porous media can vary depending on the size of the pore and the structure of the solid skeleton. Porous media are found in the nature (sandstone, volcanic rocks, etc) or can be manufactured (concrete, polyurethane foam, etc) as depicted in [68]. Instead of modeling such media as strongly heterogeneous, homogenization is used to describe the material on a macroscopic scale. Biot's theory describes the solid skeleton according to linear elasticity and adds to this the Navier-Stokes equation for a viscous fluid and Darcy's law governing the motion of the fluid [63], [61]. For simplified linear elasticity, there are one equation of motion and one constitutive law, with the unknowns being the displacement field in the solid and the solid stress. In poro-elasticity, the added unknowns are the fluid displacement relative to the solid and the fluid pressure. There are two equations of motion, coupled with two constitutive laws. By plane wave analysis, one obtains three types of waves: S wave, fast P wave and slow P wave (Biot's wave). While the first two types are similar to those existing in elastic solid, the existence of a third wave with drastically smaller speed adds to the complications already encountered in elasticity. This is obviously even more challenging for conducting poroelastic media where the three poroelastic waves are coupled with an electric field. In this case, it is not realistic to use a unique scheme for all the waves. Standard finite element methods coupled with time schemes have indeed difficulties to deliver accurate solutions because there is a need of adapting the mesh size to the smallest wave velocity and the time discretization to the largest wave velocity. It is then tricky to numerically reproduce the Biot's wave while approximating correctly the regular elastic waves P and S. Moreover, there is a challenging question about the boundary condition to be used for limiting the computational domain. We have launched a Ph.D project (Rose-Cloé Meyer) aiming at developing a new piece of software for the simulation of time-harmonic waves in conducting porous media. This project is developed in collaboration with Steve Pride from the Lawrence Berkeley National Laboratory who has elaborated the corresponding physical theory [83], [87], [73], [74]. Next, once a new numerical method is developed, it is validated by comparing the numerical solution to an analytical one. This is a key step to us for assessing the accuracy of our simulations. Nevertheless, analytical solutions are not available for realistic media such as poroelastic or viscoelastic media represented by heterogeneous parameters. Engineers still argue that simulations may be inaccurate and could lead to wrong conclusions. Fortunately, it is possible to produce experimentally quite complex configurations where multi-physics measurements are used to monitor the wave propagation. There is thus a possibility of moving further on the validation of the numerical methods by comparing simulations and experiments. What is very exciting is that experiments are used to validate numerical methods which have the objective of simulating new phenomena that are not possible to reproduce in a lab. We have launched two Ph.D thesis (Chengyi Shen and Victor Martins Gomes) in collaboration with Daniel Brito (LFCR-UPPA) on the comparison of simulations with experiments. This topic is connected to another project that we have with Total on the use of waves for characterizing carbonates.

3.3. Understanding the interior of the Earth and the Sun by solving inverse problems

Even if the Earth and the Sun are actually very different media, their imaging is based on the same solution methodology [64]. However, our knowledge on Earth inversion is far more developed than for the Sun. Earth inversion is in the continuation of previous MAGIQUE-3D achievements while Sun inversion requires developing new technologies based on modeling, numerical analysis and implementation of a piece of software which is able to ask for new developments. For instance, we would like to develop a HDG software package for solving Galbrun and Linearized Euler equations. To the best of our knowledge, this has never be done and would be a major milestone for tackling vectorial equations. Regarding the modeling, we are pursuing our collaboration with the Max Planck Institute for Solar System Research (Göttingen, Germany) in the framework of the associate team ANTS. This partnership is essential to us for understanding a complex (and new to us) physics including gravity waves that we have never considered in the past. Even if we dispose of advanced solvers dealing with elasticity, the development of fast and accurate solvers for reproducing waves travelling in large 3D domains is still one of the positive developments towards realistic simulations. In particular, the techniques for the forward discretization and linear system solver must evolve accordingly to resolve large scale time-harmonic problems. For instance, we have elaborated a space-time Trefftz-DG formulation of the elasto-acoustic problem [58], which performs very well regarding the number of dofs and the order of convergence. We have also coupled spectral and DG elements to take advantage of both methods and we have performed some simulations which are very promising [57]. The formulation of FWI is in progress in the framework of Pierre Jacquet thesis launched in November 2017. Finally, we have also initiated research on seismology at the planetary scale, with the arrival of Yder Masson on the subject and new collaborators (such as Berkeley lab). This will further help widen our expertise on inverse wave problems and will feed all the four research axes of the future team-project. Regarding industrial partnerships, we have collaboration with Total and the SME RealtimeSeismic (Pau, France). We also continue to work with the UPV, the BCAM and the BSC, namely in the framework of Mathrocks project.

3.4. Hybrid time discretizations of high-order

Most of the meshes we consider are composed of cells greatly varying in size. This can be due to the physical characteristics (propagation speed, topography, ...) which may require to refine the mesh locally, very unstructured meshes can also be the result of dysfunction of the mesher. For practical reasons which are essentially guided by the aim of reducing the number of matrix inversions, explicit schemes are generally privileged. However, they work under a stability condition, the so-called Courant Friedrichs Lewy (CFL) condition which forces the time step being proportional to the size of the smallest cell. Then, it is necessary to perform a huge number of iterations in time and in most of the cases because of a very few number of small cells. This implies to apply a very small time step on grids mainly composed of coarse cells and thus, there is a risk of creating numerical dispersion that should not exist. However, this drawback can be avoided by using low degree polynomial basis in space in the small meshes and high degree polynomials in the coarse meshes. By this way, it is possible to relax the CFL condition and in the same time, the dispersion effects are limited. Unfortunately, the cell-size variations are so important that this strategy is not sufficient. One solution could be to apply implicit and unconditionally stable schemes, which would obviously free us from the CFL constraint. Unfortunately, these schemes require inverting a linear system at each iteration and thus needs huge computational burden that can be prohibitive in 3D. Moreover, numerical dispersion may be increased. Then, as second solution is the use of local time stepping strategies for matching the time step to the different sizes of the mesh. There are several attempts [65], [60], [82], [79], [71] and Magique 3D has proposed a new time stepping method which allows us to adapt both the time step and the order of time approximation to the size of the cells. Nevertheless, despite a very good performance assessment in academic configurations, we have observed to our detriment that its implementation inside industrial codes is not obvious and in practice, improvements of the computational costs are disappointing, especially in a HPC framework. Indeed, the local time stepping algorithm may strongly affect the scalability of the code. Moreover, the complexity of the algorithm is increased when dealing with lossy media [76].

Recently, Dolean *et al* [70] have considered a novel approach consisting in applying hybrid schemes combining second order implicit schemes in the thin cells and second order explicit discretization in the coarse mesh. Their numerical results indicate that this method could be a good alternative but the numerical dispersion is still present. It would then be interesting to implement this idea with high-order time schemes to reduce the numerical dispersion. The recent arrival in the team of J. Chabassier should help us to address this problem since she has the expertise in constructing high-order implicit time scheme based on energy preserving Newmark schemes [62]. We propose that our work be organized around the two following tasks. The first one is the extension of these schemes to the case of lossy media because applying existing schemes when there is attenuation is not straightforward. This is a key issue because there is artificial attenuation when absorbing boundary conditions are introduced and if not, there are cases with natural attenuation like in visco-elastic media. The second one is the coupling of high-order implicit schemes with high-order explicit schemes. These two tasks can be first completed independently, but the ultimate goal is obviously to couple the schemes for lossy media. We will consider two strategies for the coupling. The first one will be based on the method proposed by Dolean *et al*, the second one will consist in using Lagrange multiplier on the interface between the coarse and fine grids and write a novel coupling condition that ensures the high order consistency of the global scheme. Besides these theoretical aspects, we will have to implement the method in industrial codes and our discretization methodology is very suitable for parallel computing since it involves Lagrange multipliers. We propose to organize this task as follows. There is first the crucial issue of a systematic distribution of the cells in the coarse/explicit and in the fine/implicit part. Based on our experience on local time stepping, we claim that it is necessary to define a criterion which discriminates thin cells from coarse ones. Indeed, we intend to develop codes which will be used by practitioners, in particular engineers working in the production department of Total. It implies that the code will be used by people who are not necessarily experts in scientific computing. Considering real-world problems means that the mesh will most probably be composed of a more or less high number of subsets arbitrarily distributed and containing thin or coarse cells. Moreover, in the prospect of solving inverse problems, it is difficult to assess which cells are thin or not in a mesh which varies at each iteration.

Another important issue is the load balancing that we can not avoid with parallel computing. In particular, we will have to choose one of these two alternatives: dedicate one part of processors to the implicit computations and the other one to explicit calculus or distribute the resolution with both schemes on all processors. A collaboration with experts in HPC is then mandatory since we are not expert in parallel computing. We will thus continue to collaborate with the team-projects Hiepacs and Runtime with whom we have a long-term experience of collaborations. The load-balancing leads then to the issue of mesh partitioning. Main mesh partitioners are very efficient for the coupling of different discretizations in space but to the best of our knowledge, the case of non-uniform time discretization has never been addressed. The study of meshes being out of the scopes of Magique-3D, we will collaborate with experts on mesh partitioning. We get already on to François Pellegrini who is the principal investigator of Scotch (http://www.labri.fr/perso/pelegrin/scotch) and permanent member of the team project Bacchus (Inria Bordeaux Sud Ouest Research Center).

In the future, we aim at enlarging the application range of implicit schemes. The idea will be to use the degrees of freedom offered by the implicit discretization in order to tackle specific difficulties that may appear in some systems. For instance, in systems involving several waves (as P and S waves in porous elastic media, or coupled wave problems as previously mentioned) the implicit parameter could be adapted to each wave and optimized in order to reduce the computational cost. More generally, we aim at reducing numeric bottlenecks by adapting the implicit discretization to specific cases.

3.5. Full waveform inversion for the optimal design of wind musical instruments

Makers have improved wind musical instruments (as flutes, trumpets, clarinets, bassoons, ...) in the past by a “trial and error” procedure, where the final sound and ease of the instrument in playing conditions are the main criteria. Although the playing context should still be the final reference, we can consider intermediate measurements of the pipe entry impedance [75], [69], which quantifies the Dirichlet-to-Neumann map of the wave propagation in the pipe, and relies on mathematical simulations based on accurate and concise models of the pipe [84], [59] and the embouchure [77], [59], [55], [56], [86] in order to foresee the behavior of a given instrument, and therefore optimize it. A strong interaction with makers and players is necessary for defining both operable criteria quantified as a cost function and a design parameters space. We aim at building efficient musical instrument via handcrafted techniques but also modern tools as additive synthesis (3D printers). We plan to implement state-of-the-art numerical methods (finite elements, full waveform inversion, neuronal networks fed by numerical simulations, diverse optimization techniques...) that are versatile (in terms of models, formulations, couplings...) in order to solve the optimization problem, after a proper modeling of the linear and nonlinear coupled phenomena. We wish to take advantage of the fact that sound waves in musical instruments satisfy the laws of acoustics in pipes (PDEs), which leads to use FWI technique, in harmonic or temporal regime. We propose to implement an iterative process between instrument making and optimal design in order to build instruments that optimize tone quality and playability. We are currently collaborating with musical acoustics teams who have a strong experimental background on this question [66], [67] [DCY12, DF07, GPP98], we wish to strenghten the links we have with other teams [78], [72], [80], [81], [85], we will participate to professional clusters [ITE], and we are currently collaborating with makers and museums directly : Augustin Humeau (Dordogne) for the bassoon, Luc Gallois (Oise) and the Museum of Cité de la Musique - Philharmonie de Paris for the brass instruments. This research axis is surely the most exploratory of our research program and follows the successful ”Exploratory Research Program” Inria grant obtained in 2017. It could pave the way for significant progresses in inverse problem solving. Indeed, the problem depends on a few number of parameters unlike geophysical or astrophysical problems. We can thus use it to test different methods like neuronal networks, statistical methods, coupling with nonlinear phenomena, and decide if it could be applied to large scale applications.

4. Application Domains

4.1. Seismic Imaging

The main objective of modern seismic processing is to find the best representation of the subsurface that can fit the data recorded during the seismic acquisition survey. In this context, the seismic wave equation is the most appropriate mathematical model. Numerous research programs and related publications have been devoted to this equation. An acoustic representation is suitable if the waves propagate in a fluid. But the subsurface does not contain fluids only and the acoustic representation is not sufficient in the general case. Indeed the acoustic wave equation does not take some waves into account, for instance shear waves, turning waves or the multiples that are generated after several reflections at the interfaces between the different layers of the geological model. It is then necessary to consider a mathematical model that is more complex and resolution techniques that can model such waves. The elastic or viscoelastic wave equations are then reference models, but they are much more difficult to solve, in particular in the 3D case. Hence, we need to develop new high-performance approximation methods.

Reflection seismics is an indirect measurement technique that consists in recording echoes produced by the propagation of a seismic wave in a geological model. This wave is created artificially during seismic acquisition surveys. These echoes (i.e., reflections) are generated by the heterogeneities of the model. For instance, if the seismic wave propagates from a clay layer to sand, one will observe a sharp reflected signal in the seismic data recorded in the field. One then talks about reflection seismics if the wave is reflected at the interface between the two media, or talks about seismic refraction if the wave is transmitted along the interface. The arrival time of the echo enables one to locate the position of this transition, and the amplitude of the echo gives information on some physical parameters of the two geological media that are in contact. The first petroleum exploration surveys were performed at the beginning of the 1920’s and for instance, the Orchard Salt Dome in Texas (USA) was discovered in 1924 by the seismic-reflection method.

4.2. Imaging complex media with ultrasonic waves

The acoustic behavior of heterogeneous or composite materials attracts considerable excitement. Indeed, their acoustic response may be extremely different from the single constituents responses. In particular, dispersions of resonators in a matrix are the object of large research efforts, both experimentally and theoretically. However it is still a challenge to dispose of numerical tools with sufficient abilities to deal with the simulation and imaging of such materials behavior. Indeed, not only acoustic simulations are very time-consuming, but they have to be performed on realistic enough solution domains, i.e. domains which capture well enough the structural features of the considered materials.

This collaboration with I2M, University of Bordeaux aims at addressing this type of challenges by developing numerical and experimental tools in order to understand the propagation of ultrasonic waves in complex media, image these media, and in the future, help design composite materials for industrial purposes.

4.3. Helioseismology

This collaboration with the Max Planck Institute for Solar System, Göttingen, Germany, which started in 2014, aims at designing efficient numerical methods for the wave propagation problems that arise in helioseismology in the context of inverse problems. The final goal is to retrieve information about the structure of the Sun i.e. inner properties such as density or pressure via the inversion of a wave propagation problem. Acoustic waves propagate inside the Sun which, in a first approximation and regarding the time scales of physical phenomena, can be considered as a moving fluid medium with constant velocity of motion. Some other simplifications lead to computational saving, such as supposing a radial or axisymmetric geometry of the Sun. Aeroacoustic equations must be adapted and efficiently solved in this context, this has been done in the finite elements code Montjoie. In other situations, a full 3D simulation is required and demands large computational resources. Ultimately, we aim at modeling the coupling with gravity potential and electromagnetic waves (MHD equations) in order to be able to better understand Sun spots.

5. Highlights of the Year

5.1. Highlights of the Year

Inria's Autumn school, November 4-8 2019, Inria Bordeaux Sud-Ouest co-organized by E. Agullo (HiePACS), H. Beaugendre (CARDAMOM) and J. Diaz The school aimed at simulating a physical problem, from its modeling to its implementation in a high performance computing (HPC) framework. The school offered both plenary courses and hands-on sessions that involved many members of the three teams. The physical problem considered was the harmonic wave propagation.

The first day was dedicated to the modeling of the problem and its discretization using a Discontinuous Galerkin scheme. The following two days were dedicated to linear algebra for solving large sparse systems. Background on direct, iterative and hybrid methods for sparse linear systems were discussed. Hands-on on related parallel solvers were then be proposed. Has followed a session dedicated to advanced parallel schemes using task-based paradigms, including a hands-on with the starpu runtime system. The ultimate hands-on session was devoted to the use of parallel profiling tools. The school was closed with plenary talks illustrating the usage of such a workflow in an industrial context.

The hands-on session were conducted on the Federative Platform for Research in Computer Science and Mathematics (PlaFRIM) machine in a guix-hpc reproducible environment

The school was attended by about 40 participants mostly PhDs and postdocs from Inria teams.

6. New Software and Platforms

6.1. Elasticus

KEYWORDS: Discontinuous Galerkin - Acoustic equation - Elastodynamic equations - Elastoacoustic - 2D - 3D - Time Domain

SCIENTIFIC DESCRIPTION: Elasticus simulate acoustic and elastic wave propagation in 2D and in 3D, using Discontinuous Galerkin Methods. The space discretization is based on two kind of basis functions, using Lagrange or Jacobi polynomials. Different kinds of fluxes (upwind and centered) are implemented, coupled with RK2 and RK4 time schemes.

FUNCTIONAL DESCRIPTION: Elasticus is a sequential library, independent of Total plateform and developped in Fortran, to simulate wave propagation in geophysical environment, based on a DG method. It is meant to help PhD students and post-doctoral fellows to easily implement their algorithms in the library. Thus, readability of the code is privileged to optimization of its performances. Developped features should be easily transferred in the computing platform of Total. Elasticus manages arbitrary orders for the spatial discretization with DG method.

NEWS OF THE YEAR: In 2018, we implemented the coupling between hexahedra and tetrahedra and the coupling between Discontinuous Galerkin methods and Spectral Element methods in 2D and in 3D. We also introduced Perfectly Matched layers in the Spectral Element kernel.

- Participants: Julien Diaz, Lionel Boillot and Simon Ettouati
- Contact: Julien Diaz
- Publications: Spectral Element Method and Discontinuous Galerkin approximation for elasto-acoustic problems - Hybrid space discretization to solve elasto-acoustic coupling - On the coupling of Spectral Element Method with Discontinuous Galerkin approximation for elasto-acoustic problems - SEM-DG Approximation for elasto-acoustics

6.2. Hou10ni

KEYWORDS: 2D - 3D - Elastodynamic equations - Acoustic equation - Elastoacoustic - Frequency Domain - Time Domain - Discontinuous Galerkin

SCIENTIFIC DESCRIPTION: Hou10ni simulates acoustic and elastic wave propagation in time domain and in harmonic domain, in 2D and in 3D. It is also able to model elasto acoustic coupling. It is based on the second order formulation of the wave equation and the space discretization is achieved using Interior Penalty Discontinuous Galerkin Method. Recently, the harmonic domain solver has been extended to handle Hybridizable Discontinuous Galerkin Methods.

FUNCTIONAL DESCRIPTION: This software simulates the propagation of waves in heterogeneous 2D and 3D media in time-domain and in frequency domain. It is based on an Interior Penalty Discontinuous Galerkin Method (IPDGM) and allows for the use of meshes composed of cells of various order (p-adaptivity in space).

NEWS OF THE YEAR: In 2019, we have implemented the elasto-acoustic coupling and the poroelastic equations for the HDG formulation.

- Participants: Conrad Hillairet, Elodie Estecahandy, Julien Diaz, Lionel Boillot and Marie Bonnasse
- Contact: Julien Diaz
- Publications: Hybridizable discontinuous Galerkin method for the two-dimensional frequency-domain elastic wave equations - Convergence of seismic full waveform inversion and extension to Cauchy data - Convergence Analysis for Seismic Full Waveform Inversion - Stability and convergence analysis for seismic depth imaging using FWI - On the use of a laser ablation as a laboratory seismic source - Towards Energy-Efficient Storage Servers - Equivalent Robin Boundary Conditions for Acoustic and Elastic Media - Comparison of solvers performance when solving the 3D Helmholtz elastic wave equations over the Hybridizable Discontinuous Galerkin method - Comparison of solvers performance when solving the 3D Helmholtz elastic wave equations using the Hybridizable Discontinuous Galerkin method - Resolution strategy for the Hybridizable Discontinuous Galerkin system for solving Helmholtz elastic wave equations - Seismic imaging in laboratory trough laser Doppler vibrometry - Absorbing Boundary Conditions for 3D Elastic TTI Modeling, Application to Time-Based and Time-Harmonic Simulations - Shape and material parameter reconstruction of an isotropic or anisotropic solid immersed in a fluid - Modelling and advanced simulation

of wave propagation phenomena in 3D geophysical media. - Multi-level explicit local time-stepping methods for second-order wave equations - Absorbing Boundary Conditions for 3D elastic TTI modeling - Modeling of elastic Helmholtz equations by hybridizable discontinuous Galerkin method (HDG) for geophysical applications - Performance Assessment on Hybridizable Dg Approximations for the Elastic Wave Equation in Frequency Domain - High-Order IPDG Approximations for Elasto-Acoustic Problems - High-order Discontinuous Galerkin approximations for elasto-acoustic scattering problems - Modelling of seismic waves propagation in harmonic domain by hybridizable discontinuous Galerkin method (HDG) - Absorbing Boundary Conditions for 3D Tilted Transverse Isotropic media - Performance comparison between hybridizable DG and classical DG methods for elastic waves simulation in harmonic domain - Polynomial speeds in a Discontinuous Galerkin code - Hybridizable Discontinuous Galerkin method for the simulation of the propagation of the elastic wave equations in the frequency domain - Discontinuous Galerkin methods for the simulation of the propagation of the elastic wave equations in the frequency domain - High order discontinuous Galerkin methods for time-harmonic elastodynamics - Hybridizable discontinuous Galerkin method for the two-dimensional frequency-domain elastic wave equations - Efficient DG-like formulation equipped with curved boundary edges for solving elasto-acoustic scattering problems - Numerical schemes for the simulation of seismic wave propagation in frequency domain - Performance analysis of DG and HDG methods for the simulation of seismic wave propagation in harmonic domain - Hybridizable Discontinuous Galerkin method for solving Helmholtz elastic wave equations - Discontinuous Galerkin methods for solving Helmholtz elastic wave equations for seismic imaging - Performance comparison of HDG and classical DG method for the simulation of seismic wave propagation in harmonic domain - Contributions to the mathematical modeling and to the parallel algorithmic for the optimization of an elastic wave propagator in anisotropic media - Contribution to the mathematical analysis and to the numerical solution of an inverse elasto-acoustic scattering problem

- URL: https://team.inria.fr/magique3d/software/hou10ni/

6.3. MONTJOIE

KEYWORDS: High order finite elements - Edge elements - Aeroacoustics - High order time schemes

SCIENTIFIC DESCRIPTION: Montjoie is designed for the efficient solution of time-domain and time-harmonic linear partial differential equations using high-order finite element methods. This code is mainly written for quadrilateral/hexahedral finite elements, partial implementations of triangular/tetrahedral elements are provided. The equations solved by this code, come from the ”wave propagation” problems, particularly acoustic, electromagnetic, aeroacoustic, elastodynamic problems.

FUNCTIONAL DESCRIPTION: Montjoie is a code that provides a C++ framework for solving partial differential equations on unstructured meshes with finite element-like methods (continuous finite element, discontinuous Galerkin formulation, edge elements and facet elements). The handling of mixed elements (tetrahedra, prisms, pyramids and hexahedra) has been implemented for these different types of finite elements methods. Several applications are currently available : wave equation, elastodynamics, aeroacoustics, Maxwell's equations.

- Participants: Gary Cohen, Juliette Chabassier, Marc Duruflé and Morgane Bergot
- Contact: Marc Duruflé
- URL: http://montjoie.gforge.inria.fr/

6.4. tmodeling-DG

Time-domain Wave-equation Modeling App

KEYWORDS: 2D - 3D - Elastoacoustic - Elastodynamic equations - Discontinuous Galerkin - Time Domain

SCIENTIFIC DESCRIPTION: tmodeling-DG simulate acoustic and elastic wave propagation in 2D and in 3D, using Discontinuous Galerkin Methods. The space discretization is based on two kind of basis functions, using Lagrange or Jacobi polynomials. Different kinds of fluxes (upwind and centered) are implemented, coupled with RK2 and RK4 time schemes.

FUNCTIONAL DESCRIPTION: tmodelling-DG is the follow up to DIVA-DG that we develop in collaboration with our partner Total. Its purpose is more general than DIVA-DG and should contains various DG schemes, basis functions and time schemes. It models wave propagation in acoustic media, elastic (isotropic and TTI) media and elasto-acoustic media, in two and three dimensions.

NEWS OF THE YEAR: In 2018, we have coupled the code with a Reverse Time Migration algorithm.

- Participants: Julien Diaz, Lionel Boillot, Simon Ettouati and Hélène Barucq
- Partner: TOTAL
- Contact: Julien Diaz

6.5. OpenWind

Open Wind Instrument Design

KEYWORDS: Wave propagation - Inverse problem - Experimental mechanics - Image processing

FUNCTIONAL DESCRIPTION: Computes resonating pipes' impedance using one-dimensional finite element method with tonholes and fingering chart.

RELEASE FUNCTIONAL DESCRIPTION: account for toneholes as a pipe network using transmission matrices for pipe junctions [Chaigne & Kergomard]

- Authors: Robin Tournemenne, Juliette Chabassier, Alexis Thibault, Augustin Ernoult and Guillaume Castera
- Contact: Juliette Chabassier
- Publication: hal-01963674v2
- URL: https://gitlab.inria.fr/openwind/release

6.6. ffwi

Frequency-domain Full Waveform Inversion

KEYWORDS: 2D - 3D - Discontinuous Galerkin - Inverse problem - Frequency Domain - Acoustic equation - Elasticity

FUNCTIONAL DESCRIPTION: ffwi is developed in partnership with Total in the context of the Depth Imaging Partnership (DIP). It is devoted to perform seismic imaging using the Full Waveform Inversion method, in the frequency domain. It is based upon the software Fmodeling, which is itself dedicated to the forward problem. In FWI, the forward problem is solved using Hybridizable Discontinuous Galerkin Methods. The reconstruction of medium parameter is conducted with an iterative minimization scheme, which uses gradient descent techniques. The software can work with acoustic and elastic media, in two and three dimensions.

- Partner: TOTAL
- Contact: Florian Faucher

7. New Results

7.1. High-order numerical methods for modeling wave propagation in complex media: development and implementation

7.1.1. High order discretization of seismic waves-problems based upon DG-SE methods

Participants: Hélène Barucq, Julien Diaz, Aurélien Citrain.

Accurate wave propagation simulations require selecting numerical schemes capable of taking features of the medium into account. In case of complex topography, unstructured meshes are the most adapted and in that case, Discontinuous Galerkin Methods (DGm) have demonstrated great performance. Off-shore exploration involves propagation media which can be well represented by hybrid meshes combining unstructured meshes with structured grids that are best for representing homogeneous media like water layers. Then it has been shown that Spectral Element Methods (SEm) deliver very accurate simulations on structured grids with much lower computational costs than DGms.

We have developed a DG-SEm numerical method for solving time-dependent elasto- acoustic wave problems. We consider the first-order coupled formulation for which we propose a DG-SEm formulation which turns out to be stable.

While the 2D case is almost direct, the 3D case requires a particular attention on the coupling boundary on which it is necessary to manage the possible positions of the faces of the tetrahedrons with respect to that of the neighboring hexaedra.

In the framework of this DG-SEm coupling, we are also interested in the Perfectly Matched Layer (PML) in particular the use of the SEm inside it to stabilize it in cases where the use of DGm leads to instabilities.

These results have been obtained in collaboration with Henri Calandra (TOTAL) and Christian Gout (INSA Rouen) and have been presented at Journées Ondes Sud-Ouest (JOSO) in Le Barp, the 14th International Conference on Mathematical and Numerical Aspects of Wave Propagation (WAVES) in Vienna (Austria) and MATHIAS conference in Paris [21], [26]

7.1.2. Isogeometric analysis of sharp boundaries in full waveform inversion

Participants: Hélène Barucq, Julien Diaz, Stefano Frambati.

Efficient seismic full-waveform inversion simultaneously demands a high efficiency per degree of freedom in the solution of the PDEs, and the accurate reproduction of the geometry of sharp contrasts and boundaries. Moreover, it has been shown that the stability constant of the FWI minimization grows exponentially with the number of unknowns. Isogeometric analysis has been shown to possess a higher efficiency per degree of freedom, a better convergence in high energy modes (Helmholtz) and an improved CFL condition in explicit-time wave propagation, and it seems therefore a good candidate for FWI.

In the first part of the year, we have focused on a small-scale one-dimensional problem, namely the inversion over a multi-step velocity model using the Helmholtz equation. By exploiting a relatively little-known connection between B-splines ad Dirichlet averages, we have added the knot positions as degrees of freedom in the inversion. We have shown that arbitrarily-placed discontinuities in the velocity model can be recovered using a limited amount of degrees of freedom, as the knots can coalesce at arbitrary positions, obviating the need for a very fine mesh and thus improving the stability of the inversion.

In order to reproduce the same results in two and three dimensions, the usual tensor-product structure of B-splines cannot be used. We have therefore focused on the construction of (unstructured) multivariate B-spline bases. We have generalized a known B-spline basis construction through the language of oriented matroids, showing that multivariate spline bases can be easily constructed with repeated knots and that the construction algorithm can be extended to three dimensions. This gives the freedom to locally reduce the regularity of the basis functions and to place internal boundaries in the domain. The resulting mass matrix is block-dagonal, with adjustable block size, providing an avenue for a simple unstructured multi-patch DG-IGA scheme that is being investigated. With this goal in mind, more efficient quadrature schemes for multivariate B-splines exploiting the connection to oriented matroids are also being investigated.

A research report is in preparation.

7.1.3. Seismic wave propagation in carbonate rocks at the core scale

Participants: Julien Diaz, Florian Faucher, Chengyi Shen.

Reproduction of large-scale seismic exploration at lab-scale with controllable sources is a promising approach that could not only be applied to study small-scale physical properties of the medium, but also contribute to significant progress in wave-propagation understanding and complex media imaging at exploration scale via upscaling methods. We propose to apply a laser-generated seismic point source for core-scale new geophysical experiments. This consists in generating seismic waves in various media by well-calibrated pulsed-laser impacts and measuring precisely the wavefield (displacement) by Laser Doppler Vibrometer (LDV). The point-source-LDV configuration is convenient to model numerically. It can also favor the incertitude estimate of the source and receiver locations. Parallel 2D/3D simulations featuring the Discontinuous Galerkin discretization method with Interior Penalties (IPDG) are done to match the experimental data. The IPDG method is of particular interest when it comes to solve wave propagation problems in highly heterogeneous media, such as the limestone cores that we are studying.

Current seismic data allowed us to retrieve V_p tomography slices. Further more, qualitative/quantitative comparisons between simulations and experimental data validated the experiment protocol and vice-versa the high-order FEM schemes, opening the possibility of performing FWI on dense, high frequency and large band-width data.

This work is in collaboration with Clarisse Bordes, Daniel Brito, Federico Sanjuan and Deyuan Zhang (LFCR, UPPA) and with Stéphane Garambois (ISTerre). Ii is one of the topic of the PhD. thesis of Chengyi Shen.

7.1.4. Simulation of electro-seismic waves using advanced numerical methods

Participants: Hélène Barucq, Julien Diaz, Ha Howard Faucher, Rose-Cloé Meyer.

We study time-harmonic waves propagation in conducting poroelastic media, in order to obtain accurate images for complex media with high-order methods. In these kind of media, we observe the coupling between electromagnetic and seismic wave fields, which is called seismokinetic effect. The converted waves are very interesting because they are heavily sensitive to the medium properties, and the modeling of seismo-electric conversion can allow to detect interfaces in the material where the seismic field would be blind. To the best of our knowledge, the numerical simulation of this phenomenon has never been achieved with high-order finite element methods. Simulations are difficult to perform in time domain, because the time step and the mesh size have to be adapted to the huge variations of wave velocities. To ease the numerical implementation, we work in the frequency domain. We can then include physical parameters that depend non-linearly on the frequencies. Then, we have developed a new Hybridizable Discontinuous Galerkin method for discretizing the equations. This allows us to reduce the computational costs by considering only degrees of freedom on the skeleton of the mesh. We have validated the numerical method thanks to comparison with analytical solutions. We have obtained numerical results for 2D realistic poroelastic media and conducting poroelastic media is under investigation.

Results on analytical solutions for poroelasticity are presented in the research report [44].

7.1.5. Quasinormal mode expansion of electromagnetic Lorentz dispersive materials

Participants: Marc Duruflé, Alexandre Gras.

We have studied the electromagnetic scattering of optical waves by dispersive materials governed by a Drude-Lorentz model. The electromagnetic fields can be decomposed onto the eigenmodes of the system, known as quasinormal modes. In [51], a common formalism is proposed to obtain different formulas for the coefficients of the modal expansion. In this paper, it is also explained how to handle dispersive Perfectly Matched Layers and degenerate eigenvectors. Lately, we have investigated the use of an interpolation method in order to compute quickly the diffracted field for a large number of frequencies.

7.1.6. A Hybridizable Galerkin Discontinuous formulation for elasto-acoustic coupling in frequency-domain

Participants: Hélène Barucq, Julien Diaz, Vinduja Vasanthan.

We are surrounded by many solid-fluid interactions, such as the seabed or red blood cells. Indeed, the seabed represents the ocean floors immersed in water, and red blood cells are coreless hemoglobin-filled cells. Hence, when wanting to study the propagation of waves in such domains, we need to take into account the interactions at the solid-fluid interface. Therefore, we need to implement an elasto-acoustic coupling. Many methods have already tackled with the elasto-acoustic coupling, particularly the Discontinuous Galerkin method. However, this method needs a large amount of degrees of freedom, which increases the computational cost. It is to overcome this drawback that the Hybridizable Discontinuous Galerkin (HDG) has been introduced. The implementations of HDG for the elastic wave equations, as well as partially for the acoustic ones, have been done previously. Using these, we have performed in this work the elasto-acoustic coupling for the HDG methods in 1D, 2D and 3D. The results are presented in Vinduja Vasanthan's master's thesis [54].

7.1.7. Absorbing Radiation Conidition in elongated domains

Participants: Hélène Barucq, Sébastien Tordeux.

We develop and analyse a high-order outgoing radiation boundary condition for solving three-dimensional scattering problems by elongated obstacles. This Dirichlet-to-Neumann condition is constructed using the classical method of separation of variables that allows one to define the scattered field in a truncated domain. It reads as an infinite series that is truncated for numerical purposes. The radiation condition is implemented in a finite element framework represented by a large dense matrix. Fortunately, the dense matrix can be decomposed into a full block matrix that involves the degrees of freedom on the exterior boundary and a sparse finite element matrix. The inversion of the full block is avoided by using a Sherman–Morrison algorithm that reduces the memory usage drastically. Despite being of high order, this method has only a low memory cost. This work has been published in [13].

7.1.8. Discontinuous Galerkin Trefftz type method for solving the Maxwell equations

Participants: Margot Sirdey, Sébastien Tordeux.

Trefftz type methods have been developed in Magique 3D to solve Helmholtz equation and it has been presented in [25].These methods reduce the numerical dispersion and the condition number of the linear system. This work aims in pursuing this development for electromagnetic scattering. We have adapted and tested the method for an academical 2D configuration. This is the topic of the PhD thesis of Margot Sirdey.

7.1.9. Reduced models for multiple scattering of electromagnetic waves

Participants: Justine Labat, Victor Péron, Sébastien Tordeux.

In this project, we develop fast, accurate and efficient numerical methods for solving the time-harmonic scattering problem of electromagnetic waves by a multitude of obstacles for low and medium frequencies in 3D. First, we consider a multi-scale diffraction problem in low-frequency regimes in which the characteristic length of the obstacles is small compared to the incident wavelength. We use the matched asymptotic expansion method which allows for the model reduction. Then, small obstacles are no longer considered as geometric constraints and can be modelled by equivalent point-sources which are interpreted in terms of electromagnetic multipoles. Second, we justify the Generalized Multiparticle Mie-solution method (Xu, 1995) in the framework of spherical obstacles at medium-frequencies as a spectral boundary element method based on the Galerkin discretization of a boundary integral equation into local basis composed of the vector spherical harmonics translated at the center of each obstacle. Numerically, a clever algorithm is implemented in the context of periodic structures allowing to avoid the global assembling of the matrix and so, reduce memory usage. The reduced asymptotic models of the first problem can be adapted for this regime by incorporating non-trivial corrections appearing in the Mie theory. Consequently, a change in variable between the two formulations can be made explicit, and an inherent advantage of the asymptotic formulation is that the basis and the shape can be separated with a semi-analytical expression of the polarizability tensors. A comparison of these different methods in terms of their accuracy has been carried out. Finally, for both methods and in the context of large numbers of obstacles, we implement an iterative resolution with preconditionning in a GMRES framework.

These results have been presented at Journées Ondes Sud-Ouest (JOSO) in Le Barp (France) and the 14th International Conference on Mathematical and Numerical Aspects of Wave Propagation (WAVES) in Vienna (Austria), see [22], [39]. Part of this work has been published in Wave Motion [17].

7.1.10. Boundary Element Method for 3D Conductive Thin Layer in Eddy Current Problems

Participant: Victor Péron.

Thin conducting sheets are used in many electric and electronic devices. Solving numerically the eddy current problems in presence of these thin conductive sheets requires a very fine mesh which leads to a large system of equations, and becoming more problematic in case of high frequencies. In this work we show the numerical pertinence of asymptotic models for 3D eddy current problems with a conductive thin layer of small thickness based on the replacement of the thin layer by its mid-surface with impedance transmission conditions that satisfy the shielding purpose, and by using an efficient discretization with the Boundary Element Method in order to reduce the computational cost. These results have been obtained in collaboration with M. Issa, R. Perrussel and J-R. Poirier (LAPLACE, CNRS/INPT/UPS, Univ. de Toulouse) and O. Chadebec (G2Elab, CNRS/INPG/UJF, Institut Polytechnique de Grenoble). This work has been published in COMPEL - The international journal for computation and mathematics in electrical and electronic engineering, [16].

7.1.11. Asymptotic Models and Impedance Conditions for Highly Conductive Sheets in the Time-Harmonic Eddy Current Model

Participant: Victor Péron.

This work is concerned with the time-harmonic eddy current problem for a medium with a highly conductive thin sheet. We present asymptotic models and impedance conditions up to the second order of approximation for the electromagnetic field. The conditions are derived asymptotically for vanishing sheet thickness where the skin depth is scaled like thickness parameter. The first order condition is the perfect electric conductor boundary condition. The second order condition turns out to be a Poincaré-Steklov map between tangential components of the magnetic field and the electric field. This work has been published in SIAM Journal on Applied Mathematics, [18].

7.2. Understanding the interior of the Earth and the Sun by solving inverse problems

7.2.1. Time-Domain Full Waveform Inversion based on high order discontinuous numerical schemes

Participants: Hélène Barucq, Julien Diaz, Pierre Jacquet.

Full Waveform Inversion (FWI) allows retrieving the physical parameters (e.g. the velocity, the density) from an iterative procedure underlying a global optimization technique. The recovering of the medium corresponds to the minimum of a cost function quantifying the difference between experimental and numerical data. In this study we have considered the adjoint state method to compute the gradient of this cost function.

The adjoint state can be both defined as the adjoint of the continuous equation or the discrete problem. This choice is still under study and complementary results has been presented at WAVES 2019 conference in Vienna [38].

The FWI has been largely developed for time-harmonic wave problems essentially because of computational time which is clearly below the one of corresponding time-dependent problems. However, the memory cost in large 3D domain is overflowing the computer capabilities, which motivates us to develop a FWI algorithm in the time-domain. To fully exploit the information from the seismic traces, while preserving the computational cost, it is important to use an accurate and flexible discretization. For that purpose we study several time schemes such as Runge-Kutta 2/4 or Adam-Bashforth 3 and regarding the space discretization, we employ Discontinuous Galerkin (DG) elements which are well-known not only for their h and p adaptivities but also for their massively parallel computation properties.

In the work-flow of DIP a Reverse Time Migration (RTM) code has been developed in collaboration with Total using their Galerkin Discontinuous acoustic time domain solver. Then this code served as a prototype of the time domain FWI code called utFWI (Unstructured Time-Domain Full Waveform Inversion) (https://bil.inria.fr/fr/software/view/3740/tab). Thanks to this code, 2D acoustic multi-scale reconstructions has been performed. Several optimizers such as gradient descent, non linear conjugate gradient and limited BFGS have also been developed.

This work is a collaboration with Henri Calandra (TOTAL). The time domain FWI results has been presented at Total conference MATHIAS 2019 in Paris [37] and also during the Fall Meeting 2019 AGU in San Francisco [47].

7.2.2. *Box-Tomography imaging in the deep mantle*

Participant: Yder Masson.

Box Tomography is a seismic imaging method (Masson and Romanowicz, 2017) that allows the imaging of localized geological structures buried at arbitrary depth inside the Earth, where neither seismic sources nor receivers are necessarily present. The big advantage of box-tomography over standard tomographic methods is that the numerical modelling (i.e. the ray tracing in travel time tomography and the wave propagation in waveform tomography or full waveform inversion) is completely confined within the small box-region imaged. Thus, box tomography is a lot more efficient than global tomography (i.e. where we invert for the velocity in the larger volume that encompasses all the sources and receivers), for imaging localized objects in the deep Earth. Following a successful, yet partial, application of box tomography to the imaging of the North American continent (i.e. Clouzet et al, 2018), together with Barbara Romanowicz and Sevan Adourian at the Berkeley Seismological Laboratory, we finished implementing the necessary tools for imaging localized structure in the Earth's lower mantle. The following tasks have been completed:

- Modify the global wave propagation solver Specfem_3D_globe in order to compute Green's functions in our current reference Earth model (SEMUCB).
- Modify the local wave propagation solver RegSEM_globe so that the wavefield can be recorded and stored at the surface of the modeling domain.
- Implement real-time compression for an improved management of computed data.

Preliminary results have been presented at the American geophysical union fall meeting 2019 [24]. In the near Future, the latest implementation of Box-Tomography will be deployed to investigate the deep structure under the Yellowstone hotspot down to 20 seconds period.

7.2.3. *Wave-propagation modeling using the distributional finite difference method (DFD).*

Participant: Yder Masson.

In the last decade, the Spectral Element Method (SEM) has become a popular alternative to the Finite Difference method (FD) for modeling wave propagation in heterogeneous geological media. Though this can be debated, SEM is often considered to be more accurate and flexible than FD. This is because SEM has exponential convergence, it allows to accurately model material discontinuities, and complex structures can be meshed using multiple elements. In the mean time, FD is often thought to be simpler and more computationally efficient, in particular because it relies on structured meshed that are well adapted to computational architectures. This motivated us to develop a numerical scheme called the Distributional Finite

Difference method (DFD), which combines the efficiency and the relative simplicity of the finite difference method together with an accuracy that compares to that of the finite/spectral element method. Similarly to SEM, the DFD method divides the computational domain in multiple elements but their size can be arbitrarily large. Within each element, the computational operations needed to model wave propagation closely resemble that of FD which makes the method very efficient, in particular when large elements are employed. Further, large elements may be combined with smaller ones to accurately mesh certain regions of space having complex geometry and material discontinuities, thus ensuring higher flexibility. An exploratory code allowing to model 2D and 3D wave propagation in complex media has been developed and demonstrated the interest of the proposed scheme. We presented numerical examples showing the accuracy and the interest of the DFD method for modeling wave propagation through the Earth at the EGU general assembly, 2019 and at the AGU fall meeting 2019 [41].

7.2.4. Time-harmonic seismic inverse problem

Participants: Hélène Barucq, Florian Faucher.

We study the inverse problem associated with the propagation of time-harmonic wave. In the seismic context, the available measurements correspond with partial reflection data, obtained from one side illumination (only the Earth surface is available). The inverse problem aims at recovering the subsurface Earth medium parameters and we employ the Full Waveform Inversion (FWI) method, which employs an iterative minimization algorithm of the difference between the measurement and simulation.

In particular, we investigate the use of new misfit functionals, based upon the *reciprocity-gap*. The use of such functional is only possible when specific measurements are available, and relates to Green's identity. The feature of the cost function is to allow a separation between the observational and numerical sources. In fact, the numerical sources do not have to coincide with the observational ones, offering new possibilities to create adapted computational acquisitions, and possibilities to reduce the numerical burden.

This work is a collaboration with Giovanni Alessandrini (Università di Trieste), Maarten V. de Hoop (Rice University), Romina Gaburro (University of Limerick) and Eva Sincich (Università di Trieste).

This work has given rise to a publication [11] and a preprint [53]. It has also been presented in several conferences [32], [35], [33], [34].

7.2.5. Convergence analysis for the seismic inverse problem

Participants: Hélène Barucq, Florian Faucher.

The determination of background velocity by Full Waveform Inversion (FWI) is known to be hampered by the local minima of the data misfit caused by the phase shifts associated with background perturbations. Attraction basins for the underlying optimization problems can be computed around any nominal velocity model and guarantee that the misfit functional has only one (global) minimum. The attraction basins are further associated with tolerable error levels which represent the maximal allowed distance between the (observed) data and the simulations (i.e., the acceptable noise level). The estimates are defined a priori, and only require the computation of (possibly many) first and second order directional derivatives of the (model to synthetic) forward map. The geometry of the search direction and the frequency influence the size of the attraction basins, and complex frequency can be used to enlarge the basins. The size of the attraction basins for the perturbation of background velocities in the classical FWI (global model parametrization) and the data space reflectivity (MBTT) reformulation are compared: the MBTT reformulation increases substantially the size of the attraction basins. Practically, this reformulation compensates for the lack of low frequency data.
This work is a collaboration with Guy Chavent (Inria Rocquencourt) and Henri Calandra (TOTAL). The results have been published in Inverse Problems [12] and in the Research Report [43].

7.2.6. Eigenvector representation for the seismic inverse problem

We study the seismic inverse problem for the recovery of subsurface properties in acoustic media. In order to reduce the ill-posedness of the problem, the heterogeneous wave speed parameter is represented using a limited number of coefficients associated with a basis of eigenvectors of a diffusion equation, following the regularization by discretization approach. We compare several choices for the diffusion coefficient in the partial differential equations, which are extracted from the field of image processing. We first investigate their efficiency for image decomposition (accuracy of the representation with respect to the number of variables and denoising). Next, we implement the method in the quantitative reconstruction procedure for seismic imaging, following the Full Waveform Inversion method.
This work is a collaboration with Otmar Scherzer (University of Vienna) and the results have been documented in [49].

7.2.7. Outgoing solutions for the scalar wave equation in Helioseismology

Participants: Hélène Barucq, Florian Faucher, Ha Pham.

We study the construction and uniqueness of physical solutions for the time-harmonic scalar wave equation arising in helioseismology. The definition of outgoing solutions to the equation in consideration or their construction and uniqueness has not been discussed before in the context of helieoseismology. In our work, we use the Liouville transform to conjugate the original equation to a potential scattering problem for Schrödinger operator, with the new problem containing a Coulomb-type potential. Under assumptions (in terms of density and background sound speed) generalizing ideal atmospheric behavior, we obtain existence and uniqueness of variational solutions.

Solutions obtained in this manner are characterized uniquely by a Sommerfeld-type radiation condition at a new wavenumber. The appearance of this wavenumber is only clear after applying the Liouville transform. Another advantage of the conjugated form is that it makes appear the Whittaker special functions, when ideal atmospheric behavior is extended to the whole domain. This allows for the explicit construction of the outgoing Green kernel and the exact Dirichlet-to-Neumann map and hence reference solutions and radiation boundary condition.

This work has given rise to a report of 135 pages, [45]. Some part have been extracted for a publication which has recently been accepted in ESAIM: M2AN.

Consequently to this work, ongoing research includes the fast construction of the Green's kernel, which is possible thanks to the family of special functions obtained from the previous analytical study, [36]. As part of the ANTS associate team, applications to helioseismology is also ongoing. This work is a collaboration with Damien Fournier and Laurent Gizon (Max Planck Institute at Göttingen). The "Ants workshop on computational helioseismology" has also been organized in this context.

7.2.8. Modeling the propagation of acoustic wave in the Sun

Participants: Hélène Barucq, Juliette Chabassier, Marc Duruflé, Nathan Rouxelin.

We study time-harmonic propagation of acoustic waves in the Sun in the presence of gravity forces.

Galbrun's equation, a Lagrangian description of acoustic wave propagation, is usually used in helioseismology. However, the discretization of this equation with high-order discontinuous Galerkin methods leads to poor numerical results for solar-like background flow and geometries. As better numerical results were obtained by using another model, the Linearized Euler's Equations, we investigate the equivalence between those two models.If compatible boundary conditions are chosen, it should be possible to reconstruct the solution of Galbrun's equation by solving the Linearized Euler's Equations and then a vectorial transport equation. It turns out that finding those boundary conditions is quite difficult and not always possible.

We also have constructed a reduced model for acoustic wave propagation in the presence of gravity. Under some additional assumptions on the background flow and for high frequencies, the Linearized Euler's Equations can be reduced to a scalar equation on the pressure perturbation. This equation is well-posed in a usual variational framework and it will provide a useful reference solution to validate our numerical methods. It also seems that a similar process could be used in more realistic cases.

7.2.9. *Equivalent boundary conditions for acoustic media with exponential densities. Application to the atmosphere in helioseismology*

Participants: Juliette Chabassier, Marc Duruflé, Victor Péron.

We present equivalent boundary conditions and asymptotic models for the solution of a transmission problem set in a domain which represents the sun and its atmosphere. This problem models the propagation of an acoustic wave in time-harmonic regime. The specific non-standard feature of this problem lies in the presence of a small parameter δ which represents the inverse rate of the exponential decay of the density in the atmosphere. This problem is well suited for the notion of equivalent conditions and the effect of the atmosphere on the sun is as a first approximation local. This approach leads to solve only equations set in the sun. We derive rigorously equivalent conditions up to the fourth order of approximation with respect to δ for the exact solution u. The construction of equivalent conditions is based on a multiscale expansion in power series of δ for u. Numerical simulations illustrate the theoretical results. Finally we measure the boundary layer phenomenon by introducing a characteristic length that turns out to depend on the mean curvature of the interface between the subdomains. This work has been published in Applied Mathematics and Computation [15].

7.3. Hybrid time discretizations of high-order

7.3.1. *Construction and analysis of a fourth order, energy preserving, explicit time discretization for dissipative linear wave equations.*

Participants: Juliette Chabassier, Julien Diaz.

A paper was accepted in M2AN [14]. This paper deals with the construction of a fourth order, energy preserving, explicit time discretization for dissipative linear wave equations. This family of schemes is obtained by replacing the inversion of a matrix, that comes naturally after using the technique of the Modified Equation on the second order Leap Frog scheme applied to dissipative linear wave equations, by an explicit approximation of its inverse. The series can be truncated at different orders, which leads to several schemes. The stability of the schemes is studied. Numerical results in 1D illustrate the good behavior regarding space/time convergence and the efficiency of the newly derived scheme compared to more classical time discretizations. A loss of accuracy is observed for non smooth profiles of dissipation, and we propose an extension of the method that fixes this issue. Finally, we assess the good performance of the scheme for a realistic dissipation phenomenon in Lorentz's materials. This work has been done in collaboration with Sébastien Imperiale (Inria Project-Team M3DISIM).

7.3.2. *Space-Time Discretization of Elasto-Acoustic Wave Equation in Polynomial Trefftz-DG Bases*

Participants: Hélène Barucq, Julien Diaz.

In the context of the strategic action "Depth Imaging Partnership" between Inria and Total we have investigated to the development of an explicit Trefftz-DG formulation for elasto-acoustic problem, solving the global sparse matrix by constructing an approximate inverse obtained from the decomposition of the global matrix into a block-diagonal one. The inversion is then justified under a CFL-type condition. This idea allows for reducing the computational costs but its accuracy is limited to small computational domains. According to the limitations of the method, we have investigated the potential of Tent Pitcher algorithms following the recent works of Gopalakrishnan et al. It consists in constructing a space-time mesh made of patches that can be solved independently under a causality constraint. We have obtained very promising numerical results illustrating the potential of Tent Pitcher in particular when coupled with a Trefftz-DG method involving only surface terms. In this way, the space-time mesh is composed of elements which are 3D objects at most. It is also worth noting that this framework naturally allows for local time-stepping which is a plus to increase the accuracy while decreasing the computational burden. The results of this work [28] have been presented during the ICIAM conference (Valencia, July 15-19).

7.4. Modeling and design of wind musical instruments

7.4.1. Full Waveform inversion for bore reconstruction of woodwind instruments

Participants: Juliette Chabassier, Augustin Ernoult.

Several techniques can be used to reconstruct the internal geometry of a wind instrument from acoustics measurements. One possibility is to simulate the passive linear acoustic response of an instrument and to use an optimization process to fit the simulation to the measurements. This technique can be seen as a first step toward the design of wind instruments, where the targeted acoustics properties come no more longer from measurements but are imposed by the designer. We applied the FWI methodology, along with 1D spectral finite element discretization in space [19], to the woodwind instruments (with tone holes, losses and radiation). The algorithm have been implemented in Pyhton3 and is know operational to reconstruct the bore of real instrument. This functionality will be available in an upcoming version of the toolbox OpenWind.

7.4.2. Computation of the entry impedance of a wind instrument with toneholes and radiation

Participants: Guillaume Castera, Juliette Chabassier, Augustin Ernoult, Alexis Thibault, Robin Tournemenne.

Modeling the entry impedance of wind instruments pipes is essential for sound synthesis or instrument qualification. Based on a one-dimensional model of acoustic propagation ("telegraphist's equations") we find approximate solutions using a high-order Finite Element Method (FEM1D). Contrary to the more standard semi-analytic Transfer Matrix Method (TMM), the FEM1D can take into account arbitrarily complex and variable coefficients [19]. It is therefore well-suited for the realistic cases involving boundary losses, smooth waveguide geometry, and possibly even a temperature gradient along the instrument's bore. We model toneholes as junctions of one-dimensional waveguides, and an acoustic radiation impedance models the radiation of all open tube ends. A global matrix is assembled to connect all these elements together, and solved for each frequency to compute the impedance curve. Source code is available in our Python3 toolbox OpenWind.

7.4.3. Time-domain simulation of a reed instrument with toneholes

Participants: Juliette Chabassier, Augustin Ernoult, Alexis Thibault, Robin Tournemenne.

As part of the project aiming at providing practical tools for instrument design, we have been developing a sound synthesis module for reed instruments. We model a reed music instrument, such as the oboe or the bassoon, as a coupled system composed of a nonlinear source mechanism (the reed), and a linear resonating part (the air within the instrument's bore). Acoustic wave propagation inside of the instrument is reduced to a one-dimensional model, on which a variational approximation is performed, yielding high-order finite elements in space. Tone holes on the side of the instrument are taken into account using junctions of one-dimensional waveguides. The acoustic radiation impedance is written as a positive Padé approximation, so that it leads to a stable time domain model even when opening and closing holes during the simulation. For the reed, a one-degree-of-freedom lumped model is used, in which the reed opening follows a second order ODE and acts as a valve, modulating the flow that enters the pipe based on the pressure difference between the player's mouth and the inside of the instrument. Energy-consistent time discretization schemes have been derived for each component, so that it is possible to simulate instruments with an arbitrary geometry with good numerical accuracy and stability. The simulations have been implemented in Python3 and will be made available in an upcoming version of the toolbox OpenWind.

7.4.4. Time-domain simulation of 1D acoustic wave propagation with boundary layer losses

Participants: Juliette Chabassier, Augustin Ernoult, Alexis Thibault.

Energy dissipation effects are of critical importance in musical acoustics. Boundary layer losses occurring in acoustic waveguides are usually modeled in the frequency domain, leading to slowly-decreasing kernels in the time domain similar to fractional derivatives. We have developed an energy-consistent time-domain model based on positive fraction approximation of the dissipative operators, leading to the use of $2N+1$ additional variables per degree of freedom. Coefficients for these new variables depend only on N so that they can be tabulated without any prior knowledge of the waveguide geometry. They are found with an optimization procedure. This model can be discretized using 1D finite elements [19], and an energy-consistent time-stepping scheme can be found. The resulting numerical scheme has been implemented numerically, and source code will be made available in an upcoming version of the toolbox OpenWind. An article is being written and will be submitted soon to JASA.

7.4.5. *Numerical libraries for hybrid meshes in a discontinuous Galerkin context*

Participants: Hélène Barucq, Aurélien Citrain, Julien Diaz.

Elasticus team code has been designed for triangles and tetrahedra mesh cell types. The first part of this work was dedicated to add quadrangle libraries and then to extend them to hybrid triangles-quadrangles (so in 2D). This implied to work on polynomials to form functions basis for the (discontinuous) finite element method, to finally be able to construct reference matrices (mass, stiffness, ...).

A complementary work has been done on mesh generation. The goal was to encircle an unstructured triangle mesh, obtained by third-party softwares, with a quadrangle mesh layer. At first, we built scripts to generate structured triangle meshes, quadrangle meshes and hybrid meshes (triangles surrounded by quadrangles). In 2018, we have implemented the coupling between Discontinuous Galerkin methods (using the triangles/tetrahedra) and Spectral Element methods (using quadrangles/hexahedra). We have also implemented the PML in the SEM part, and we are now working on the local time-stepping feature.

8. Bilateral Contracts and Grants with Industry

8.1. Contracts with TOTAL

- Depth Imaging Partnership (DIP)
- Depth Imaging Partnership (DIP2)

  Period: 2014 May - 2019 April , Management: Inria Bordeaux Sud-Ouest, Amount: 120000 euros/year.
- Depth Imaging Partnership (DIP3)

  Period: 2019 May - 2021 December , Management: Inria Bordeaux Sud-Ouest, Amount: 120000 euros/year.
- Tent Pitcher algorithm for space-time integration of wave problems Period: 2019 November - 2022 October, Management: Inria Bordeaux Sud-Ouest, Amount: 165000 euros.
- Isogeometric analysis of sharp boundaries in fullwaveform inversion Period: 2019 January - 2021 December, Management: Inria Bordeaux Sud-Ouest, Amount: 55000 euros.
- FWI (Full Waveform Inversion) dans le domaine temporel utilisant des méthodes numériques hybrides pour la caractérisation de milieux élasto-acoustiques. Period: 2017 October - 2020 December , Management: Inria Bordeaux Sud-Ouest, Amount: 180000 euros.
- Petrophysics in pre-salt carbonate rocks

  Period: 2019 November - 2021 June, Management: Inria Bordeaux Sud-Ouest, Amount: 142000 euros.

9. Partnerships and Cooperations

9.1. Regional Initiatives

9.1.1. *Partnership with I2M in Bordeaux supported by Conseil Régional d'Aquitaine*

title: COFIMUS.
Coordinator:Juliette Chabassier
Other partners: I2M CNRS Université Bordeaux I

The objective is to develop a virtual workshop for wind musical instrument makers.

This project is supported by the Conseil Régional d'Aquitaine, for a duration of 2 years and has funded the postdoctoral position of Augustin Ernoult since March 2019.

9.2. National Initiatives

9.2.1. Depth Imaging Partnership

Magique-3D maintains active collaborations with Total. In the context of Depth Imaging, Magique-3D coordinates research activities dealing with the development of high-performance numerical methods for solving wave equations in complex media. This project has involved 2 other Inria Team-Projects (Hiepacs and Nachos) which have complementary skills in mathematics, computing and in geophysics. DIP is fully funded by Total by the way of an outline agreement with Inria .

In 2014, the second phase of DIP has begun. Lionel Boillot has been hired as engineer to work on the DIP platform. Six PhD students have defended their PhD since 2014 and they are now post-doctoral researchers or engineers in Europe. DIP is currently employing 2 PhD students and one post-doctoral researcher.

9.2.2. PRE Concert

Magique 3D is hosting an Inria "exploratory research project" (PRE) about modeling and designing wind musical instruments. This project has funded the post-doctoral position of Robin Tournemenne from July 2017 until July 2019.

9.2.3. ANR Num4Sun

The ANR has launched a specific program for supporting and promoting applications to European or more generally International projects. Magique-3D has been selected in 2016 after proposing a project to be applied as a FET project on the occasion of a call that will open in 2017 April. This project will gather researchers of the MPS (https://www.mps.mpg.de/en), of the BSC (https://www.bsc.es/), of the BCAM (http://www.bcamath.org/en/), of Heriot-Watt University (https://www.hw.ac.uk/) and Inria teams.
A kick-off meeting has been held in November 2016 in Strasbourg and a second one in Paris in July 2017. Thanks to this support, we have submitted a ETPHPC proposal in September 2017 The project is funded for 18 months starting from August 2016. The funding amounts 30000€.

9.2.4. Grant from Fondation Blaise Pascal

The project Louis 14.0 has been selected by the Fondation Blaise Pascal as one of their supported projects for 2019. See more about the project at https://project.inria.fr/louis14point0/, in french.

9.3. European Initiatives

9.3.1. FP7 & H2020 Projects

9.3.1.1. Mathrocks

Title: Multiscale Inversion of Porous Rock Physics using High-Performance Simulators: Bridging the Gap between Mathematics and Geophysics

Program: H2020

Duration: April 2018 - March 2022

Coordinator: Universidad Del Pais Vasco (EHU UPV)

Partners:

- Bcam - Basque Center for Applied Mathematics Asociacion (Spain)
- Barcelona Supercomputing Center - Centro Nacional de Supercomputacion (Spain)
- Universidad Del Pais Vasco Ehu Upv (Spain)
- Universitat Politecnica de Catalunya (Spain)

REPSOL SA (Spain)

Pontificia Universidad Catolica de Valparaiso (Chile)

Curtin University of Technology (Australia)

The University of Texas System (USA)

University Nacional de Columbia (Colombia)

Pontificia Universidad Catolica de Chile (Chile)

Universidad Central de Venezuela (Venezuela)

University de Buenos Aires (Argentina)

Macquarie University (Australia)

Inria contact: Hélène BARUCQ

We will develop and exchange knowledge on applied mathematics, high-performance computing (HPC), and geophysics to better characterize the Earth´s subsurface. We aim to better understand porous rocks physics in the context of elasto-acoustic wave propagation phenomena. We will develop parallel high-continuity isogeometric analysis (IGA) simulators for geophysics. We will design and implement fast and robust parallel solvers for linear equations to model multi-physics electromagnetic and elasto-acoustic phenomena. We seek to develop a parallel joint inversion workflow for electromagnetic and seismic geophysical measurements. To verify and validate these tools and methods, we will apply the results to: characterise hydrocarbon reservoirs, determine optimal locations for geothermal energy production, analyze earthquake propagation, and jointly invert deep-azimuthal resistivity and elasto-acoustic borehole measurements. Our target computer architectures for the simulation and inversion software infrastructure consists of distributed-memory parallel machines that incorporate the latest Intel Xeon Phi processors. Thus, we will build a hybrid OpenMP and MPI software framework. We will widely disseminate our collaborative research results through publications, workshops, postgraduate courses to train new researchers, a dedicated webpage with regular updates, and visits to companies working in the area. Therefore, we will perform a significant role in technology transfer between the most advanced numerical methods and mathematics, the latest super-computer architectures, and the area of applied geophysics.

9.4. International Initiatives

9.4.1. Inria Associate Teams Not Involved in an Inria International Labs

9.4.1.1. ANTS

Title: Advanced Numerical meThods for helioSeismology

International Partner (Institution - Laboratory - Researcher):

Max Plank Institut für Sonnensystemforschung (Germany) – Department Solar and Stellar Interiors – Laurent Gizon.

Start year: 2019

See also: https://team.inria.fr/ants/

Magique-3D has started an Associate Team project, ANTS (Advanced Numerical meThods for helioSeismology), with the Max Planck Institute for Solar System Research (MPS), led by Laurent Gizon. This helps promote the collaboration between Magique3D and the Solar group at the Max Planck Institute for Solar System Research at Göttingen (MPS) for the direct and inversion of solar models from Doppler data obtained at the surface of the Sun. The scientific project benefits from the expertise of Magique-3D in seismic imaging, and the expert knowledge of the MPS group on Solar physics, in order to design accurate and efficient methodology. A joint workshop was held at Inria Bordeaux Sud-Ouest in December 2019: https://project.inria.fr/antsworkshop201912/.

9.4.2. Inria International Partners

9.4.2.1. New international partner: The Berkeley Seismological Laboratory, University of California, Berkeley.

In September 2019, together with Barbara Romanowicz at the University of California Berkeley https://seismo.berkeley.edu/, we initiated a collaboration aiming at developing and deploying novel tomographic methods for imaging localized structures in the deep Earth that are either blurred out or not visible in the current global models.This effort is supported by the France-Berkeley Fund which granted our project for a period of 2 years. Amount: 11000€, Management: Berkeley University url: https://fbf.berkeley.edu/project/development-and-application-advanced-seismic-imaging-techniques-key-target-structures-deep

9.4.2.2. Declared Inria International Partners

9.4.2.2.1. MAGIC2

Title: Advance Modeling in Geophysics

International Partner (Institution - Laboratory - Researcher):

California State University at Northridge (United States) - Department of Mathematics - Djellouli Rabia

The Associated Team MAGIC was created in January 2006 and renewed in January 2009. At the end of the program in December 2011, the two partners, MAGIQUE-3D and the California State University at Northridge (CSUN) decided to continue their collaboration and obtained the “Inria International Partner” label in 2013.

See also: https://project.inria.fr/magic/

The ultimate objective of this research collaboration is to develop efficient solution methodologies for solving inverse problems arising in various applications such as geophysical exploration, underwater acoustics, and electromagnetics. To this end, the research program will be based upon the following three pillars that are the key ingredients for successfully solving inverse obstacle problems. 1) The design of efficient methods for solving high-frequency wave problems. 2) The sensitivity analysis of the scattered field to the shape and parameters of heterogeneities/scatterers. 3) The construction of higher-order Absorbing Boundary Conditions. In the framework of Magic2, Rabia Djellouli (CSUN) visited Magique 3D in February 2018

9.5. International Research Visitors

9.5.1. Visits of International Scientists

- Vianey Villamizar (Department of Mathematics, Brigham Young University) visited the team in September 2019
- Mounir Tlemcani (Université d’Oran, Algeria) visited Magique 3D in March 2019.
- Sevan Adourian (Univesity of California, Berkeley) visited Magique 3D for a week in June 2019, this visit has been sponsored by the France-Berkeley Fund.

9.5.2. Visits to International Teams

9.5.2.1. Research Stays Abroad

- Nathan Rouxelin visited MPS at Göttingen in April 2019, during a month.
- Rose-Cloé Meyer visited prof. Steve Pride from Lawrence Berkeley National Laboratory in June 2019 during 1 month and in December 2019 during 3 weeks.
- In the framework of DIP, Pierre Jacquet visited Total Research Center at Houston, USA, in December 2019 during 1 week.
- Yder Masson, visited Barbara Romanowicz at the Berkeley Seismological Laboratory and Steve R. Pride at the Lawrence Berkeley Laboratory for two days the week following the AGU Fall Meeting Dec 9-13, 2019 , San Francisco, CA, USA)

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events: Organisation

10.1.1.1. Member of the Organizing Committees

- Hélène Barucq co-organized committee of "Journées Ondes du Sud-Ouest" (JOSO 2019), March, 12-14. https://hal.archives-ouvertes.fr/JOSO2019
- Hélène Barucq, Florian Faucher and Ha Pham organized the "Ants workshop on computational helioseismology" in Bordeaux, December, 3-5, https://project.inria.fr/antsworkshop201912/
- Hélène Barucq coorganized a minisymposium on "Geophysical Applications" at ICIAM 2019 in Valence, July, 15-19, https://iciam2019.org/
- Julien Diaz and Sébastien Tordeux coorganized a minisymposium on "Advanced numerical tools for wave propagation simulation" at ICIAM 2019 in Valence, July, 15-19, https://iciam2019.org/
- Julien Diaz coorganized an autumn school on "High performance numerical simulation", https://project.inria.fr/hpcschool2019/, in Bordeaux, November, 4-8. This school gathered 30 participants, mainly PhD students and post-doc. It aimed at simulating a physical problem, from its modeling to its implementation in an high performance computing (HPC) framework. The physical problem considered was the harmonic wave propagation. The hands-on sessions were conducted on the Federative Platform for Research in Computer Science and Mathematics (PlaFRIM) machine.

10.1.2. Scientific Events: Selection

10.1.2.1. Member of the Conference Program Committees

- Hélène Barucq and Julien Diaz were members of the scientific committee of Waves 2019 https://waves2019.at
- Sébastien Tordeux was member of the scientific committee of The international Russian-french workshop, Differential equations and Mathematical Modeling, Khanty-Mansiisk, Russia 25-29 août 2019

10.1.3. Journal

10.1.3.1. Reviewer

Members of Magique 3D have been reviewers for the following journals:

- Computer Methods in Applied Mechanics and Engineering
- Geophysics
- Journal of Computational Physics
- Journal of Scientific Computing
- Numerical Methods in Engineering
- Geophysical Journal International
- Computational Geosciences (COMG)

10.1.4. Leadership within the Scientific Community

Hélène Barucq is elected member of the Liaison Committee of SMAI-GAMNI (Society of Applied and Industrial Mathematics - Group for promoting the Numerical Methods for Engineers).

10.1.5. Scientific Expertise

- Julien Diaz was expert for the evaluation of Millennium Science Initiative project for the government of Chile.
- Since 2017, Hélène Barucq has been chairwoman of a committee which evaluates research projects in Mathematics, Computer Science, Electronics and Optics to be funded by the Regional Council New Aquitaine
- Since 2018, Hélène Barucq has been scientific officer for E2S project. She participates in the evaluation of each E2S call. She is also member of a committee having in charge the recruitment of non permanent researchers for E2S.

10.1.6. Research Administration

- Julien Diaz is elected member of the Inria Technical Committee and of the Inria Administrative Board. Since 2018, he has been the head of the Mescal team of LMAP.
- Justine Labat is elected member of Laboratory Commitee of LMAP.
- Victor Péron is appointed member of the CER (Commission des emplois de recherche) of Inria Bordeaux Sud-Ouest.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

Master : Julien Diaz, Transformées, 24h Eq. TD, M1, EISTIA, France

Licence : Rose-Cloé Meyer, Mathématiques appliquées, 22.5h Eq. TD, L1, UPPA, France

Licence : Rose-Cloé Meyer, Développements limités, suites et séries, 19.5h Eq. TD, L2, UPPA, France

Licence : Marc Duruflé, Équations différentielles, 20h Eq. TD, L3, Enseirb-MatMeca, France

Licence : Marc Duruflé, Algorithmique Numérique, 50h Eq. TD, L3, Enseirb-MatMeca, France

Licence : Marc Duruflé, Outils Mathématiques 3-D, 37h Eq. TD, L3, Enscpb, France

Master : Marc Duruflé, Calcul scientifique en C++, 96h Eq. TD, M1, Enseirb-MatMeca, France

Licence : Marc Duruflé, Calcul scientifique en Fortran90, 20h Eq. TD, L3, Enseirb-MatMeca, France

Licence : Nathan Rouxelin, Mathématiques appliquées, 22.5h Eq. TD, L1, UPPA, France

Licence : Nathan Rouxelin, Modèles mathématiques pour l'informatique, 19.5h Eq. TD, L1, UPPA, France

Master : Florian Faucher, Inversion / optimisation, 10.5h Eq. Cours et TD, M2, Université de Pau et des Pays de l'Adour, France

Licence : Justine Labat, Algèbre pour l'informatique, 19.5h Eq. TD, L1, UPPA, France

Licence : Justine Labat, Introduction aux Probabilités, 12.5h Eq. TD, L2, UPPA, France

Licence : Victor Péron, Analyse 2, 39 Eq. TD, L1, UPPA, France

Licence : Victor Péron, Mathématiques appliquées, 15 Eq. TD, L1, UPPA, France

Licence : Victor Péron, Mathématiques appliquées, 19.5 Eq. TD, L1, UPPA, France

Licence : Victor Péron, Analyse numérique des systèmes linéaires, 48.75 Eq. TD, L3, UPPA, France

Licence: Géométrie analytique, 20h Eq. TD, UPPA, France

Master : Victor Péron and Sébastien Tordeux, Analyse numérique des EDP 1: différences finies, 75 eq. TD, Master1, UPPA, France

Master : Victor Péron and Sébastien Tordeux, Introduction aux phénomènes de propagation d'ondes, 38 eq. TD, Master 2, UPPA, France

Master : Robin Tournemenne, Math-Info, 64h eq. TD, L3+M1, ENSAM Bordeaux, France

10.2.2. Supervision

PhD : Aurélien Citrain, Méthode d'éléments finis hybride pour la simulation des ondes sismiques : couplage des discrétisations Galerkine Discontinue et éléments spectraux, December 16th, Hélène Barucq and Christian Gout (Insa Rouen).

PhD : Justine Labat, Modélisation multi-échelle de la diffraction des ondes électromagnétiques par de petits obstacles, November 28th, Victor Péron and Sébastien Tordeux.

PhD in progress : Alexandre Gras, Hybrid resonance for sensing applications, IOGS, October 2017, Philippe Lalanne(IOGS), Marc Duruflé, Hélène Barucq (Magique 3D)

PhD in progress : Pierre Jacquet, Time domain Full Waveform Inversion involving hybrids numerical method to characterize elasto-acoustic media. ,October 2017, Hélène Barucq and Julien Diaz.

PhD in progress: Victor Martins Gomez, Experimental characterization and modeling of seismo-electromagnetic waves, Université de Pau et des Pays de l'Adour, October 2018, Hélène Barucq and daniel brito (LFCR)

PhD in progress : Rose-Cloé Meyer, Modeling of conducting poro-elastic media using advanced numerical methods , Université de Pau et des Pays de l'Adour, October 2018, Hélène Barucq and Julien Diaz

PhD in progress : Nathan Rouxelin, Advanced numerical modeling of acoustic waves propagating below the surface of the Sun, Université de Pau et des Pays de l'Adour, October 2018, Hélène Barucq and Juliette Chabassier

PhD in progress : Chengyi Shen, Approches expérimentale et numérique de la propagation d'ondes sismiques dans les roches carbonatées, October 2016, Julien Diaz and Daniel Brito (LFCR).

PhD in progress : Margot Sirdey, Méthode de Trefftz pour l'électromagnétisme, October 2019, Sébastien Tordeux and Sébastien Pernet (Onera).

PhD in progress : Vinduja Vasanthan, Tent Pitcher algorithm for space-time integration of wave problems, October 2019, Hélène Barucq and Julien Diaz.

PhD in progress : Stefano Frambati, Isogeometric analysis of sharp boundaries in full waveform inversion, January 2019, Hélène Barucq and Julien Diaz.

Master 2 internship : Ilyas Bouchni, Optimisation de maillage pour l'imagerie sismique, Université de Montpellier, Sept. 2019.

Master 2 internship : Vinduja Vasanthan, Couplage élasto-acoustique en domaine fréquentiel par des méthodes de type Galerkine Discontinues Hybride , Insa Rouen, Sept. 2019.

10.2.3. Juries

- Victor Péron : Jérôme Tomezyk (Université Polytechnique Hauts-de-France), Résolution numérique de quelques problèmes du type Helmholtz avec conditions au bord d'impédance ou des couches absorbantes (PML), July 2nd 2019
- Julien Diaz : Soumaya Oueslati (Université de Cergy-Pontoise), "A new variational formulation for electromagnetic scattering problem using integral method with high order impedance boundary condition – Small perturbation of an interface for Stokes system", PhD thesis, June 12th 2019
- Julien Diaz : Aurélien Citrain (Insa de Rouen), "Méthode d'éléments finis hybride pour la simulation des ondes sismiques : couplage des discrétisations Galerkine Discontinue et éléments spectraux", PhD thesis, December 16th 2019
- Sébastien Tordeux : Pierre Schickele (Université de Toulouse),"Modélisation de l'émission EM de faisceaux de câbles complexes dans un environnement 3D", december 18th 2019

10.3. Popularization

10.3.1. Interventions

- Justine Labat participated in scientific 'speed datings' during the 'Filles et Maths' day at Pau in February 2019.
- Juliette Chabassier participated to the festival Club Med'iation in May 2019.
- Juliette Chabassier participated to many interventions of Louis 14.0, a scientific and artistic show.
- Juliette Chabassier animated a workshop around the virtual piano in La Couronne in Nov 2019.
- Juliette Chabassier, Augustin Ernoult and Alexis Thibault participated to the "Articulations workshop" in Dec 2019.
- Juliette Chabassier participated to a workshop around the Meta-Piano-Teq with Jean Haury in Dec 2019.
- Sébastien Tordeux gave a talk on numerical analysis in the Cercle Sofia Kovalevskaïa of Toulouse in May 2019
- Sébastien Tordeux was member of the judging comittee for the "Tournois Français des Jeunes Mathématiciennes et Mathématiciens" in May 2019

10.3.2. Creation of media or tools for science outreach

Juliette Chabassier co-created with the Ensemble Les Précieuses the show Louis 14.0 that presents how ancient instruments can be restored via numerical techniques, and played in real time in a musical and theatral show.

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Major publications by the team in recent years

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[10] J. LABAT.*Modélisation multi-échelle de la diffraction des ondes électromagnétiques par de petits obstacles*, UPPA, 2019

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[11] G. ALESSANDRINI, M. V. DE HOOP, F. FAUCHER, R. GABURRO, E. SINCICH.*Inverse problem for the Helmholtz equation with Cauchy data: reconstruction with conditional well-posedness driven iterative regularization*, in "ESAIM: Mathematical Modelling and Numerical Analysis", May 2019, vol. 53, n^o 3, p. 1005-1030 [*DOI :* 10.1051/M2AN/2019009], https://hal.archives-ouvertes.fr/hal-02168474

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[23] B. FABRE, P. DE LA CUADRA, A. ERNOULT.*How do flute players adapt their control to modifications of the flute bore ?*, in "ISMA 2019 - International Symposium on Music Acoustics", Detmold, Germany, September 2019, https://hal.archives-ouvertes.fr/hal-02428022

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Project-Team MANAO

Melting the frontiers between Light, Shape and Matter

IN COLLABORATION WITH: Laboratoire Bordelais de Recherche en Informatique (LaBRI)

IN PARTNERSHIP WITH:
CNRS

Université de Bordeaux

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Interaction and visualization

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Creation of the Team: 2012 January 01, updated into Project-Team: 2014 July 01

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A5.1.6. - Tangible interfaces
A5.3.5. - Computational photography
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2. Overall Objectives

2.1. General Introduction

Computer generated images are ubiquitous in our everyday life. Such images are the result of a process that has seldom changed over the years: the optical phenomena due to the propagation of *light* in a 3D environment are simulated taking into account how light is scattered [51], [28] according to *shape* and *material* characteristics of objects. The **intersection of optics** (for the underlying laws of physics) and **computer science** (for its modeling and computational efficiency aspects) provides a unique opportunity to tighten the links between these domains in order to first improve the image generation process (computer graphics, optics and virtual reality) and next to develop new acquisition and display technologies (optics, mixed reality and machine vision).

Most of the time, light, shape, and matter properties are studied, acquired, and modeled separately, relying on realistic or stylized rendering processes to combine them in order to create final pixel colors. Such modularity, inherited from classical physics, has the practical advantage of permitting to reuse the same models in various contexts. However, independent developments lead to un-optimized pipelines and difficult-to-control solutions since it is often not clear which part of the expected result is caused by which property. Indeed, the most efficient solutions are most often the ones that **blur the frontiers between light, shape, and matter** to lead to specialized and optimized pipelines, as in real-time applications (like Bidirectional Texture Functions [61] and Light-Field rendering [26]). Keeping these three properties separated may lead to other problems. For instance:

- Measured materials are too detailed to be usable in rendering systems and data reduction techniques have to be developed [59], [62], leading to an inefficient transfer between real and digital worlds;
- It is currently extremely challenging (if not impossible) to directly control or manipulate the interactions between light, shape, and matter. Accurate lighting processes may create solutions that do not fulfill users' expectations;
- Artists can spend hours and days in modeling highly complex surfaces whose details will not be visible [82] due to inappropriate use of certain light sources or reflection properties.

Most traditional applications target human observers. Depending on how deep we take into account the specificity of each user, the requirement of representations, and algorithms may differ.

Auto-stereoscopy display ©Nintendo | HDR display ©Dolby Digital | Printing both geometry and material [43]

Figure 1. Examples of new display technologies. Nowadays, they are not limited to a simple array of 2D low-dynamic RGB values.

With the evolution of measurement and display technologies that go beyond conventional images (e.g., as illustrated in Figure 1, High-Dynamic Range Imaging [72], stereo displays or new display technologies [47], and physical fabrication [17], [35], [43]) the frontiers between real and virtual worlds are vanishing [31]. In this context, a sensor combined with computational capabilities may also be considered as another kind of observer. Creating separate models for light, shape, and matter for such an extended range of applications and observers is often inefficient and sometimes provides unexpected results. Pertinent solutions must be able to **take into account properties of the observer** (human or machine) and application goals.

2.2. Methodology

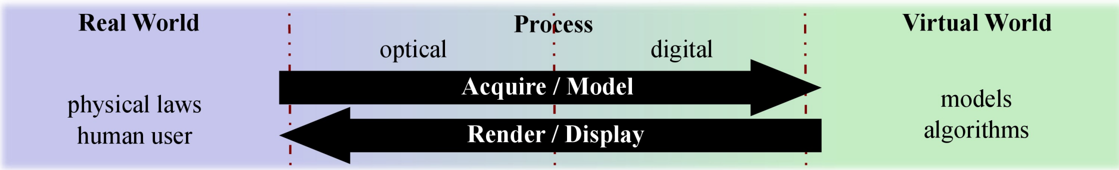


Figure 2. Interactions/Transfers between real and virtual worlds. One of our goal is to combine optical instruments with processes from computer science in order to blend the two worlds.

2.2.1. Using a global approach

The main goal of the *MANAO* project is to study phenomena resulting from the interactions between the three components that describe light propagation and scattering in a 3D environment: light, shape, and matter. Improving knowledge about these phenomena facilitates the adaption of the developed digital, numerical, and analytic models to specific contexts. This leads to the development of new analysis tools, new representations, and new instruments for acquisition, visualization, and display.

To reach this goal, we have to first increase our understanding of the different phenomena resulting from the interactions between light, shape, and matter. For this purpose, we consider how they are captured or perceived by the final observer, taking into account the relative influence of each of the three components. Examples include but are not limited to:

- The manipulation of light to reveal reflective [23] or geometric properties [88], as mastered by professional photographers;

- The modification of material characteristics or lighting conditions [89] to better understand shape features, for instance to decipher archaeological artifacts;
- The large influence of shape on the captured variation of shading [70] and thus on the perception of material properties [85].

Based on the acquired knowledge of the influence of each of the components, we aim at developing new models that combine two or three of these components. Examples include the modeling of Bidirectional Texture Functions (BTFs) [34] that encode in a unique representation effects of parallax, multiple light reflections, and also shadows without requiring to store separately the reflective properties and the meso-scale geometric details, or Light-Fields that are used to render 3D scenes by storing only the result of the interactions between light, shape, and matter both in complex real environments and in simulated ones.

One of the strengths of *MANAO* is that we are inter-connecting computer graphics and optics. On one side, the laws of physics are required to create images but may be bent to either increase performance or user's control: this is one of the key advantage of computer graphics approach. It is worth noticing that what is not possible in the real world may be possible in a digital world. However, on the other side, the introduced approximations may help to better comprehend the physical interactions of light, shape, and matter.

2.2.2. Taking observers into account

The *MANAO* project specifically aims at considering information transfer, first from the real world to the virtual world (acquisition and creation), then from computers to observers (visualization and display). For this purpose, we use a larger definition of what an observer is: it may be a human user or a physical sensor equipped with processing capabilities. Sensors and their characteristics must be taken into account in the same way as we take into account the human visual system in computer graphics. Similarly, computational capabilities may be compared to cognitive capabilities of human users. Some characteristics are common to all observers, such as the scale of observed phenomena. Some others are more specifics to a set of observers. For this purpose, we have identified two classes of applications.

- **Physical systems** Provided our partnership that leads to close relationships with optics, one novelty of our approach is to extend the range of possible observers to physical sensors in order to work on domains such as *simulation, mixed reality, and testing*. Capturing, processing, and visualizing complex data is now more and more accessible to everyone, leading to the possible convergence of real and virtual worlds through visual signals. This signal is traditionally captured by cameras. It is now possible to augment them by projecting (e.g., the infrared laser of Microsoft Kinect) and capturing (e.g., GPS localization) other signals that are outside the visible range. These supplemental information replace values traditionally extracted from standard images and thus lower down requirements in computational power [58]. Since the captured images are the result of the interactions between light, shape, and matter, the approaches and the improved knowledge from *MANAO* help in designing interactive acquisition and rendering technologies that are required to merge the real and the virtual world. With the resulting unified systems (optical and digital), transfer of pertinent information is favored and inefficient conversion is likely avoided, leading to new uses in interactive computer graphics applications, like augmented reality [22], [31] and computational photography [71].
- **Interactive visualization** This direction includes domains such as *scientific illustration and visualization, artistic or plausible rendering*. In all these cases, the observer, a human, takes part in the process, justifying once more our focus on real-time methods. When targeting average users, characteristics as well as limitations of the human visual system should be taken into account: in particular, it is known that some configurations of light, shape, and matter have masking and facilitation effects on visual perception [82]. For specialized applications, the expertise of the final user and the constraints for 3D user interfaces lead to new uses and dedicated solutions for models and algorithms.

3. Research Program

3.1. Related Scientific Domains

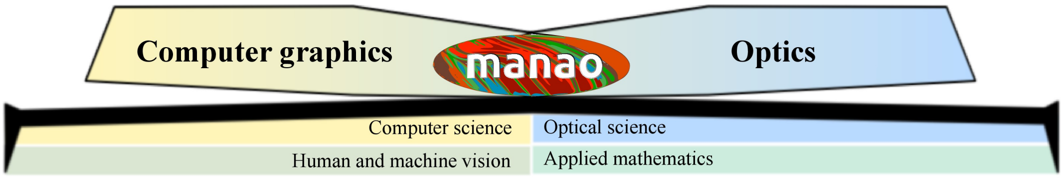


Figure 3. Related scientific domains of the MANAO project.

The *MANAO* project aims at studying, acquiring, modeling, and rendering the interactions between the three components that are light, shape, and matter from the viewpoint of an observer. As detailed more lengthily in the next section, such a work will be done using the following approach: first, we will tend to consider that these three components do not have strict frontiers when considering their impacts on the final observers; then, we will not only work in **computer graphics**, but also at the intersection of computer graphics and **optics**, exploring the mutual benefits that the two domains may provide. It is thus intrinsically a **transdisciplinary** project (as illustrated in Figure 3) and we expect results in both domains.

Thus, the proposed team-project aims at establishing a close collaboration between computer graphics (e.g., 3D modeling, geometry processing, shading techniques, vector graphics, and GPU programming) and optics (e.g., design of optical instruments, and theories of light propagation). The following examples illustrate the strengths of such a partnership. First, in addition to simpler radiative transfer equations [36] commonly used in computer graphics, research in the later will be based on state-of-the-art understanding of light propagation and scattering in real environments. Furthermore, research will rely on appropriate instrumentation expertise for the measurement [48], [49] and display [47] of the different phenomena. Reciprocally, optics researches may benefit from the expertise of computer graphics scientists on efficient processing to investigate interactive simulation, visualization, and design. Furthermore, new systems may be developed by unifying optical and digital processing capabilities. Currently, the scientific background of most of the team members is related to computer graphics and computer vision. A large part of their work have been focused on simulating and analyzing optical phenomena as well as in acquiring and visualizing them. Combined with the close collaboration with the optics laboratory LP2N (http://www.lp2n.fr) and with the students issued from the "Institut d'Optique" (http://www.institutoptique.fr), this background ensures that we can expect the following results from the project: the construction of a common vocabulary for tightening the collaboration between the two scientific domains and creating new research topics. By creating this context, we expect to attract (and even train) more trans-disciplinary researchers.

At the boundaries of the *MANAO* project lie issues in **human and machine vision**. We have to deal with the former whenever a human observer is taken into account. On one side, computational models of human vision are likely to guide the design of our algorithms. On the other side, the study of interactions between light, shape, and matter may shed some light on the understanding of visual perception. The same kind of connections are expected with machine vision. On the one hand, traditional computational methods for acquisition (such as photogrammetry) are going to be part of our toolbox. On the other hand, new display technologies (such as the ones used for augmented reality) are likely to benefit from our integrated approach and systems. In the *MANAO* project we are mostly users of results from human vision. When required, some experimentation might be done in collaboration with experts from this domain, like with the European PRISM project. For machine vision, provided the tight collaboration between optical and digital systems, research will be carried out inside the *MANAO* project.

Analysis and modeling rely on **tools from applied mathematics** such as differential and projective geometry, multi-scale models, frequency analysis [38] or differential analysis [70], linear and non-linear approximation techniques, stochastic and deterministic integrations, and linear algebra. We not only rely on classical tools, but also investigate and adapt recent techniques (e.g., improvements in approximation techniques), focusing on their ability to run on modern hardware: the development of our own tools (such as Eigen) is essential to control their performances and their abilities to be integrated into real-time solutions or into new instruments.

3.2. Research axes

The *MANAO* project is organized around four research axes that cover the large range of expertise of its members and associated members. We briefly introduce these four axes in this section. More details and their inter-influences that are illustrated in the Figure 2 will be given in the following sections.

Axis 1 is the theoretical foundation of the project. Its main goal is to increase the understanding of light, shape, and matter interactions by combining expertise from different domains: optics and human/machine vision for the analysis and computer graphics for the simulation aspect. The goal of our analyses is to identify the different layers/phenomena that compose the observed signal. In a second step, the development of physical simulations and numerical models of these identified phenomena is a way to validate the pertinence of the proposed decompositions.

In Axis 2, the final observers are mainly physical captors. Our goal is thus the development of new acquisition and display technologies that combine optical and digital processes in order to reach fast transfers between real and digital worlds, in order to increase the convergence of these two worlds.

Axes 3 and 4 focus on two aspects of computer graphics: rendering, visualization and illustration in Axis 3, and editing and modeling (content creation) in Axis 4. In these two axes, the final observers are mainly human users, either generic users or expert ones (e.g., archaeologist [74], computer graphics artists).

3.3. Axis 1: Analysis and Simulation

Challenge: Definition and understanding of phenomena resulting from interactions between light, shape, and matter as seen from an observer point of view.

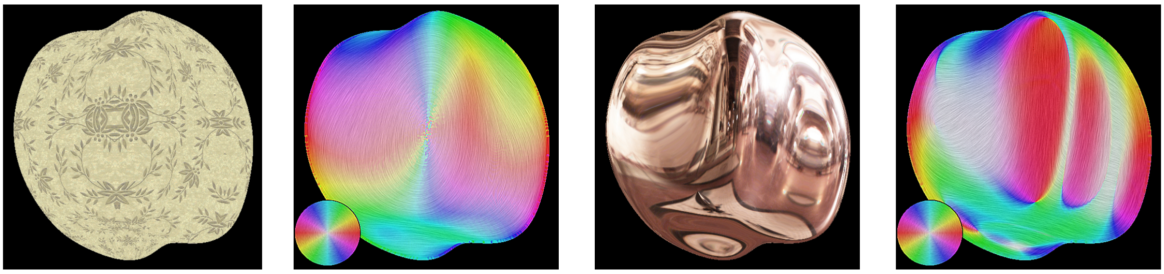
Results: Theoretical tools and numerical models for analyzing and simulating the observed optical phenomena.

To reach the goals of the *MANAO* project, we need to **increase our understanding** of how light, shape, and matter act together in synergy and how the resulting signal is finally observed. For this purpose, we need to identify the different phenomena that may be captured by the targeted observers. This is the main objective of this research axis, and it is achieved by using three approaches: the simulation of interactions between light, shape, and matter, their analysis and the development of new numerical models. This resulting improved knowledge is a foundation for the researches done in the three other axes, and the simulation tools together with the numerical models serve the development of the joint optical/digital systems in Axis 2 and their validation.

One of the main and earliest goals in computer graphics is to faithfully reproduce the real world, focusing mainly on light transport. Compared to researchers in physics, researchers in computer graphics rely on a subset of physical laws (mostly radiative transfer and geometric optics), and their main concern is to efficiently use the limited available computational resources while developing as fast as possible algorithms. For this purpose, a large set of theoretical as well as computational tools has been introduced to take a **maximum benefit of hardware** specificities. These tools are often dedicated to specific phenomena (e.g., direct or indirect lighting, color bleeding, shadows, caustics). An efficiency-driven approach needs such a classification of light paths [44] in order to develop tailored strategies [86]. For instance, starting from simple direct lighting, more complex phenomena have been progressively introduced: first diffuse indirect illumination [42], [78], then more generic inter-reflections [51], [36] and volumetric scattering [75], [33]. Thanks to this search for efficiency and this classification, researchers in computer graphics have developed a now recognized expertise in fast-simulation of light propagation. Based on finite elements (radiosity techniques) or on unbiased Monte

Carlo integration schemes (ray-tracing, particle-tracing, ...), the resulting algorithms and their combination are now sufficiently accurate to be used-back in physical simulations. The *MANAO* project will continue the search for **efficient and accurate simulation** techniques, but extending it from computer graphics to optics. Thanks to the close collaboration with scientific researchers from optics, new phenomena beyond radiative transfer and geometric optics will be explored.

Search for algorithmic efficiency and accuracy has to be done in parallel with **numerical models**. The goal of visual fidelity (generalized to accuracy from an observer point of view in the project) combined with the goal of efficiency leads to the development of alternative representations. For instance, common classical finite-element techniques compute only basis coefficients for each discretization element: the required discretization density would be too large and to computationally expensive to obtain detailed spatial variations and thus visual fidelity. Examples includes texture for decorrelating surface details from surface geometry and high-order wavelets for a multi-scale representation of lighting [32]. The numerical complexity explodes when considering directional properties of light transport such as radiance intensity (Watt per square meter and per steradian - $W.m^{-2}.sr^{-1}$), reducing the possibility to simulate or accurately represent some optical phenomena. For instance, Haar wavelets have been extended to the spherical domain [77] but are difficult to extend to non-piecewise-constant data [80]. More recently, researches prefer the use of Spherical Radial Basis Functions [83] or Spherical Harmonics [69]. For more complex data, such as reflective properties (e.g., BRDF [63], [52] - 4D), ray-space (e.g., Light-Field [60] - 4D), spatially varying reflective properties (6D - [73]), new models, and representations are still investigated such as rational functions [66] or dedicated models [20] and parameterizations [76], [81]. For each (newly) defined phenomena, we thus explore the space of possible numerical representations to determine the **most suited one for a given application**, like we have done for BRDF [66].



Texuring | 1st order gradient field | Environment reflection | 2st order gradient field

Figure 4. First-oder analysis [87] have shown that shading variations are caused by depth variations (first-order gradient field) and by normal variations (second-order fields). These fields are visualized using hue and saturation to indicate direction and magnitude of the flow respectively.

Before being able to simulate or to represent the different **observed phenomena**, we need to define and describe them. To understand the difference between an observed phenomenon and the classical light, shape, and matter decomposition, we can take the example of a highlight. Its observed shape (by a human user or a sensor) is the resulting process of the interaction of these three components, and can be simulated this way. However, this does not provide any intuitive understanding of their relative influence on the final shape: an artist will directly describe the resulting shape, and not each of the three properties. We thus want to decompose the observed signal into models for each scale that can be easily understandable, representable, and manipulable. For this purpose, we will rely on the **analysis** of the resulting interaction of light, shape, and matter as observed by a human or a physical sensor. We first consider this analysis from an **optical point of view**, trying to identify the different phenomena and their scale according to their mathematical properties (e.g., differential [70] and frequency analysis [38]). Such an approach has leaded us to exhibit the influence of surfaces flows (depth and normal gradients) into lighting pattern deformation (see Figure 4). For a **human observer**, this correspond to one recent trend in computer graphics that takes into account the human visual systems [39] both to evaluate the results and to guide the simulations.

3.4. Axis 2: From Acquisition to Display

Challenge: Convergence of optical and digital systems to blend real and virtual worlds.

Results: Instruments to acquire real world, to display virtual world, and to make both of them interact.

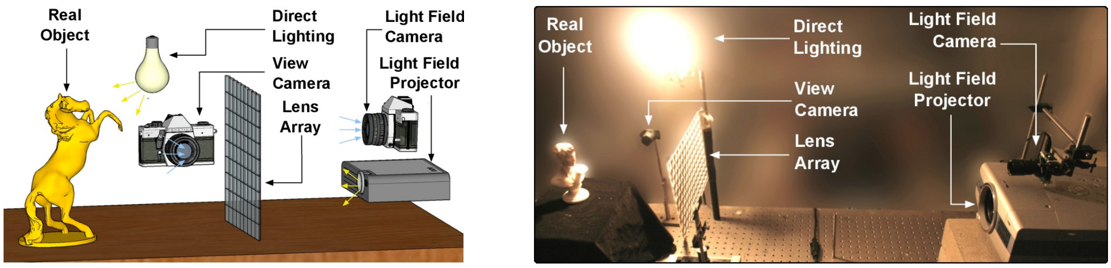


Figure 5. Light-Field transfer: global illumination between real and synthetic objects [31]

In this axis, we investigate *unified acquisition and display systems*, that is systems which combine optical instruments with digital processing. From digital to real, we investigate new display approaches [60], [47]. We consider projecting systems and surfaces [27], for personal use, virtual reality and augmented reality [22]. From the real world to the digital world, we favor direct measurements of parameters for models and representations, using (new) optical systems unless digitization is required [41], [40]. These resulting systems have to acquire the different phenomena described in Axis 1 and to display them, in an efficient manner [45], [21], [46], [49]. By efficient, we mean that we want to shorten the path between the real world and the virtual world by increasing the data bandwidth between the real (analog) and the virtual (digital) worlds, and by reducing the latency for real-time interactions (we have to prevent unnecessary conversions, and to reduce processing time). To reach this goal, the systems have to be designed as a whole, not by a simple concatenation of optical systems and digital processes, nor by considering each component independently [50].

To increase data bandwidth, one solution is to **parallelize more and more the physical systems**. One possible solution is to multiply the number of simultaneous acquisitions (e.g., simultaneous images from multiple viewpoints [49], [68]). Similarly, increasing the number of viewpoints is a way toward the creation of full 3D displays [60]. However, full acquisition or display of 3D real environments theoretically requires a continuous field of viewpoints, leading to huge data size. Despite the current belief that the increase of computational power will fill the missing gap, when it comes to visual or physical realism, if you double the processing power, people may want four times more accuracy, thus increasing data size as well. To reach the best performances, a trade-off has to be found between the amount of data required to represent accurately the reality and the amount of required processing. This trade-off may be achieved using **compressive sensing**. Compressive sensing is a new trend issued from the applied mathematics community that provides tools to accurately reconstruct a signal from a small set of measurements assuming that it is sparse in a transform domain (e.g., [67], [92]).

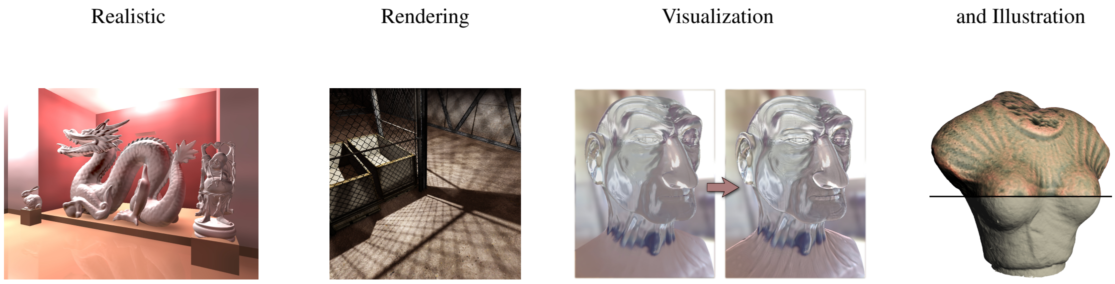
We prefer to achieve this goal by avoiding as much as possible the classical approach where acquisition is followed by a fitting step: this requires in general a large amount of measurements and the fitting itself may consume consequently too much memory and preprocessing time. By **preventing unnecessary conversion** through fitting techniques, such an approach increase the speed and reduce the data transfer for acquisition but also for display. One of the best recent examples is the work of Cossairt et al. [31]. The whole system is designed around a unique representation of the energy-field issued from (or leaving) a 3D object, either virtual or real: the Light-Field. A Light-Field encodes the light emitted in any direction from any position on an object. It is acquired thanks to a lens-array that leads to the capture of, and projection from, multiple simultaneous viewpoints. A unique representation is used for all the steps of this system. Lens-arrays, parallax barriers, and coded-aperture [57] are one of the key technologies to develop such acquisition (e.g., Light-Field camera [0] [50] and acquisition of light-sources [41]), projection systems (e.g., auto-stereoscopic displays). Such an approach is versatile and may be applied to improve classical optical instruments [55]. More generally, by designing unified optical and digital systems [64], it is possible to leverage the requirement of processing power, the memory footprint, and the cost of optical instruments.

Those are only some examples of what we investigate. We also consider the following approaches to develop new unified systems. First, similar to (and based on) the analysis goal of Axis 1, we have to take into account as much as possible the characteristics of the measurement setup. For instance, when fitting cannot be avoided, integrating them may improve both the processing efficiency and accuracy [66]. Second, we have to integrate signals from multiple sensors (such as GPS, accelerometer, ...) to prevent some computation (e.g., [58]). Finally, the experience of the group in surface modeling help the design of optical surfaces [53] for light sources or head-mounted displays.

3.5. Axis 3: Rendering, Visualization and Illustration

Challenge: How to offer the most legible signal to the final observer in real-time?

Results: High-level shading primitives, expressive rendering techniques for object depiction, real-time realistic rendering algorithms



(a) Global illumination [65] (b) Shadows [93] (c) Shape enhancement [89] (d) Shape depiction [19]

Figure 6. In the MANAO project, we are investigating rendering techniques from realistic solutions (e.g., inter-reflections (a) and shadows (b)) to more expressive ones (shape enhancement (c) with realistic style and shape depiction (d) with stylized style) for visualization.

The main goal of this axis is to offer to the final observer, in this case mostly a human user, the most legible signal in real-time. Thanks to the analysis and to the decomposition in different phenomena resulting from interactions between light, shape, and matter (Axis 1), and their perception, we can use them to convey essential information in the most pertinent way. Here, the word *pertinent* can take various forms depending on the application.

In the context of scientific illustration and visualization, we are primarily interested in tools to convey shape or material characteristics of objects in animated 3D scenes. **Expressive rendering** techniques (see Figure 6c,d) provide means for users to depict such features with their own style. To introduce our approach, we detail it from a shape-depiction point of view, domain where we have acquired a recognized expertise. Prior work in this area mostly focused on stylization primitives to achieve line-based rendering [90], [54] or stylized shading [25], [89] with various levels of abstraction. A clear representation of important 3D **object features** remains a

[0]Lytro, http://www.lytro.com/

major challenge for better shape depiction, stylization and abstraction purposes. Most existing representations provide only local properties (e.g., curvature), and thus lack characterization of broader shape features. To overcome this limitation, we are developing higher level descriptions of shape [18] with increased robustness to sparsity, noise, and outliers. This is achieved in close collaboration with Axis 1 by the use of higher-order local fitting methods, multi-scale analysis, and global regularization techniques. In order not to neglect the observer and the material characteristics of the objects, we couple this approach with an analysis of the appearance model. To our knowledge, this is an approach which has not been considered yet. This research direction is at the heart of the *MANAO* project, and has a strong connection with the analysis we plan to conduct in Axis 1. Material characteristics are always considered at the light ray level, but an understanding of **higher-level primitives** (like the shape of highlights and their motion) would help us to produce more legible renderings and permit novel stylizations; for instance, there is no method that is today able to create stylized renderings that follow the motion of highlights or shadows. We also believe such tools also play a fundamental role for geometry processing purposes (such as shape matching, reassembly, simplification), as well as for editing purposes as discussed in Axis 4.

In the context of **real-time photo-realistic rendering** ((see Figure 6a,b), the challenge is to compute the most plausible images with minimal effort. During the last decade, a lot of work has been devoted to design approximate but real-time rendering algorithms of complex lighting phenomena such as soft-shadows [91], motion blur [38], depth of field [79], reflexions, refractions, and inter-reflexions. For most of these effects it becomes harder to discover fundamentally new and faster methods. On the other hand, we believe that significant speedup can still be achieved through more clever use of **massively parallel architectures** of the current and upcoming hardware, and/or through more clever tuning of the current algorithms. In particular, regarding the second aspect, we remark that most of the proposed algorithms depend on several parameters which can be used to **trade the speed over the quality**. Significant speed-up could thus be achieved by identifying effects that would be masked or facilitated and thus devote appropriate computational resources to the rendering [56], [37]. Indeed, the algorithm parameters controlling the quality vs speed are numerous without a direct mapping between their values and their effect. Moreover, their ideal values vary over space and time, and to be effective such an auto-tuning mechanism has to be extremely fast such that its cost is largely compensated by its gain. We believe that our various work on the analysis of the appearance such as in Axis 1 could be beneficial for such purpose too.

Realistic and real-time rendering is closely related to Axis 2: real-time rendering is a requirement to close the loop between real world and digital world. We have to thus develop algorithms and rendering primitives that allow the integration of the acquired data into real-time techniques. We have also to take care of that these real-time techniques have to work with new display systems. For instance, stereo, and more generally multi-view displays are based on the multiplication of simultaneous images. Brute force solutions consist in independent rendering pipeline for each viewpoint. A more energy-efficient solution would take advantages of the computation parts that may be factorized. Another example is the rendering techniques based on image processing, such as our work on augmented reality [29]. Independent image processing for each viewpoint may disturb the feeling of depth by introducing inconsistent information in each images. Finally, more dedicated displays [47] would require new rendering pipelines.

3.6. Axis 4: Editing and Modeling

Challenge: Editing and modeling appearance using drawing- or sculpting-like tools through high level representations.

Results: High-level primitives and hybrid representations for appearance and shape.

During the last decade, the domain of computer graphics has exhibited tremendous improvements in image quality, both for 2D applications and 3D engines. This is mainly due to the availability of an ever increasing amount of shape details, and sophisticated appearance effects including complex lighting environments. Unfortunately, with such a growth in visual richness, even so-called *vectorial* representations (e.g., subdivision surfaces, Bézier curves, gradient meshes, etc.) become very dense and unmanageable for the end user who has to deal with a huge mass of control points, color labels, and other parameters. This is becoming a major challenge, with a necessity for novel representations. This Axis is thus complementary of Axis 3: the focus is the development of primitives that are easy to use for modeling and editing.

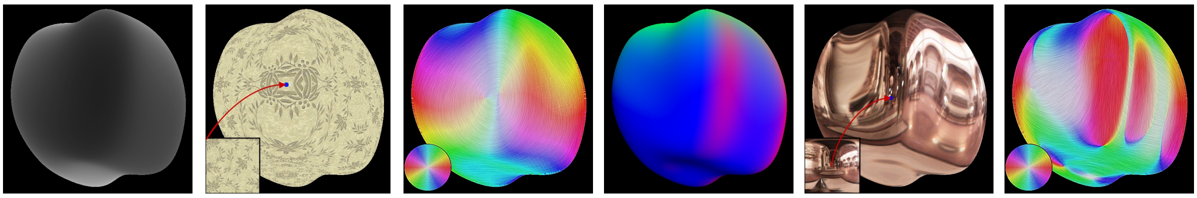
More specifically, we plan to investigate *vectorial representations* that would be amenable to the production of rich shapes with a minimal set of primitives and/or parameters. To this end we plan to build upon our insights on dynamic local reconstruction techniques and implicit surfaces [30] [24]. When working in 3D, an interesting approach to produce detailed shapes is by means of procedural geometry generation. For instance, many natural phenomena like waves or clouds may be modeled using a combination of procedural functions. Turning such functions into triangle meshes (main rendering primitives of GPUs) is a tedious process that appears not to be necessary with an adapted vectorial shape representation where one could directly turn procedural functions into implicit geometric primitives. Since we want to prevent unnecessary conversions in the whole pipeline (here, between modeling and rendering steps), we will also consider *hybrid representations* mixing meshes and implicit representations. Such research has thus to be conducted while considering the associated editing tools as well as performance issues. It is indeed important to keep *real-time performance* (cf. Axis 2) throughout the interaction loop, from user inputs to display, via editing and rendering operations. Finally, it would be interesting to add *semantic information* into 2D or 3D geometric representations. Semantic geometry appears to be particularly useful for many applications such as the design of more efficient manipulation and animation tools, for automatic simplification and abstraction, or even for automatic indexing and searching. This constitutes a complementary but longer term research direction.

In the *MANAO* project, we want to investigate representations beyond the classical light, shape, and matter decomposition. We thus want to directly control the appearance of objects both in 2D and 3D applications (e.g., [84]): this is a core topic of computer graphics. When working with 2D vector graphics, digital artists must carefully set up color gradients and textures: examples range from the creation of 2D logos to the photo-realistic imitation of object materials. Classic vector primitives quickly become impractical for creating illusions of complex materials and illuminations, and as a result an increasing amount of time and skill is required. This is only for still images. For animations, vector graphics are only used to create legible appearances composed of simple lines and color gradients. There is thus a need for more complex primitives that are able to accommodate complex reflection or texture patterns, while keeping the ease of use of vector graphics. For instance, instead of drawing color gradients directly, it is more advantageous to draw flow lines that represent local surface concavities and convexities. Going through such an intermediate structure then allows to deform simple material gradients and textures in a coherent way (see Figure 7), and animate them all at once. The manipulation of 3D object materials also raises important issues. Most existing material models are tailored to faithfully reproduce physical behaviors, not to be *easily controllable* by artists. Therefore artists learn to tweak model parameters to satisfy the needs of a particular shading appearance, which can quickly become cumbersome as the complexity of a 3D scene increases. We believe that an alternative approach is required, whereby material appearance of an object in a typical lighting environment is directly input (e.g., painted or drawn), and adapted to match a plausible material behavior. This way, artists will be able to create their own appearance (e.g., by using our shading primitives [84]), and replicate it to novel illumination environments and 3D models. For this purpose, we will rely on the decompositions and tools issued from Axis 1.

4. Application Domains

4.1. Physical Systems

Given our close relationships with researchers in optics, one novelty of our approach is to extend the range of possible observers to physical sensors in order to work on domains such as simulation, mixed reality, and testing. Capturing, processing, and visualizing complex data is now more and more accessible to everyone, leading to the possible convergence of real and virtual worlds through visual signals. This signal is traditionally captured by cameras. It is now possible to augment them by projecting (e.g., the infrared laser of Microsoft Kinect) and capturing (e.g., GPS localization) other signals that are outside the visible



(a) (b) (c) (d) (e) (f)

Figure 7. Based on our analysis [87] (Axis 1), we have designed a system that mimics texture (left) and shading (right) effects using image processing alone. It takes depth (a) and normal (d) images as input, and uses them to deform images (b-e) in ways that closely approximate surface flows (c-f). It provides a convincing, yet artistically controllable illusion of 3D shape conveyed through texture or shading cues.

range. This supplemental information replaces values traditionally extracted from standard images and thus lowers down requirements in computational power. Since the captured images are the result of the interactions between light, shape, and matter, the approaches and the improved knowledge from *MANAO* help in designing interactive acquisition and rendering technologies that are required to merge the real and the virtual worlds. With the resulting unified systems (optical and digital), transfer of pertinent information is favored and inefficient conversion is likely avoided, leading to new uses in interactive computer graphics applications, like **augmented reality**, **displays** and **computational photography**.

4.2. Interactive Visualization and Modeling

This direction includes domains such as **scientific illustration and visualization**, **artistic or plausible rendering**, and **3D modeling**. In all these cases, the observer, a human, takes part in the process, justifying once more our focus on real-time methods. When targeting average users, characteristics as well as limitations of the human visual system should be taken into account: in particular, it is known that some configurations of light, shape, and matter have masking and facilitation effects on visual perception. For specialized applications (such as archeology), the expertise of the final user and the constraints for 3D user interfaces lead to new uses and dedicated solutions for models and algorithms.

5. Highlights of the Year

5.1. Highlights of the Year

5.1.1. Public exhibitions

Textile(s) 3D, exhibition at the Musée Ethnographique de Bordeaux (MEB), until May 29th, 2020: measurement and reproduction of textiles.

The program has targeted the faithful reproduction of the appearance of fragile textiles. To this end, an optical appearance measurement setup has been developped and installed in the basement of the museum. Several textiles have been measured, including ancient asian textiles from the MEB collection; the originals along with their digital reproduction have been shown to the visitors of the museum.

5.1.2. Demonstration

SID Display Week I-Zone, San José Convention Center, May 14-16, 2019: Prototype of an autostereoscopic transparent display

We have showcased a 5-view, full-color, autostereoscopic transparent display prototype that we have developed [8], [13]. Its solution is much like a window that is able to superimpose autostereoscopic 3D data over the real world without the need of any wearables. There are many potential applications in augmented reality and head-up display fields; for example, in automotive, advertisement, and educational areas.

6. New Software and Platforms

6.1. Eigen

KEYWORD: Linear algebra

FUNCTIONAL DESCRIPTION: Eigen is an efficient and versatile C++ mathematical template library for linear algebra and related algorithms. In particular it provides fixed and dynamic size matrices and vectors, matrix decompositions (LU, LLT, LDLT, QR, eigenvalues, etc.), sparse matrices with iterative and direct solvers, some basic geometry features (transformations, quaternions, axis-angles, Euler angles, hyperplanes, lines, etc.), some non-linear solvers, automatic differentiations, etc. Thanks to expression templates, Eigen provides a very powerful and easy to use API. Explicit vectorization is performed for the SSE, AltiVec and ARM NEON instruction sets, with graceful fallback to non-vectorized code. Expression templates allow to perform global expression optimizations, and to remove unnecessary temporary objects.

RELEASE FUNCTIONAL DESCRIPTION: In 2017, we released three revisions of the 3.3 branch with few fixes of compilation and performance regressions, some doxygen documentation improvements, and the addition of transpose, adjoint, conjugate methods to SelfAdjointView to ease writing generic code.

- Participant: Gaël Guennebaud
- Contact: Gaël Guennebaud
- URL: http://eigen.tuxfamily.org/

6.2. Spectral Viewer

KEYWORD: Image

FUNCTIONAL DESCRIPTION: An open-source (spectral) image viewer that supports several images formats: ENVI (spectral), exr, png, jpg.

- Partner: LP2N (CNRS - UMR 5298)
- Contact: Romain Pacanowski
- URL: https://adufay.gitlabpages.inria.fr/SpectralViewer/index.html

6.3. otmap

C++ optimal transport solver on 2D grids

KEYWORDS: Optimal transportation - Eigen - C++ - Image processing - Numerical solver

FUNCTIONAL DESCRIPTION: This is a lightweight implementation of "Instant Transport Maps on 2D Grids".

It currently supports L2-optimal maps from an arbitrary density defined on a uniform 2D grid (aka an image) to a square with uniform density. Inverse maps and maps between pairs of arbitrary images are then recovered through numerical inversion and composition resulting in density preserving but approximately optimal maps.

This code also includes with 3 mini applications:

- otmap: computes the forward and backward maps between one image and a uniform square or between a pair of images. The maps are exported as .off quad meshes. - stippling: adapt a uniformly distributed point cloud to a given image. - barycenters: computes linear (resp. bilinear) approximate Wasserstein barycenters between a pair (resp. four) images.

- Contact: Gaël Guennebaud

7. New Results

7.1. Analysis and Simulation

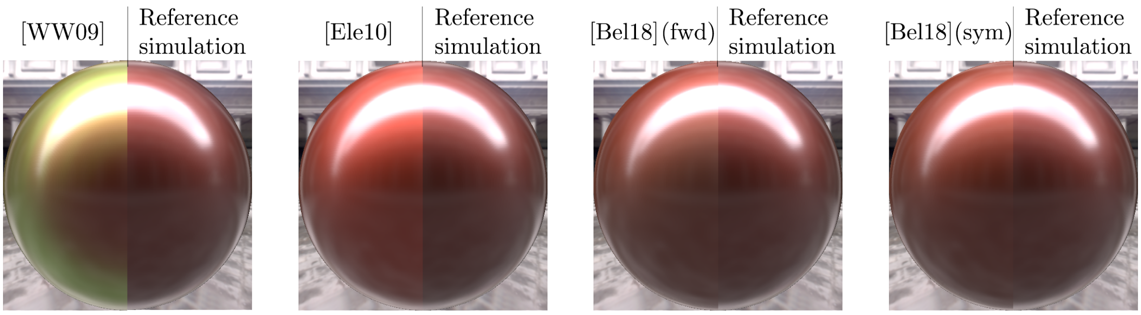


Figure 8. We study how the approximations made by layered material models impact their accuracy, and ultimately material appearance. Here we compare four models side by side with our reference simulation on a frosted metal – one of the 60 material configurations we have considered in our study. This specific choice is particularly problematic for the model of Weidlich and Wilkie [WW09], which creates oddly-colored reflections away from normal incidence. The variant of Elek [Ele10] is devoid of these artefacts, but clearly overestimates the intensity of the metallic base. Belcour's models [Bel18] (forward and symmetric) produce more accurate results, even though the intensity of the metallic base remains slightly higher. They still deviate from the reference simulation, especially at grazing angles as seen for instance at the bottom of the spheres. Our analysis in BRDF (and BTDF) space provides explanations for such departures from the reference.

7.1.1. Numerical Analysis of Layered Materials Models ,

Publications: [12], [14]

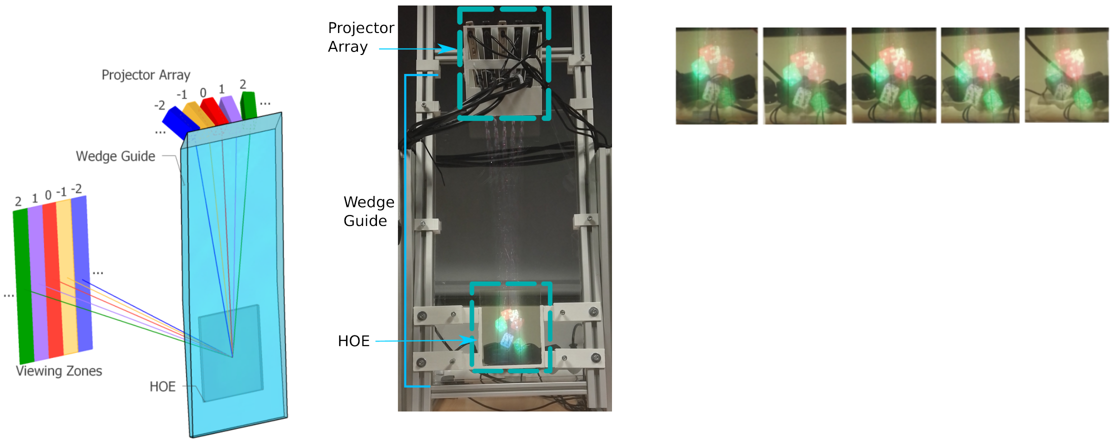
Most real-world materials are composed of multiple layers, whose physical properties impact the appearance of objects. The accurate reproduction of layered material properties is thus an important part of physically-based rendering applications. Since no exact analytical model exists for arbitrary configurations of layer stacks, available models make a number of approximations. In this technical report, we propose to evaluate these approximations with a numerical approach: we simulate BRDFs and BTDFs for layered materials in order to compare existing models against a common reference. More specifically, we consider 60 layered material configurations organized in three categories: plastics, metals and transparent slabs. Our results (see Figure 8) show that: (1) no single model systematically outperforms the others on all categories; and (2) significant discrepancies remain between simulated and modeled materials. We analyse the reasons for these discrepancies and introduce immediate corrections that improve models accuracy with little effort. Finally, we provide a few challenging cases for future layered material models.

7.1.2. A systematic approach to testing and predicting light-material interactions

Publication: [11]

Photographers and lighting designers set up lighting environments that best depict objects and human figures to convey key aspects of the visual appearance of various materials, following rules drawn from experience. Understanding which lighting environment is best adapted to convey which key aspects of materials is an important question in the field of human vision. The endless range of natural materials and lighting environments poses a major problem in this respect. Here we present a systematic approach to make this problem tractable for lighting–material interactions, using optics-based models composed of canonical lighting and material modes. In two psychophysical experiments, different groups of inexperienced observers judged the material qualities of the objects depicted in the stimulus images. In the first experiment, we took photographs of real objects as stimuli under canonical lightings. In a second experiment, we selected three generic natural lighting environments on the basis of their predicted lighting effects and made computer renderings of the objects. The selected natural lighting environments have characteristics similar to the canonical lightings, as computed using a spherical harmonic analysis. Results from the two experiments correlate strongly, showing (a) how canonical material and lighting modes associate with perceived material qualities; and (b) which lighting is best adapted to evoke perceived material qualities, such as softness, smoothness, and glossiness. Our results demonstrate that a system of canonical modes spanning the natural range of lighting and materials provides a good basis to study lighting–material interactions in their full natural ecology.

7.2. From Acquisition to Display



(a) Illustration (b) Photograph (c) 5 views

Figure 9. The autostereoscopic transparent display: light beams from multiple laser beam steering picoprojectors are coupled into a transparent wedge guide, and then the light from each projector is redirected to separate viewing zones using a transparent HOE.

7.2.1. Autostereoscopic transparent display using a wedge light guide and a holographic optical element

Publications: [8], [13]

We designed and developed a novel transparent autostereoscopic display consisting of laser picoprojectors, a wedge light guide, and a custom holographic optical element (HOE). Such a display can superimpose 3D data on the real world without any wearable.

The principle of our display, as depicted in Figure 9, is to couple beams from multiple laser beam steering picoprojectors into a transparent wedge guide and then to redirect each beam to separate viewing zones using a transparent HOE. The HOE is wavelength-multiplexed for full-color efficiency, but only one angular grating is recorded and multiple viewing zones are reconstructed with several projector positions due to the high angular bandwidth. Our current prototype has 5 views but is theoretically able to generate 9 views. The views are located 50cm in front of the display, they are 3cm wide and 10cm high. These values are fixed once the HOE is recorded; they result from our choices and can be changed in the recording step.

This display has great potential for augmented reality applications such as augmented exhibitions in museums or shops, head-up displays for vehicles or aeronautics, and industrial maintenance, among others.

7.2.2. Wedge cameras for minimally invasive archaeology

Publication: [9]

Acquiring images of archaeological artifacts is an essential step for the study and preservation of cultural heritage. In constrained environments, traditional acquisition techniques may fail or be too invasive. We present an optical device including a camera and a wedge waveguide that is optimized for imaging within confined spaces in archeology. The major idea is to redirect light by total internal reflection to circumvent the lack of room, and to compute the final image from the raw data. We tested various applications onsite during an archaeological mission in Medamoud (Egypt). Our device was able to successfully record images of the underground from slim trenches, including underwater trenches, and between rocks composing a wall temple. Experts agreed that the acquired images were good enough to get useful information that cannot be obtained as easily with traditional techniques.

7.2.3. Study of contrast variations with depth in focused plenoptic cameras

Publication: [10]

A focused plenoptic camera has the ability to record and separate spatial and directional information of the incoming light. Combined with the appropriate algorithm, a 3D scene could be reconstructed from a single acquisition, over a depth range called plenoptic depth-of-field. We have studied the contrast variations with depth as a way to assess plenoptic depth-of-field. We take into account the impact of diffraction, defocus, and magnification on the resulting contrast. We measure the contrast directly on both simulated and acquired images. We demonstrate the importance of diffraction and magnification in the final contrast. Contrary to classical optics, the maximum of contrast is not centered around the main object plane, but around a shifted position, with a fast and nonsymmetric decrease of contrast.

7.2.4. Unifying the refocusing algorithms and parameterizations for traditional and focused plenoptic cameras

Publication: [16]

We propose a unique parameterization of the light rays in a plenoptic setup, allowing the development of a unique refocusing algorithm valid for any plenoptic configurations, based on this parameterization. With this method we aim at refocusing images at any distances from the camera, without previous discontinuity due to change of optical configuration. We aim to obtain reconstructed images visually similar to the results of the other algorithms, but quantitatively more accurate.

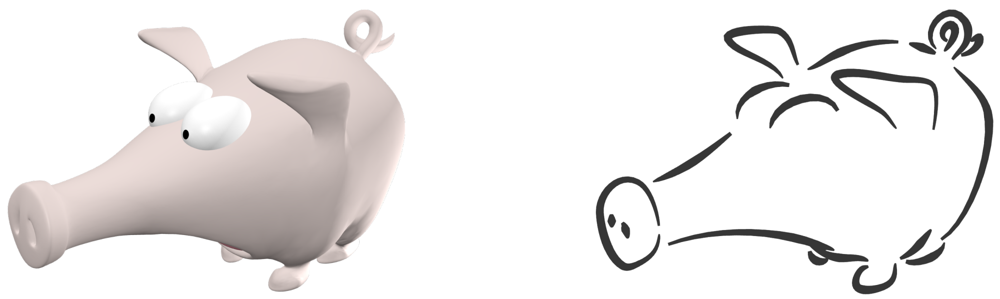
7.3. Rendering, Visualization and Illustration

7.3.1. Line drawings from 3D models: a tutorial

Publication: [7]

This tutorial describes the geometry and algorithms for generating line drawings from 3D models, focusing on occluding contours. The geometry of occluding contours on meshes and on smooth surfaces is described in detail, together with algorithms for extracting contours, computing their visibility, and creating stylized renderings and animations. Exact methods and hardware-accelerated fast methods are both described, and the trade-offs between different methods are discussed. The tutorial brings together and organizes material that, at present, is scattered throughout the literature. It also includes some novel explanations, and implementation tips. A thorough survey of the field of non-photorealistic 3D rendering is also included, covering other kinds of line drawings and artistic shading (Figure 10). In addition, we provide an interactive viewer at https://benardp.github.io/contours_viewer/.

7.4. Editing and Modeling



(a) 3D object with diffuse shading (b) Stylized curves

Figure 10. The occluding contours of the 3D model “Origins of the Pig” by Keenan Crane, shown in (a) with diffuse shading, are depicted in (b) with calligraphic brush strokes.

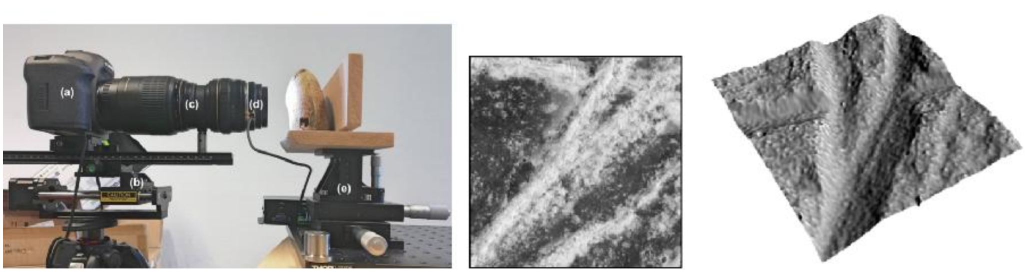


Figure 11. Left: our low-cost depth-from-focus acquisition setup. Right: result of our reconstruction algorithm for the sample shown in the middle image. The width of grooves are about 500 micrometers.

7.4.1. Depth from focus stacks at micrometer scale

In this work we designed a low-cost acquisition setup and a new algorithm for the digitalization of micro reliefs. The setup is based on a common digital camera equipped with a special assembly of different lenses designed to enable a $\times 2$ magnification factor with a very shallow depth of field (fig. 11). A micro-metric motor rail allows us to acquire dense focus stacks with depth information that can be reconstructed through image processing and analysis techniques. To enhance the accuracy of this reconstruction step, we designed novel focus estimators as well as novel focus-point analysis algorithms exploiting novel 3D invariants. Our initial results show that we are able to reconstruct depth maps with sub-step length accuracy.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

8.1.1. CIFRE PhD contract with Imaging Optics (2017-2020)

Participants: C. Herzog & X. Granier

For this project, we aim at developing 3 dimensions X-rays imaging techniques for medical applications.

9. Partnerships and Cooperations

9.1. National Initiatives

9.1.1. ANR

9.1.1.1. "Young Researcher" VIDA (2017-2021)

LP2N-CNRS-IOGS Inria
Leader R. Pacanowski (LP2N-CNRS-IOGS)
Participant P. Barla
This project aims at establishing a framework for direct and inverse design of material appearance for objects of complex shape. Since the manufacturing processes are always evolving, our goal is to establish a framework that is not tied to a fabrication stage.

9.1.1.2. MATERIALS (2015-2019)

MAVERICK, LP2N-CNRS (MANAO), Musée d'Ethnographie de Bordeaux, OCÉ-Print
Leader N. Holzschuch (MAVERICK)
Participant A. Lucat
Museums are operating under conflicting constraints: they have to preserve the artifacts they are storing, while making them available to the public and to researchers. Cultural artifacts are so fragile that simply exposing them to light degrades them. 3D scanning, combined with virtual reality and 3D printing has been used for the preservation and study of sculptures. The approach is limited: it acquires the geometry and the color, but not complex material properties. Current 3D printers are also limited in the range of colors they can reproduce. Our goal in this project is to address the entire chain of material acquisition and restitution. Our idea is to scan complex cultural artifacts, such as silk cloths, capturing all the geometry of their materials at the microscopic level, then reproduce them for study by public and researchers. Reproduction can be either done through 2.5D printing or virtual reality displays.

9.1.1.3. FOLD-Dyn (2017-2021)

IRIT, IMAGINE, MANAO, TeamTo, Mercenaries
Leader L. Barthe (IRIT)
Local Leader G. Guennebaud

The FOLD-Dyn project proposes the study of new theoretical approaches for the effective generation of virtual characters deformations, when they are animated. These deformations are two-folds: character skin deformations (skinning) and garment simulations. We propose to explore the possibilities offered by a novel theoretical way of addressing character deformations: the implicit skinning. This method jointly uses meshes and volumetric scalar functions. By improving the theoretical properties of scalar functions, the study of their joint use with meshes, and the introduction of a new approach and its formalism - called multi-layer 3D scalar functions - we aim at finding effective solutions allowing production studios to easily integrate in their pipeline plausible character deformations together with garment simulations.

9.1.1.4. CaLiTrOp (2017-2021)

IRIT, LIRIS, MANAO, MAVERICK
Leader: M. Paulin (IRIT)
Participant D. Murray
What is the inherent dimensionality, topology and geometry of light-paths space? How can we leverage this information to improve lighting simulation algorithms? These are the questions that this project wants to answer from a comprehensive functional analysis of light transport operators, with respect to the 3D scene's geometry and the reflectance properties of the objects, but also, to link operators with screen-space visual effects, with respect to the resulting picture.

9.2. International Research Visitors

9.2.1. Visits of International Scientists

Masatake Sawayama, Research Scientist, NTT Communication Science Laboratories, Japan (from March 2019 until October 2019)

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events: Selection

10.1.1.1. Member of the Conference Program Committees

Eurographics Workshop on Graphics and Cultural Heritage (GCH), Eurographics 2019, Eurographics Symposium on Rendering 2019 (EGSR), ACM Siggraph Asia 2019 talks and posters.

10.1.1.2. Reviewer

ACM Siggraph 2019, ACM Siggraph Asia 2019, ACM SIGGRAPH Symposium on Interactive 3D Graphics and Games 2019 (I3D), Eurographics Workshop on Graphics and Cultural Heritage (GCH), Pacific Graphics 2019, SIBGRAPI 2019.

10.1.2. Journal

10.1.2.1. Reviewer - Reviewing Activities

ACM Transactions on Graphics (TOG), Computer Graphics Forum (CGF), Computer and Graphics, ACM Journal on Computing and Cultural Heritage (JOCCH).

10.1.3. Invited Talks

Talk at the DYVITO workshop 2019, in Giessen, Germany.
Talk at the Shitsukan workshop 2019, in Kyoto, Japan.

10.1.4. Leadership within the Scientific Community

One member of the team is member of the Steering Board of the Eurographics Workshop on Graphics and Cultural Heritage.

10.1.5. Scientific Expertise

We review project submissions of the Horizon 2020 - Research and Innovation Action of the European Commission.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

The members of our team are involved in teaching computer science at University of Bordeaux and Institut d'Optique Graduate School (IOGS). General computer science is concerned, as well as the following graphics related topics:

Master : Pierre Bénard, Gaël Guennebaud, Advanced Image Synthesis, 50 HETD, M2, Univ. Bdx, France.

Master : Antoine Lucat, Simulations Radiométriques avancées, 20 HETD, M2, IOGS, France

Master : Gaël Guennebaud, Geometric Modeling, 31 HETD, M2, IOGS, France

Master : Gaël Guennebaud and Pierre Bénard, 3D Worlds, 60 HETD, M1, Univ. Bdx and IOGS, France.

Master : Pierre Bénard, Patrick Reuter, Virtual Reality, 20 HETD, M2, Univ. Bdx, France.

Master : Patrick Reuter, Graphical user interfaces and Spatial augmented reality seminars, M2, ESTIA, France.

Licence : Patrick Reuter, Digital Imaging, 30 HETD, L3, Univ. Bdx, France.

One member is also in charge of a field of study:

Master : Pierre Bénard, M2 “Informatique pour l'Image et le Son”, Univ de Bordeaux, France.

Pierre Bénard was also part of the education team of the DIU (Diplôme Inter-Universitaire) titled “Numérique et Sciences Informatiques” which is opened to secondary professors that are teaching Computer Science in high school. The first session took place during the last three weeks of June.

10.2.2. Supervision

PhD: Thomas Crespel, Optical and software tools for the design of a new transparent 3D display, Inria & Univ. Bordeaux, P. Reuter & X. Granier, 9 December 2019

PhD in progress: Antoine Lucat, Appearance Acquisition and Rendering, IOGS & Univ. Bordeaux, R. Pacanowski & X. Granier

PhD in progress: Charlotte Herzog, 3 dimensions X-rays imaging for medical applications, Imaging Optics, IOGS & Univ. Bordeaux, X. Granier

PhD in progress: Camille Brunel, Real-Time Animation and Deformation of 3D Characters, Inria & Univ. Bordeaux, P. Barla, G. Guennebaud & P. Bénard

PhD in progress: Megane Bati, Inverse Design for Complex Material Apperance, IOGS & Univ. Bordeaux, R. Pacanowski & P. Barla

PhD in progress: Charlie Schlick, Augmented reality with transparent multi-view screens, Inria & Univ. Bordeaux, P. Reuter

PhD in progress: Corentin Cou, Characterization of visual appearance for 3D restitution and exploration of monumental heritage, Inria & IOGS & CNRS/INHA, G. Guennebaud, X. Granier, M. Volait, R. Pacanowski.

10.2.3. Juries

PhD (jury member) : Johanna Delanoy, Université Côte d'Azur (June 4th).

PhD (jury member) : Fan Zhang, TU Delft, Netherlands (October 29th).

PhD (reviewer) : Xavier Chermain, Université de Limoges (November 27th).

Pierre Bénard was the president of a jury for the Professional Baccalauréat (June 4th and 9th).

10.3. Popularization

10.3.1. Interventions

- “Textile 3D” exhibition at the MEB (Musée Ethnographique de Bordeaux, from October 1st 2019 to May 29th 2020).
- During the national “Fête de la Science” event at Inria Bordeaux Sud-Ouest, Pierre Bénard gave a 30 minutes talk titled *L'art et la science des films d'animation 3D*, and Camille Brunel presented her background and Phd topic to schoolchildren (October 8th to 10th).
- During the national “Fête de la Science” event at Musée Ethnographique de Bordeaux, Pascal Barla helped organise a workshop for high school students on the topic of the appearance of textiles, in conjunction of the “Textile 3D” exhibition. With Mégane Bati, they have participated during the workshop as scientific animators (October 7th to 8th).
- We organized a Mini-forum 3D to gather Master students together with researches and companies from the Bordeaux area (November 19th).
- Pierre Bénard presented the team research activities to 3rd year Bachelor students from ENS Lyon (December 5th).

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Articles in International Peer-Reviewed Journal

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Project-Team MEMPHIS

Modeling Enablers for Multi-PHysics and InteractionS

IN PARTNERSHIP WITH:
Université de Bordeaux

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Numerical schemes and simulations

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Project-Team MEMPHIS

Creation of the Team: 2015 January 01, updated into Project-Team: 2016 October 01

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Anne-Laure Gautier [Inria, Administrative Assistant]

2. Overall Objectives

2.1. Multi-physics numerical modeling

We aim at a step change in multi-physics numerical modeling by developing two fundamental enablers:

- **reduced-order models**;
- **hierarchical Cartesian schemes**.

Reduced-order models (ROMs) are simplified mathematical models derived from the full set of PDEs governing the physics of the phenomenon of interest. ROMs can be obtained exploiting first principles or be data-driven. With ROMs one trades accuracy for speed and scalability, and counteracts the curse of dimensionality of traditional high-fidelity solvers by significantly reducing the computational complexity. ROMs represent an ideal building block for systems with real-time requirements, like interactive decision support systems that offer the possibility to rapidly explore various alternatives.

Hierarchical Cartesian schemes allow the multi-scale solution of PDEs on non body-fitted meshes with a drastic reduction of the computational setup overhead. These methods are easily parallelizable and they can efficiently be mapped to high-performance computer architectures. They avoid dealing with grid generation, a prohibitive task when the boundaries are moving and the topology is complex and unsteady.

3. Research Program

3.1. Reduced-order models

Massive parallelization and rethinking of numerical schemes will allow the use of mathematical models for a broader class of physical problems. For industrial applications, there is an increasing need for rapid and reliable numerical simulators to tackle design and control tasks. To provide a concrete example, in the design process of an aircraft, the flight conditions and manoeuvres, which provide the largest aircraft loads, are not known *a priori*. Therefore, the aerodynamic and inertial forces are calculated for a large number of conditions to give an estimate of the maximum loads, and hence stresses, that the structure of the detailed aircraft design might experience in service. As a result, the number of simulations required for a realistic design problem could easily be in the order of tens of millions. Even with simplistic models of the aircraft behavior this is an unfeasible number of separate simulations. However, engineering experience is used to identify the most likely critical load conditions, meaning that approximately hundreds of thousands simulations are required for conventional aircraft configurations. Furthermore, these analyses have to be repeated every time that there is an update in the aircraft structure.

Compared to existing approaches for ROMs [35], our interest will be focused on two axes. On the one hand, we start from the consideration that small, highly nonlinear scales are typically concentrated in limited spatial regions of the full simulation domain. So for example, in the flow past a wing, the highly non-linear phenomena take place in the proximity of the walls at the scale of a millimeter, for computational domains that are of the order of hundreds of meters. Based on these considerations, we propose in [31] a multi-scale model where the large scales are described by far-field models based on ROMs and the small scales are simulated by high-fidelity models. The whole point for this approach is to optimally decouple the far field from the near field.

A second characterizing feature of our ROM approach is non-linear interpolation. We start from the consideration that dynamical models derived from the projection of the PDE model in the reduced space are neither stable to numerical integration nor robust to parameter variation when hard non-linear multi-scale phenomena are considered.

However, thanks to Proper Orthogonal Decomposition (POD) [41], [47], [30] we can accurately approximate large solution databases using a low-dimensional base. Recent techniques to investigate the temporal evolution of the POD modes (Koopman modes [42], [28], Dynamic Mode Decomposition [45]) and allow a dynamic discrimination of the role played by each of them. This in turn can be exploited to interpolate between modes in parameter space, thanks to ideas relying on optimal transportation [50], [32] that we have started developing in the FP7 project FFAST and H2020 AEROGUST.

3.2. Hierarchical Cartesian schemes

We intend to conceive schemes that will simplify the numerical approximation of problems involving complex unsteady objects together with multi-scale physical phenomena. Rather than using extremely optimized but non-scalable algorithms, we adopt robust alternatives that bypass the difficulties linked to grid generation. Even if the mesh problem can be tackled today thanks to powerful mesh generators, it still represents a severe difficulty, in particular when highly complex unsteady geometries need to be dealt with. Industrial experience and common practice shows that mesh generation accounts for about 20% of overall analysis time, whereas creation of a simulation-specific geometry requires about 60%, and only 20% of overall time is actually devoted to analysis. The methods that we develop bypass the generation of tedious geometrical models by automatic implicit geometry representation and hierarchical Cartesian schemes.

The approach that we plan to develop combines accurate enforcement of unfitted boundary conditions with adaptive octree and overset grids. The core idea is to use an octree/overset mesh for the approximation of the solution fields, while the geometry is captured by level set functions [46], [40] and boundary conditions are imposed using appropriate interpolation methods [27], [49], [44]. This eliminates the need for boundary-conforming meshes that require time-consuming and error-prone mesh generation procedures, and opens the door for simulation of very complex geometries. In particular, it will be possible to easily import the industrial geometry and to build the associated level set function used for simulation.

Hierarchical octree grids offer several considerable advantages over classical adaptive mesh refinement for body-fitted meshes, in terms of data management, memory footprint and parallel HPC performance. Typically, when refining unstructured grids, like for example tetrahedral grids, it is necessary to store the whole data tree corresponding to successive subdivisions of the elements and eventually recompute the full connectivity graph. In the linear octree case that we develop, only the tree leaves are stored in a linear array, with a considerable memory advantage. The mapping between the tree leaves and the linear array as well as the connectivity graph is efficiently computed thanks to an appropriate space-filling curve. Concerning parallelization, linear octrees guarantee a natural load balancing thanks to the linear data structure, whereas classical unstructured meshes require sophisticated (and moreover time consuming) tools to achieve proper load distribution (SCOTCH, METIS etc.). Of course, using unfitted hierarchical meshes requires further development and analysis of methods to handle the refinement at level jumps in a consistent and conservative way, accuracy analysis for new finite-volume or finite-difference schemes, efficient reconstructions at the boundaries to recover appropriate accuracy and robustness. These subjects, that are currently virtually absent at Inria, are among the main scientific challenges of our team.

4. Application Domains

4.1. Energy conversion

4.1.1. Fluid-structure interaction

We apply the methods developed in our team to the domain of wind engineering and sea-wave converters. In Figure 1, we show results of a numerical model for a sea-wave energy converter. We here rely on a monolithic model to describe the interaction between the rigid floater, air and water; material properties such as densities, viscosities and rigidity vary across the domain. The appropriate boundary conditions are imposed at interfaces that arbitrarily cross the grid using adapted schemes built thanks to geometrical information computed via level set functions [46]. The background method for fluid-structure interface is the volume penalization method [27] where the level set functions is used to improve the degree of accuracy of the method [3] and also to follow the object. The underlined mathematical model is unsteady, and three dimensional; numerical simulations based on a grid with $\mathcal{O}(10^8)$ degrees of freedom are executed in parallel using 512 CPUs .

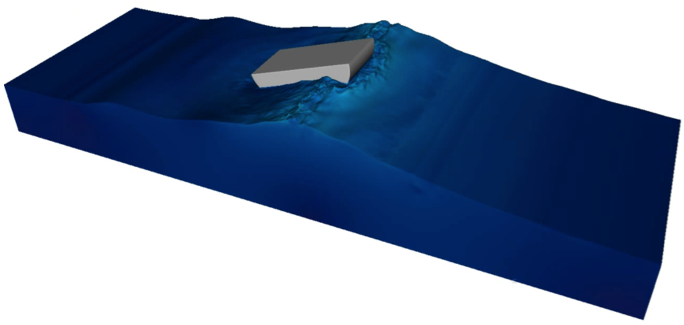

Figure 1. numerical modeling of a sea-wave converter by a monolithic model and Cartesian meshes.

In the context of the Aerogust (Aeroelastic gust modelling) European project, together with Valorem, we investigated the behavior of wind turbine blades under gust loading. The aim of the project was to optimize the design of wind turbine blades to maximize the power extracted. A meteorological mast (Figure 2(a)) has been installed in March 2017 in Brittany to measure wind on-site: data provided by the mast have been exploited to initialize the mathematical model. Due to the large cost of the full-order mathematical model, we relied on a simplified model [38] to optimize the global twist. Then, we validated the optimal configuration using the full-order Cartesian model based on the NaSCar solver. Figure 2(b) shows the flow around the optimized optimized wind turbine rotor.

4.1.2. Schemes for turbulent flow simulations using Octrees

We have initially developed and tested a 3D first-order Octree code for unsteady incompressible Navier-Stokes equations for full windmill simulations with an LES model and wall laws. We have validated this code on Occigen for complex flows at increasing Reynolds numbers. This step implied identifying stable and feasible schemes compatible with the parallel linear Octree structure. The validation has been conducted with respect to the results of a fully Cartesian code (NaSCAR) that we run on Turing (with significantly more degrees of freedom) and with respect to experimental results.

Figure 2. Aerogust project. Left: met mast after its installation. Right: flow around the optimized wind turbine rotor (as predicted by NaSCar).

Subsequently, we have developed a second-order Octree scheme that has been validated on Occigen for a sphere at a moderate Reynolds number ($\mathrm{Re} = 500$), see Table 1. Then, for a cylinder at ($\mathrm{Re} = 140000$) (Figures 3(a) and 3(b)), close to real applications, we have preliminary validation results for the second-order scheme with respect to experimental drag coefficient (Table 2). Additional resources will be asked on Occigen to complete the study.

Table 1. Flow past a sphere at Re =500. Results in the literature are spread between C D =0.48 and C D =0.52.

Mesh	Δx_{min}	number of cells	C_{D} (1^{st}-order scheme)	C_{D} (2^{nd}-order scheme)
1	0.094	$0.72 \cdot 10^5$	N.A.	0.526
2	0.047	$4.9 \cdot 10^5$	0.595	0.522
3	0.023	$4.7 \cdot 10^6$	0.546	0.492
4	0.012	$37.6 \cdot 10^6$	0.555	0.496

Table 2. Flow past a sphere at Re =14000.

Case	C_{D}
Octree, 1^{st}-order scheme	1.007
Octree, 2^{nd}-order scheme	1.157
Cartesian	1.188
Experimental estimate [34]	1.237

4.2. Vascular flows

A new research direction pursued by the team is the mathematical modelling of vascular blood flows in arteries. Together with the start-up Nurea (http://nurea-soft.com/) and the surgeon Eric Ducasse, we aim at developing reliable and automatic procedures for aneurysm segmentation and for the prediction of aneurysm rupture

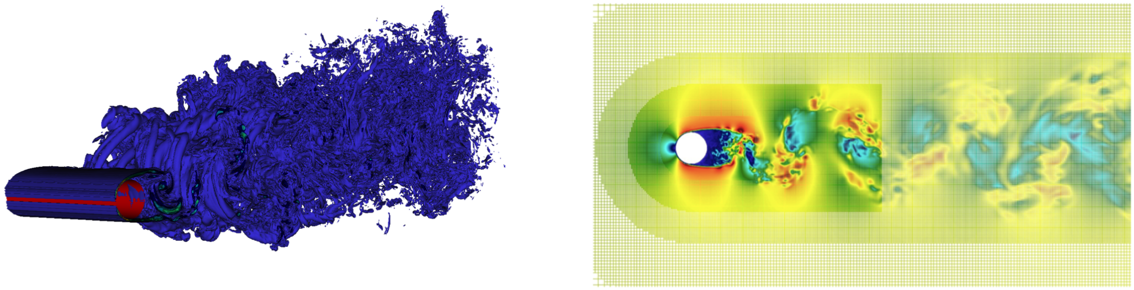

Figure 3. flow past a cylinder at $\mathrm{Re} = 140000$. *Left: vorticity contour lines. Right: streamwise velocity section and grid for the second-order Octree scheme.*

risk. Our approach exploits two sources of information: (i) numerical simulations of blood flows in complex geometries, based on an octree discretization, and (ii) computed tomography angiography (CTA) data. Figure 4 shows the force distribution on the walls of the abdominal aorta in presence of an aneurysm; results are obtained using a parallelized hierarchical Cartesian scheme based on octrees.

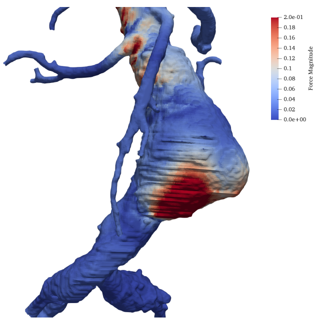

Figure 4. force distribution on the walls of the abdominal aorta in presence of an aneurysm.

4.3. Eulerian non-linear elasticity models

Mathematical and numerical modelling of continuum systems undergoing extreme regimes is challenging due to the presence of large deformations and displacements of the solid part, and due to the strongly non-linear behaviour of the fluid part. At the same time, proper experiments of impact phenomena are particularly dangerous and require expensive facilities, which make them largely impractical. For this reason, there is a growing interest in the development of predictive models for impact phenomena.

In MEMPHIS, we rely on a fully Eulerian approach based on conservation laws, where the different materials are characterized by their specific constitutive laws, to address these tasks. This approach was introduced in [37] and subsequently pursued and extended in [43], [36], [29], [33] In Figure 5, we show the results of the numerical simulation of the impact of a copper projectile immersed in air over a copper shield. Results are obtained using a fully parallel monolithic Cartesian method, based on a 4000^2 fixed Cartesian grid. Simulations are performed on a cluster of 512 processors, and benefits from the isomorphism between grid partitioning and processor topology.

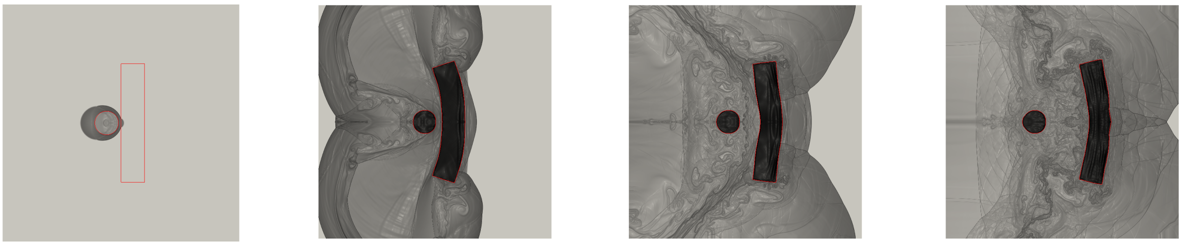

Figure 5. impact and rebound of a copper projectile on a copper plate. Interface and schlieren at $50\mu s$, $199\mu s$, $398\mu s$ and $710\mu s$.

5. Highlights of the Year

5.1. Highlights of the Year

5.1.1. 3D Numerical Model of a Zebra Fish Larva

The full reconstruction of a 3D larval zebrafish (5 days post fertilization) was realized using a serial-section electron microscopy data set combined with the technique of level-set and optimal transportation for shape interpolation. From an experimental video of zebrafish escape swimming, the kinematics of the swimming is extracted removing both translational and rotating displacements. Based on this video-extracted body deformation, 3D zebrafish snapshots of the body surface were generated deforming the 3D model according to the midline motion. The escape response of the zebrafish larva has been simulated using the NaSCar solver. The numerical simulation of the hydrodynamic zebrafish-locomotion provides a full range of the energetic performance performed by the larva during an escape response that are used by the MRGM biology lab in Bordeaux for toxicology evaluations. See figures 6 and 7.

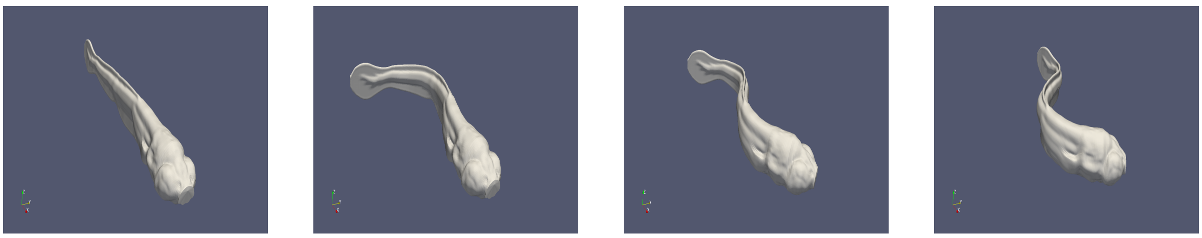

Figure 6. Snaphshots from left to right: reconstruction from electron microscopy and experimental video provided by MRGM Bordeaux of a zebra fish larva swimming movement.

6. New Software and Platforms

6.1. COCOFLOW

KEYWORDS: 3D - Elasticity - MPI - Compressible multimaterial flows

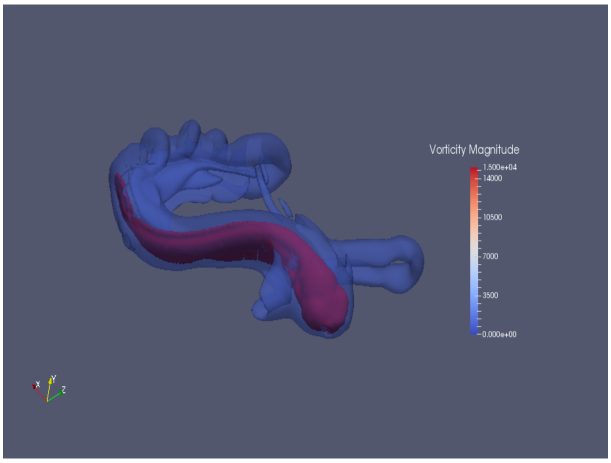

Figure 7. Numerical simulation of the swimming displacement of a zebra fish larva.

FUNCTIONAL DESCRIPTION: The code is written in fortran 95 with a MPI parallelization. It solves equations of conservation modeling 3D compressible flows with elastic models as equation of state.

- Authors: Alexia De Brauer, Florian Bernard, Yannick Gorsse, Thomas Milcent and Angelo Iollo
- Partners: CNRS - Université Bordeaux 1
- Contact: Florian Bernard
- URL: https://gforge.inria.fr/projects/cocoflow

6.2. KOPPA

Kinetic Octree Parallel PolyAtomic

KEYWORDS: C++ - 3D - MPI

FUNCTIONAL DESCRIPTION: KOPPA is a C++/MPI numerical code solving a large range of rarefied flows from external to internal flows in 1D, 2D or 3D. Different kind of geometries can be treated such as moving geometries coming from CAO files or analytical geometries. The models can be solved on Octree grids with dynamic refinement.

- Participant: Florian Bernard
- Partners: Université de Bordeaux - INP Bordeaux - CNRS
- Contact: Angelo Iollo
- URL: https://git.math.cnrs.fr/gitweb/?p=plm/fbernard/KOPPA.git;a=summary

6.3. NaSCar

Navier-Stokes Cartesian

KEYWORDS: HPC - Numerical analyse - Fluid mechanics - Langage C - PETSc

SCIENTIFIC DESCRIPTION: NaSCar can be used to simulate both hydrodynamic bio-locomotion as fish like swimming and aerodynamic flows such wake generated by a wind turbine.

FUNCTIONAL DESCRIPTION: This code is devoted to solve 3D-flows in around moving and deformable bodies. The incompressible Navier-Stokes equations are solved on fixed grids, and the bodies are taken into account thanks to penalization and/or immersed boundary methods. The interface between the fluid and the bodies is tracked with a level set function or in a Lagrangian way. The numerical code is fully second order (time and space). The numerical method is based on projection schemes of Chorin-Temam's type. The code is written in C language and use Petsc library for the resolution of large linear systems in parallel.

NaSCar can be used to simulate both hydrodynamic bio-locomotion as fish like swimming and aerodynamic flows such wake generated by a wind turbine.

- Participant: Michel Bergmann
- Partner: Université de Bordeaux
- Contact: Michel Bergmann
- URL: https://gforge.inria.fr/projects/nascar/

6.4. NS-penal

Navier-Stokes-penalization

KEYWORDS: 3D - Incompressible flows - 2D

FUNCTIONAL DESCRIPTION: The software can be used as a black box with the help of a data file if the obstacle is already proposed. For new geometries the user has to define them. It can be used with several boundary conditions (Dirichlet, Neumann, periodic) and for a wide range of Reynolds numbers.

- Partner: Université de Bordeaux
- Contact: Charles-Henri Bruneau

7. New Results

7.1. DGDD Method for Reduced-Order Modeling of Conservation Laws

Reduced-order models are attractive method to decrease significantly the computational cost of the simulations. However, the ability of reduced-order models to accurately approximate solutions containing strong convection, sharp gradients or discontinuities can be challenging. The discontinuous Galerkin domain decomposition (DGDD) reduced model for systems of conservation laws couples at the discrete level sub-domains of high-fidelity polynomial approximation to regions of low-dimensional resolution as shown in figure 8.

In this approach, the high-dimensional model solves the equations where a given degree of accuracy is required, while the reduced-order model approximates the solution elsewhere. Since the high-dimensional model is used in a small part of the domain, the computational cost is significantly reduced. To perform the coupling, we develop a reduced-order model based on Proper Orthogonal Decomposition in the offline stage and on discontinuous Galerkin method in the online stage instead of the standard Galerkin method. In this way, the domain decomposition is applied transparently thought the numerical fluxes. We investigate the prediction of unsteady flows over a NACA 0012 airfoil. The results demonstrate the accuracy of the proposed method and the significant reduction of the computational cost. In the figures (9 and 10) we show examples of predictions obtained by the low-order model compared to the actual solutions as a function of the Mach number at infintiy and the angle of attack. In the last figure we present the overall space-time L^2 errors as a function of the low-dimensional space size.

7.2. Segmentation of aortic aneurism: collaboration with Nurea

Starting from February 2019, AMIES granted a one-year contract engineer in close collaboration with the Nurea start-up.

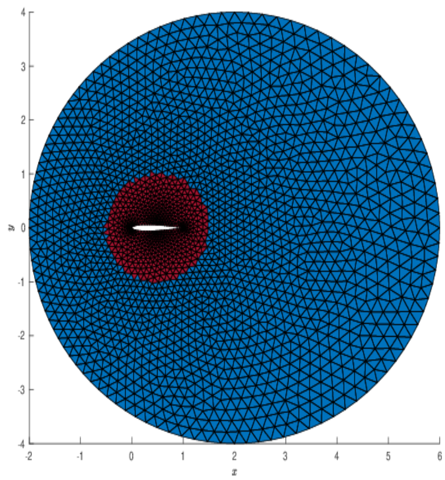

Figure 8. Decomposition of the domain: high-dimensional model (red), reduced-order model (blue).

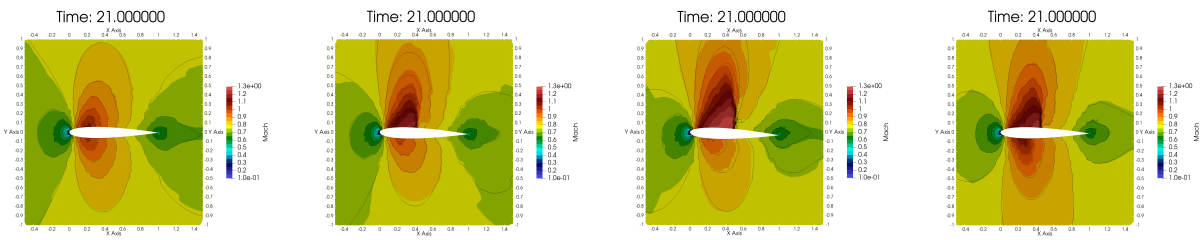

Figure 9. From left to right: $M_\infty = 0.754$ *and* $\alpha = 0.2$*,* $M_\infty = 0.763$ *and* $\alpha = 1.1$*,* $M_\infty = 0.776$ *and* $\alpha = 1.8$*,* $M_\infty = 0.784$ *and* $\alpha = 0.6$

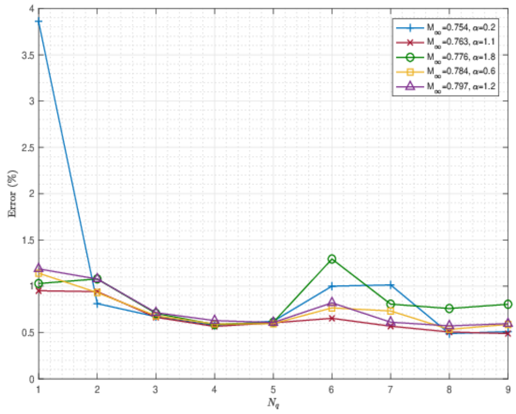

Figure 10. With $N_q = 9$ basis functions, ***the approximation error is less than 1% and the run time is reduced by approximately 72%*** *with respect to the high-fidelity solutions.*

The main objective of the project is to improve the quality and the robustness of automatic segmentation of aortic aneurism. An important part of the work was to decide if patient data needed to be pre-processed or not. To do so a criteron was developed to apply or not a smoothing filter. Several filters were tested and their performance were compared in order to choose the filter the more appropriate to our problem.
Another issue was the bones wrongly taken into the segmentation. A cleaning function was created to deal with it and remove the bones from the segmentation. An usual issue when working with medical images is to deal with the gradient of intensity. Existing tools need to be adapted to take into account these variations within images. This is currently worked out.
The code is implemented in C++ and mostly relies on itk and vtk libraries. An example in figure 11.

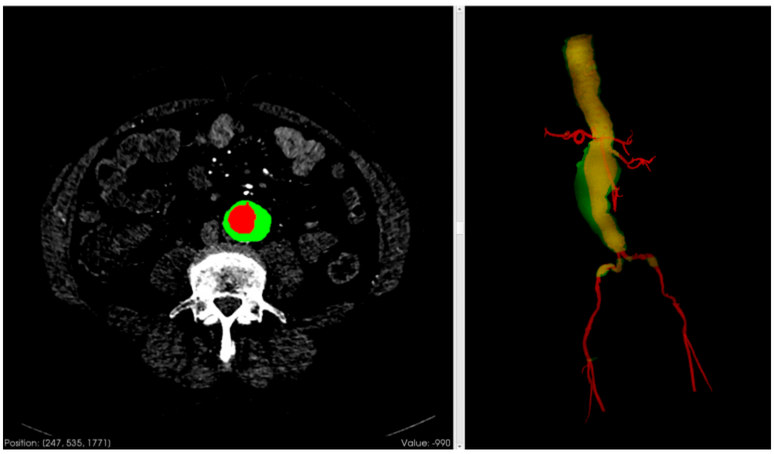

Figure 11. Example of aortic aneurism segmentation. Left: CT scan image; Right: 3D visualization. Red: blood; green: aortic wall

7.3. Fluid-structure interactions on AMR enabled quadree grids

We develop a versatile fully Eulerian method for the simulation of fluid-structure interactions. In the context of a monolithic approach, the whole system is modeled through a single continuum model. The equations are numerically solved using a finite-volume scheme with a compact stencil on AMR enabled quadtree grids where the dynamic refinement is adapted in time to the fluid-structure system.

The geometry is followed using a level-set formulation. In the Eulerian representation, a smooth Heaviside function is defined according to a level-set function on the cartesian mesh to distinguish between fluid and elastic phases. The temporal deformation of the structure is described according to the backward characteristics which are employed to express the Cauchy stress of a two-parameter hyperelastic Mooney-Rivlin material. This model is particularly adapted to elastomeric materials undergoing large deformations, see figure 12.

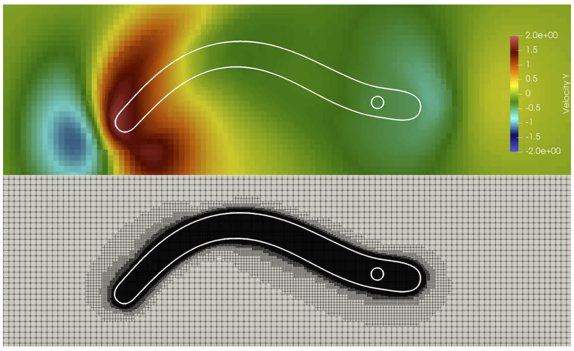

Figure 12. Y-component of the velocity for an oscillating elastomeric membrane actuated by a rigid holder at the tip, immersed in glycerin after 3 periods of oscillations. The criterion used for the dynamic AMR mesh is based on the level-set function.

7.4. Overset grids

One of the difficulties in the simulation of a fluid flow problem is the representation of the computational domain with a static mesh. As a matter of fact, not only the geometry could be particularly complex in itself, but it could change during the simulation and this necessary involves an *in itinere* geometrical adaptation of the mesh, with a consequent high computational cost. One of the ways to overcome this problem is to use multiple overlapping mesh blocks that together define a *Chimera* or *overset* grid. Once the different mesh blocks are generated, they are properly composed by the creation of holes (*hole cutting*) and, consequently, an *overlapping zone* between two overlapping blocks is defined. Figure 13 shows a Chimera grid in the computational domain $[-\pi, \pi]^2$; in black there is the background mesh, in blue the foreground mesh. In particular, the foreground mesh can move and deform (consequently, the hole in the background mesh can change its configuration). The overlapping zone is necessary for the the communication and data transfer from one mesh to another. These operations are possible through an appropriate definition of local stencils of cells, both within and at the border of the individual blocks.
The Navier-Stokes equations for incompressible flows are going to be approximated through a projection method (*Chorin-Temam*), for this reason we have studied two Finite Volume (FV) solvers, for the pure diffusive equation and the unsteady convective-diffusive equation, on Chimera configurations. The first numerical experiments were conducted on 2D problems. The order of convergence of the error of the mismatch between the exact solution and its FV approximation in L^∞- and L^2-norms is 2.

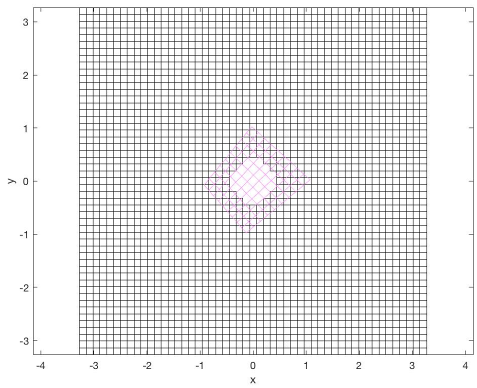

Figure 13. A Chimera grid configuration for the computational domain $[-\pi, \pi]^2$.

7.5. Collective propulsion: collaboration with ONERA

Motivated by recent studies and the locomotion of animal groups for robotics, we investigated the influence of hydrodynamic interactions on the collective propulsion of flapping wings. We studied the horizontal locomotion of an infinite array of flapping wings separated by a constant gap using unsteady non-linear simulations. Two control parameters were explored: the flapping frequency and the gap between the wings. Results obtained for different gaps at a fixed frequency are shown in Figure 14. We first observe that for a very large spacing between the wings — greater than 20 times the chord of a wing — the interaction effects are no longer present (Figure 14 (b)) and the average speed of the system tends to the speed of a single wing. For lower gaps, the average speed may become lower or higher than that of a single wing. For certain gaps, one can find two different stable solutions: one at higher propulsion speed and the other lower than a single wing. This phenomenon has already been observed for a fixed spacing and different frequencies of movement. The stability of these solutions is linked to the interaction between the vortex wake generated by the previous wings and the vortex ejected at the leading or trailing edge of the considered wing (Figure 14 (a)). We remark that propulsive efficiency is higher for the collective case both in faster and slower solutions. Understanding the key mechanisms responsible for the stable solutions will provide directions to control strategies aiming to optimize the wing horizontal speed.

7.6. Automatic registration for model reduction

As part of the ongoing team effort on ROMs, we work on the development of automatic registration procedures for model reduction. In computer vision and pattern recognition, registration refers to the process of finding a spatial transformation that aligns two datasets; in our work, registration refers to the process of finding a parametric transformation that improves the linear compressibility of a given parametric manifold. For advection-dominated problems, registration is motivated by the inadequacy of linear approximation spaces due to the presence of parameter-dependent boundary layers and travelling waves.

In [48], we proposed and analysed a computational procedure for stationary PDEs and investigated performance for two-dimensional model problems. In Figure 15, we show slices of the parametric solution for three different parameters before (cf. Left) and after (cf. Right) registration: we observe that the registration procedure is able to dramatically reduce the sensitivity of the solution to the parameter value μ. In Figure 16, we show the behaviour of the normalised POD eigenvalues (cf. Left) and of the relative L^2 error of the corresponding POD-Galerkin ROM (cf. Right) for an advection-reaction problem: also in this case, the approach

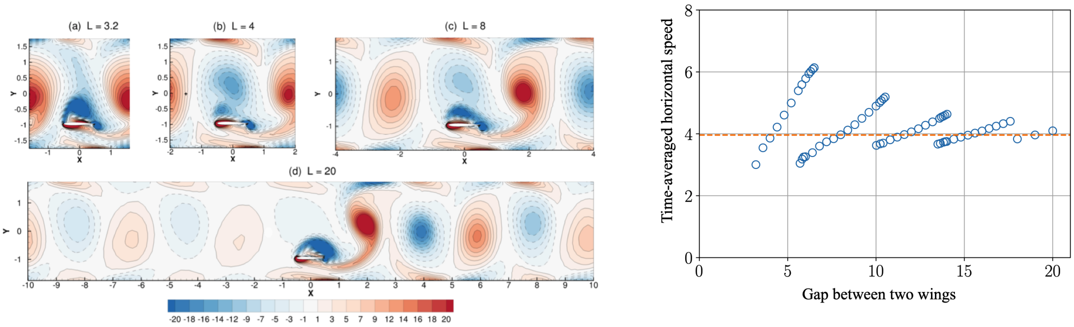

Figure 14. Vorticity contours (a) and time-averaged horizontal speed (b) for a flapping wing interacting in an infinite array. In (b) the average speed of a non interacting flapping wing is represented by a dashed orange line.

is able to improve the approximation properties of linear approximation spaces and ultimately simplify the reduction task.

We aim to extend the approach to a broad class of non-linear steady and unsteady PDEs: in October 2019, we funded a 16-month postdoc to work on the reduction of hyperbolic systems of PDEs. We are also collaborating with EDF (departments PERICLES and LNHE) to extend the approach to the Saint-Venant (shallow water) equations.

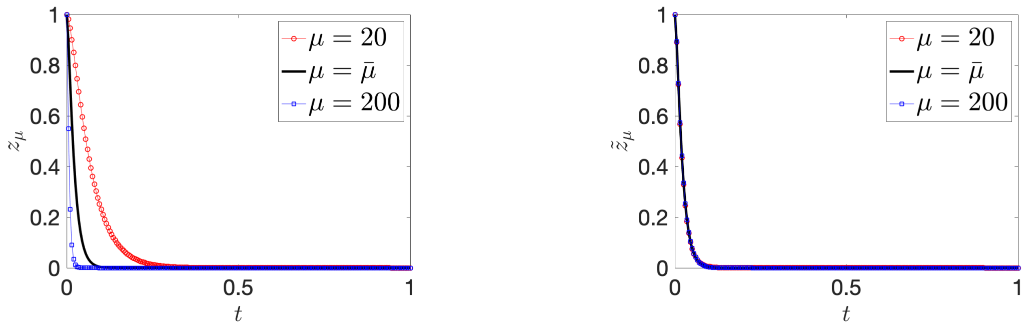

Figure 15. automatic registration for model reduction. Registration of a boundary layer ($\overline{\mu} = \sqrt{20 \cdot 200}$).

7.7. Modeling and numerical simulation of ellipsoidal particle-laden flows and self propelled swimmers in a porous enclosure

Despite being relevant in many natural and industrial processes, suspensions of non-spherical particles have been largely under-investigated compared to the extensive analyses made on the gravity-driven motions of spherical particles. One of the main reasons for this disparity is the difficulty of accurately correcting the short-range hydrodynamic forces and torques acting on complex particles. These effects, also known as lubrication, are essential to the suspension of the particles and are usually poorly captured by direct numerical simulation

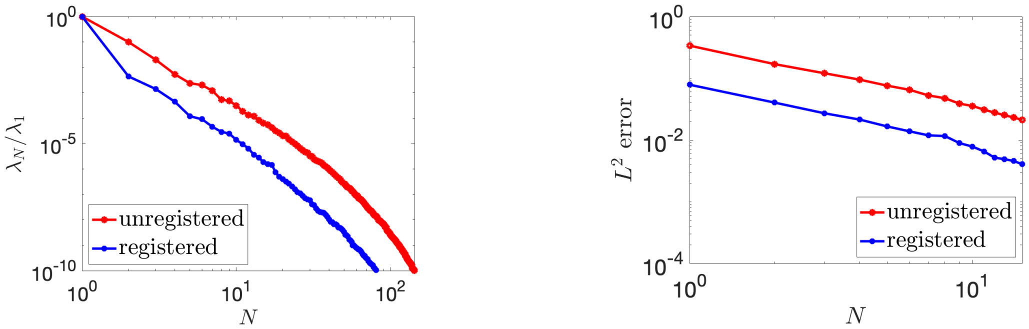

Figure 16. automatic registration for model reduction. Registration of a parameterized advection-reaction problem.

of particle-laden flows. We have proposed a partitioned VP-DEM (Volume Penalization method - Discrete Element Method) solver which estimates the unresolved hydrodynamic forces and torques. Corrections are made locally on the surface of the interacting particles without any assumption on the particle global geometry. This is an extension of our previous work [39]. Numerical validations have been made using ellipsoidal particles immersed in an incompressible Navier-Stokes flow.

Self organization of groups of several swimmers is of interest in biological applications. One of the main question is to determine if the possible organization comes from an uncontrolled or a controlled swimming behavior. This work has been motivated by the recent studies of Hamid Kellay (LOMA). Hamid Kellay has presented his results during a small workshop we organized earlier this year between members of the Memphis team (modeling and numerical methods), the MRGM (experimental zebra-fishes swimming), the LOMA (interaction between self-propelled particles) and the ONERA (flapping wings).

The collision model developed in the previous section has been developed for concave interactions like sphere-sphere or in the limit of sphere-plane wall. For non concave interactions, we have derived a simple approximation considering locally convexity as being a plane wall. We have performed numerical simulations of the interaction of several self propelled swimmers in a porous enclosure (see figure 17). Fishes are organized in small groups that are able to put into motion the enclosure. This behavior is similar to the one observed in the experimental set-up of Hamid Kellay.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry: EDF

40kEuro contract for a study on the development of projection-based reduction strategies for the shallow-water equations, for applications in Hydraulics.

8.2. Bilateral Grants with Industry: ANDRA

36kEuro contract for the development of a projection-based reduced model for a thermo-hydraulic-mechanical (THM) system.

9. Partnerships and Cooperations

9.1. National Initiatives

We are part of the GDR AMORE on ROMs.

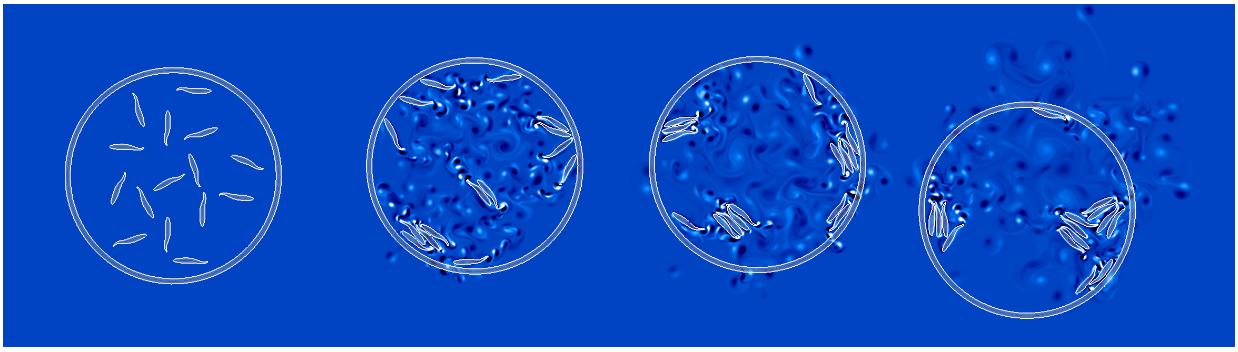

Figure 17. Organization of small self propelled fish groups in a porous enclosure (time evolution is in the usual reading direction). Colormap is the vorticity field.

9.2. European Initiatives

9.2.1. FP7 & H2020 Projects: ARIA RISE project

The overarching objective of ARIA (Accurate Roms for Industrial Applications) project is to form an international and intersectoral network of organizations working on a joint research program in numerical modelling, specifically in the fields of model reduction and convergence between data and models. Memphis team is ccordinating this 926KEuro project. 7 industrial partners are involved (VW, Valorem, Optimad, IEFluids, VirtualMech, Nurea, Esteco), 5 EU academic partners (Inria, Université de Seville, Poitecnico di Milano, Politecnico di Torino, SISSA) and 3 universities in the USA: Stanford University, Virginia Tech and University of South Carolina.

9.3. International Initiatives

9.3.1. Inria International Labs

Inria@SiliconValley

Associate Team involved in the International Lab:

9.3.1.1. MARE

Title: Multiscale Accurate Reduced-order model Enablers

International Partner (Institution - Laboratory - Researcher):

Stanford (United States) - VNU University of Engineering and Technology - Charbel Farhat

Start year: 2019

See also: https://team.inria.fr/memphis/mare-associate-team/

Reduced-order models (ROMs) are simplified mathematical models derived from the full set of partial differential equations governing the physics of the phenomenon of interest. We focus on ROMs that are data-driven as they are based on relevant solution data previously obtained. In particular we will focus on multiscale adaptive models where the large scales are governed by a PDE and the small scales are described by data driven models. To do that we will leverage on tools from data geometry, numerical PDEs and machine learning.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Reviewer - Reviewing Activities

Journal of Computational Physics, International Journal of CFD, Journal of Non-linear Analysis B, ASME Journal of Computational and Nonlinear Dynamics, Journal of Fluid Mechanics, Acta Mechanica, AIAA Journal, International Journal Numerical Methods in Fluids, Computers & Fluids, Journal of Engineering Mathematics, European Journal of Mechanics / B Fluids, Journal Européen de Systèmes Automatisés, Applied Mathematics and Computation. Nuclear Science and Engineering, Computer Methods in Applied Mechanics and Engineering, Journal of Theoretical Biology, Computational Optimization and Applications, Applied science, Meccanica, SIAM journal on scientific computing, SIAM journal on uncertainty quantification, Advances in Computational Mathematics.

10.1.2. Invited Talks

Angelo Iollo

1. June 5th, 2019. Journées scientifiques Inria, Lyon.

   https://project.inria.fr/journeesscientifiques2019/francais-programme/.
2. May 2019. CIMPA School, Tunis. Science des données pour l'ingénierie et la technologie.

   https://www.cimpa.info/fr/node/6217.
3. March 2019. Conférencier invité à la conférence « Fluid-structure interaction», Politecnico di Milano, Milano, 18/3-20/3/2019.

   http://www1.mate.polimi.it/ gazzola/fs.html.

Tommaso Taddei

1. November 2019. MORTECH 2019, Paris.

   https://mortech2019.sciencesconf.org/

10.1.3. Leadership within the Scientific Community

10.1.3.1. Scientific Expertise

Angelo Iollo is an expert for the European Union for the program FET OPEN.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

Four members of the team are Professors or Assistant Professors at Bordeaux University and have teaching duties, which consist in courses and practical exercises in numerical analysis and scientific computing. Michel Bergmann (CR) also teaches around 64 hours per year (practical exercises in programming for scientific computing). Tommaso Taddei (CR) also teaches around 50 hours per year (practical exercises in numerical analysis and scientific computing).

10.2.2. Supervision

1. 2019-2022. Giulia Sambataro. Bourse ANDRA. *Component-based reduction strategies for THM equations.* Advisors: Angelo Iollo, Tommaso Taddei.
2. 2018-2021. Michele Giuliano Carlino. Bourse Inria. *Fluid-structure models on Chimera grids.* Advisors: Michel Bergmann, Angelo Iollo.
3. 2018-2021. Antoine Fondanèche. Bourse UB. *Monolithic fluid-structure modeles on parallel hierarchical grids.* Advisors: Michel Bergmann, Angelo Iollo.
4. 2017-2020. Sebastien Riffaud. *Convergence between data and numerical models.* Advisor: Angelo Iollo.
5. 2017-2020. Luis Ramos Benetti. Bourse ERC Aeroflex (O. Marquet, ONERA). *Monolithic fluid-structure modeles on parallel hierarchical grids.* Advisors: Michel Bergmann, Angelo Iollo.

10.2.3. Juries

Angeo Iollo: reviewer of 3 PhD theses, president of one PhD jury, member of one PhD jury, in France and abroad.
Michel Bergmann: reviewer of 2 PhD theses.

11. Bibliography

Major publications by the team in recent years

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Doctoral Dissertations and Habilitation Theses

[12] M. BRAUN.*Reduced Order Modelling and Uncertainty Propagation Applied to Water Distribution Networks*, Université de Bordeaux, April 2019, https://tel.archives-ouvertes.fr/tel-02278297

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Project-Team MNEMOSYNE

Mnemonic Synergy

IN PARTNERSHIP WITH:
CNRS

Institut Polytechnique de Bordeaux

Université de Bordeaux

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Computational Neuroscience and Medicine

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Project-Team MNEMOSYNE

Creation of the Team: 2012 February 01, updated into Project-Team: 2014 July 01

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1. Team, Visitors, External Collaborators

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2. Overall Objectives

2.1. Summary

At the frontier between integrative and computational neuroscience, we propose to model the brain as a system of active memories in synergy and in interaction with the internal and external world and to simulate it *as a whole and in situation*.

In integrative and cognitive neuroscience (*cf.* § 3.1), on the basis of current knowledge and experimental data, we develop models of the main cerebral structures, taking a specific care of the kind of mnemonic function they implement and of their interface with other cerebral and external structures. Then, in a systemic approach, we build the main behavioral loops involving these cerebral structures, connecting a wide spectrum of actions to various kinds of sensations. We observe at the behavioral level the properties emerging from the interaction between these loops.

We claim that this approach is particularly fruitful for investigating cerebral structures like the basal ganglia and the prefrontal cortex, difficult to comprehend today because of the rich and multimodal information flows they integrate. We expect to cope with the high complexity of such systems, inspired by behavioral and developmental sciences, explaining how behavioral loops gradually incorporate in the system various kinds of information and associated mnesic representations. As a consequence, the underlying cognitive architecture, emerging from the interplay between these sensations-actions loops, results from a *mnemonic synergy*.

In computational neuroscience (*cf.* § 3.2), we concentrate on the efficiency of local mechanisms and on the effectiveness of the distributed computations at the level of the system. We also take care of the analysis of their dynamic properties, at different time scales. These fundamental properties are of high importance to allow the deployment of very large systems and their simulation in a framework of high performance computing Running simulations at a large scale is particularly interesting to evaluate over a long period a consistent and relatively complete network of cerebral structures in realistic interaction with the external and internal world. We face this problem in the domain of autonomous robotics (*cf.* § 3.4) and ensure a real autonomy by the design of an artificial physiology and convenient learning protocoles.

We are convinced that this original approach also permits to revisit and enrich algorithms and methodologies in machine learning (*cf.* § 3.3) and in autonomous robotics (*cf.* § 3.4), in addition to elaborate hypotheses to be tested in neuroscience and medicine, while offering to these latter domains a new ground of experimentation similar to their daily experimental studies.

3. Research Program

3.1. Integrative and Cognitive Neuroscience

The human brain is often considered as the most complex system dedicated to information processing. This multi-scale complexity, described from the metabolic to the network level, is particularly studied in integrative neuroscience, the goal of which is to explain how cognitive functions (ranging from sensorimotor coordination to executive functions) emerge from (are the result of the interaction of) distributed and adaptive computations of processing units, displayed along neural structures and information flows. Indeed, beyond the astounding complexity reported in physiological studies, integrative neuroscience aims at extracting, in simplifying models, regularities at various levels of description. From a mesoscopic point of view, most neuronal structures (and particularly some of primary importance like the cortex, cerebellum, striatum, hippocampus) can be described through a regular organization of information flows and homogenous learning rules, whatever the nature of the processed information. From a macroscopic point of view, the arrangement in space of neuronal structures within the cerebral architecture also obeys a functional logic, the sketch of which is captured in models describing the main information flows in the brain, the corresponding loops built in interaction with the external and internal (bodily and hormonal) world and the developmental steps leading to the acquisition of elementary sensorimotor skills up to the most complex executive functions.

In summary, integrative neuroscience builds, on an overwhelming quantity of data, a simplifying and interpretative grid suggesting homogenous local computations and a structured and logical plan for the development of cognitive functions. They arise from interactions and information exchange between neuronal structures and the external and internal world and also within the network of structures.

This domain is today very active and stimulating because it proposes, of course at the price of simplifications, global views of cerebral functioning and more local hypotheses on the role of subsets of neuronal structures in cognition. In the global approaches, the integration of data from experimental psychology and clinical studies leads to an overview of the brain as a set of interacting memories, each devoted to a specific kind of information processing [53]. It results also in longstanding and very ambitious studies for the design of cognitive architectures aiming at embracing the whole cognition. With the notable exception of works initiated by [50], most of these frameworks (e.g. Soar, ACT-R), though sometimes justified on biological grounds, do not go up to a *connectionist* neuronal implementation. Furthermore, because of the complexity of the resulting frameworks, they are restricted to simple symbolic interfaces with the internal and external world and to (relatively) small-sized internal structures. Our main research objective is undoubtly to build such a general purpose cognitive architecture (to model the brain *as a whole* in a systemic way), using a connectionist implementation and able to cope with a realistic environment.

3.2. Computational Neuroscience

From a general point of view, computational neuroscience can be defined as the development of methods from computer science and applied mathematics, to explore more technically and theoretically the relations between structures and functions in the brain [55], [44]. During the recent years this domain has gained an increasing interest in neuroscience and has become an essential tool for scientific developments in most fields in neuroscience, from the molecule to the system. In this view, all the objectives of our team can be described as possible progresses in computational neuroscience. Accordingly, it can be underlined that the systemic view that we promote can offer original contributions in the sense that, whereas most classical models in computational neuroscience focus on the better understanding of the structure/function relationship for isolated specific structures, we aim at exploring synergies between structures. Consequently, we target interfaces and interplay between heterogenous modes of computing, which is rarely addressed in classical computational neuroscience.

We also insist on another aspect of computational neuroscience which is, in our opinion, at the core of the involvement of computer scientists and mathematicians in the domain and on which we think we could particularly contribute. Indeed, we think that our primary abilities in numerical sciences imply that our developments are characterized above all by the effectiveness of the corresponding computations: We provide biologically inspired architectures with effective computational properties, such as robustness to noise, self-organization, on-line learning. We more generally underline the requirement that our models must also mimick biology through its most general law of homeostasis and self-adaptability in an unknown and changing environment. This means that we propose to numerically experiment such models and thus provide effective methods to falsify them.

Here, computational neuroscience means mimicking original computations made by the neuronal substratum and mastering their corresponding properties: computations are distributed and adaptive; they are performed without an homonculus or any central clock. Numerical schemes developed for distributed dynamical systems and algorithms elaborated for distributed computations are of central interest here [41], [49] and were the basis for several contributions in our group [54], [51], [56]. Ensuring such a rigor in the computations associated to our systemic and large scale approach is of central importance.

Equally important is the choice for the formalism of computation, extensively discussed in the connectionist domain. Spiking neurons are today widely recognized of central interest to study synchronization mechanisms and neuronal coupling at the microscopic level [42]; the associated formalism [47] can be possibly considered for local studies or for relating our results with this important domain in connectionism. Nevertheless, we remain mainly at the mesoscopic level of modeling, the level of the neuronal population, and consequently interested in the formalism developed for dynamic neural fields [39], that demonstrated a richness of behavior [43] adapted to the kind of phenomena we wish to manipulate at this level of description. Our group has a long experience in the study and adaptation of the properties of neural fields [51], [52] and their use for observing the emergence of typical cortical properties [46]. In the envisioned development of more complex architectures and interplay between structures, the exploration of mathematical properties such as stability and boundedness and the observation of emerging phenomena is one important objective. This objective is also associated with that of capitalizing our experience and promoting good practices in our software production. In summary, we think that this systemic approach also brings to computational neuroscience new case studies where heterogenous and adaptive models with various time scales and parameters have to be considered jointly to obtain a mastered substratum of computation. This is particularly critical for large scale deployments.

3.3. Machine Learning

The adaptive properties of the nervous system are certainly among its most fascinating characteristics, with a high impact on our cognitive functions. Accordingly, machine learning is a domain [48] that aims at giving such characteristics to artificial systems, using a mathematical framework (probabilities, statistics, data analysis, etc.). Some of its most famous algorithms are directly inspired from neuroscience, at different levels. Connectionist learning algorithms implement, in various neuronal architectures, weight update rules, generally derived from the hebbian rule, performing non supervised (e.g. Kohonen self-organizing maps), supervised (e.g. layered perceptrons) or associative (e.g. Hopfield recurrent network) learning. Other algorithms, not necessarily connectionist, perform other kinds of learning, like reinforcement learning. Machine learning is a very mature domain today and all these algorithms have been extensively studied, at both the theoretical and practical levels, with much success. They have also been related to many functions (in the living and artificial domains) like discrimination, categorisation, sensorimotor coordination, planning, etc. and several neuronal structures have been proposed as the substratum for these kinds of learning [45], [38]. Nevertheless, we believe that, as for previous models, machine learning algorithms remain isolated tools, whereas our systemic approach can bring original views on these problems.

At the cognitive level, most of the problems we face do not rely on only one kind of learning and require instead skills that have to be learned in preliminary steps. That is the reason why cognitive architectures are often referred to as systems of memory, communicating and sharing information for problem solving. Instead of the classical view in machine learning of a flat architecture, a more complex network of modules must be considered here, as it is the case in the domain of deep learning. In addition, our systemic approach brings the question of incrementally building such a system, with a clear inspiration from developmental sciences. In this perspective, modules can generate internal signals corresponding to internal goals, predictions, error signals, able to supervise the learning of other modules (possibly endowed with a different learning rule), supposed to become autonomous after an instructing period. A typical example is that of episodic learning (in the hippocampus), storing declarative memory about a collection of past episods and supervising the training of a procedural memory in the cortex.

At the behavioral level, as mentionned above, our systemic approach underlines the fundamental links between the adaptive system and the internal and external world. The internal world includes proprioception and interoception, giving information about the body and its needs for integrity and other fundamental programs. The external world includes physical laws that have to be learned and possibly intelligent agents for more complex interactions. Both involve sensors and actuators that are the interfaces with these worlds and close the loops. Within this rich picture, machine learning generally selects one situation that defines useful sensors and actuators and a corpus with properly segmented data and time, and builds a specific architecture and its corresponding criteria to be satisfied. In our approach however, the first question to be raised is to discover what is the goal, where attention must be focused on and which previous skills must be exploited, with the help of a dynamic architecture and possibly other partners. In this domain, the behavioral and the developmental sciences, observing how and along which stages an agent learns, are of great help to bring some structure to this high dimensional problem.

At the implementation level, this analysis opens many fundamental challenges, hardly considered in machine learning : stability must be preserved despite on-line continuous learning; criteria to be satisfied often refer to behavioral and global measurements but they must be translated to control the local circuit level; in an incremental or developmental approach, how will the development of new functions preserve the integrity and stability of others? In addition, this continous re-arrangement is supposed to involve several kinds of learning, at different time scales (from msec to years in humans) and to interfer with other phenomena like variability and meta-plasticity.

In summary, our main objective in machine learning is to propose on-line learning systems, where several modes of learning have to collaborate and where the protocoles of training are realistic. We promote here a *really autonomous* learning, where the agent must select by itself internal resources (and build them if not available) to evolve at the best in an unknown world, without the help of any *deus-ex-machina* to define parameters, build corpus and define training sessions, as it is generally the case in machine learning. To that end, autonomous robotics (*cf.* § 3.4) is a perfect testbed.

3.4. Autonomous Robotics

Autonomous robots are not only convenient platforms to implement our algorithms; the choice of such platforms is also motivated by theories in cognitive science and neuroscience indicating that cognition emerges from interactions of the body in direct loops with the world (*embodiment of cognition* [40]). In addition to real robotic platforms, software implementations of autonomous robotic systems including components dedicated to their body and their environment will be also possibly exploited, considering that they are also a tool for studying conditions for a real autonomous learning.

A real autonomy can be obtained only if the robot is able to define its goal by itself, without the specification of any high level and abstract cost function or rewarding state. To ensure such a capability, we propose to endow the robot with an artificial physiology, corresponding to perceive some kind of pain and pleasure. It may consequently discriminate internal and external goals (or situations to be avoided). This will mimick circuits related to fundamental needs (e.g. hunger and thirst) and to the preservation of bodily integrity. An important objective is to show that more abstract planning capabilities can arise from these basic goals.

A real autonomy with an on-line continuous learning as described in § 3.3 will be made possible by the elaboration of protocols of learning, as it is the case, in animal conditioning, for experimental studies where performance on a task can be obtained only after a shaping in increasingly complex tasks. Similarly, developmental sciences can teach us about the ordered elaboration of skills and their association in more complex schemes. An important challenge here is to translate these hints at the level of the cerebral architecture.

As a whole, autonomous robotics permits to assess the consistency of our models in realistic condition of use and offers to our colleagues in behavioral sciences an object of study and comparison, regarding behavioral dynamics emerging from interactions with the environment, also observable at the neuronal level.

In summary, our main contribution in autonomous robotics is to make autonomy possible, by various means corresponding to endow robots with an artificial physiology, to give instructions in a natural and incremental way and to prioritize the synergy between reactive and robust schemes over complex planning structures.

4. Application Domains

4.1. Overview

One of the most original specificity of our team is that it is part of a laboratory in Neuroscience (with a large spectrum of activity from the molecule to the behavior), focused on neurodegenerative diseases and consequently working in tight collaboration with the medical domain. As a consequence, neuroscientists and the medical world are considered as the primary end-users of our researches. Beyond data and signal analysis where our expertise in machine learning may be possibly useful, our interactions are mainly centered on the exploitation of our models. They will be classically regarded as a way to validate biological assumptions and to generate new hypotheses to be investigated in the living. Our macroscopic models and their implementation in autonomous robots will allow an analysis at the behavioral level and will propose a systemic framework, the interpretation of which will meet aetiological analysis in the medical domain and interpretation of intelligent behavior in cognitive neuroscience and related domains like for example educational science.

The study of neurodegenerative diseases is targeted because they match the phenomena we model. Particularly, the Parkinson disease results from the death of dopaminergic cells in the basal ganglia, one of the main systems that we are modeling. The Alzheimer disease also results from the loss of neurons, in several cortical and extracortical regions. The variety of these regions, together with large mnesic and cognitive deficits, require a systemic view of the cerebral architecture and associated functions, very consistent with our approach.

Of course, numerical sciences are also impacted by our researches, at several levels. At a global level, we will propose new control architectures aimed at providing a higher degree of autonomy to robots, as well as machine learning algorithms working in more realistic environment. More specifically, our focus on some cognitive functions in closed loop with a real environment will address currently open problems. This is obviously the case for planning and decision making; this is particularly the case for the domain of affective computing, since motivational characteristics arising from the design of an artificial physiology allow to consider not only cold rational cognition but also hot emotional cognition. The association of both kinds of cognition is undoublty an innovative way to create more realistic intelligent systems but also to elaborate more natural interfaces between these systems and human users.

At last, we think that our activities in well-founded distributed computations and high performance computing are not just intended to help us design large scale systems. We also think that we are working here at the core of informatics and, accordingly, that we could transfer some fundamental results in this domain.

5. Highlights of the Year

5.1. Highlights of the Year

We recently considered a new domain of application for our models, educational science. In a very stimulating perspective, we wonder how our cognitive models of cerebral architectures can be used to study children performing problem solving. Our first steps in this domain concern the etablishment of relations with a laboratory in educational science, designing a software platform (*cf.* § 6.4). and being associated to ongoing projects, one project with the French ANR regarding cocreativity and problem solving evaluation during a computational thinking initiation activity and one in the Erasmus+ CAI « Communauté d'Apprentissage de l'Informatique » 19PE0004 project, in link with the Erasmus+ Let'Steam project.

6. New Software and Platforms

6.1. DANA

Distributed Asynchronous Numerical and Adaptive computing framework

KEYWORD: Neural networks

FUNCTIONAL DESCRIPTION: DANA is a python framework whose computational paradigm is grounded on the notion of a unit that is essentially a set of time dependent values varying under the influence of other units via adaptive weighted connections. The evolutions of a unit's value are defined by a set of differential equations expressed in standard mathematical notation which greatly ease their definition. The units are organized into groups that form a model. Each unit can be connected to any other unit (including itself) using a weighted connection. The DANA framework offers a set of core objects needed to design and run such models. The modeler only has to define the equations of a unit as well as the equations governing the training of the connections. The simulation is completely transparent to the modeler and is handled by DANA. This allows DANA to be used for a wide range of numerical and distributed models as long as they fit the proposed framework (e.g. cellular automata, reaction-diffusion system, decentralized neural networks, recurrent neural networks, kernel-based image processing, etc.).

- Participant: Nicolas Rougier
- Contact: Nicolas Rougier
- URL: http://dana.loria.fr/

6.2. Virtual Enaction

KEYWORDS: Neurosciences - Simulation - Health

FUNCTIONAL DESCRIPTION: VirtualEnaction: A Platform for Systemic Neuroscience Simulation. The computational models studied in this project have applications that extend far beyond what is possible to experiment yet in human or non-human primate subjects. Real robotics experimentations are also impaired by rather heavy technological constraints, for instance, it is not easy to dismantle a given embedded system in the course of emerging ideas. The only versatile environment in which such complex behaviors can be studied both globally and at the level of details of the available modeling is a virtual environment, as in video games, Such a system can be implemented as “brainy-bot” (a programmed player based on our knowledge of the brain architecture) which goal is to survive in a complete manipulable environment.

In order to attain this rather ambitious objective we both (i) deploy an existing open-source video game middleware in order to be able to shape the survival situation to be studied and (ii) revisit the existing models in order to be able to integrate them as an effective brainy-bot. It consists of a platform associated to a scenario that is the closest possible to a survival situation (foraging, predator-prey relationship, partner approach to reproduction) and in which it is easy to integrate an artificial agent with sensory inputs (visual, touch and smell), emotional and somatosensory cues (hunger, thirst, fear, ..) and motor outputs (movement, gesture, ..) connected to a "brain" whose architecture will correspond to the major anatomical regions involved in the issues of learning and action selection (cortex areas detailed here, basal ganglia, hippocampus, and areas dedicated to sensorimotor processes). The internal game clock can be slowed down enough to be able to run non trivial brainy-bot implementations. This platform has already being used by two students of the team and is now a new deliverable of the KEOpS project.

- Participants: André Garenne, Frédéric Alexandre, Nicolas Rougier and Thierry Viéville
- Contact: Frédéric Alexandre

6.3. ReservoirPy

KEYWORDS: Recurrent network - Artificial intelligence - Reservoir Computing - Multi-label classification - Timeseries Prediction - Time Series - Machine learning - Classification

FUNCTIONAL DESCRIPTION: This toolbox provides a class of Echo State Networks that can be used with Python and its scientific librairies like Numpy, Scipy and Matplolib. It includes useful expertise to train recurrent neural networks of ESN architecture kind.

ESN is a particular kind of recurrent neural network (RNN) with or without leaky neurons. The input stream is projected to a random recurrent layer and a linear output layer (called "read-out") is modified by learning (which can also be done in an online fashion).

Compared to other RNNs, the input layer and the recurrent layer (called "reservoir") do not need to be trained. For other RNNs, the structure of the recurrent layer evolves in most cases by gradient descent algorithms like Backpropagation-Through-Time, which is not biologically plausible and is adapted iteratively to be able to hold a representaion of the input sequence. In contrast, the random weights of the ESN’s reservoir are not trained, but adapted to possess the "Echo State Property" (ESP) or at least suitable dynamics (e.g. ’edge of chaos’) to generalize, which includes a non-linear transformation of the input that can be learned by a linear classifier. The weights are adapted by scaling the weights based on the maximum absolute eigenvalue (also called spectral radius), which is a hyperparameter specific to the task. The states of the reservoir are linearly separable and can be mapped to the output layer by a computationally cheap linear regression, as no gradient descent is necessary. The weights of the input layer can be scaled by the input scaling hyperparameter, which also depends on the nature of the inputs.

- Partners: Université de Hamburg - University of Hamburg
- Contact: Xavier Hinaut
- URL: https://github.com/neuronalX/reservoirpy

6.4. Platforms

6.4.1. Platform AIDE

Keywords : computational thinking initiation, learning analytics, machine learning

Functional description : This package provides source files to control a tapletop setup allowing to initiate learners to computational thinking using unplugged activities and connected objects, and collecting automatically learning activities including thanks to neuroinspired machine learning mechanisms, developped in collaboration with pobot and the Inria mission of science outreach and the LINE laboratory.

7. New Results

7.1. Overview

This year we have explored the main cortico-basal loops of the cerebral architecture and their associated memory mechanisms. The limbic loop (*cf.* § 7.2) concerns the taking into account of the emotional and motivational aspects by the respondant and operant conditioning and their relations with the semantic and episodic memories. The associative loop (*cf.* § 7.3) is about mechanisms of working memory and rule manipulation. Concerning the motor loop (*cf.* § 7.4), we have studied mechanisms of song acquisition and production in birds.

We have also worked on the systemic integration of our models (*cf.* § 7.5), raising the question of the conditions of autonomous learning.

Finally, we study the links between our bio-inspired modeling work and other domains like Machine Learning, computer science and educational science (*cf.* § 7.6).

7.2. The limbic loop

Our main contribution this year to advancing our view of the limbic loop is the defense of the PhD of B. T. Nallapu [1] related to the modeling of the orbital and medial loops the two main constituents of the limbic loop, as described in [33]. In short, this work proposes, instead of a global view of the orbital loop as generally proposed, a view with two loops, one corresponding to the lateral part of the orbitofrontal cortex related to respondent conditioning and one to the medial part related to operant conditioning and closely linked to the medial loop. The work shows that such a model replicates a variety of observations in neuroscience and can be used for the autonomous behavior of an agent in the Minecraft video game.

7.3. The associative loop

The prefrontal cortex is known to be involved in many high-level cognitive functions, in particular working memory. Gated working memory is defined as the capacity of holding arbitrary information at any time in order to be used at a later time. Based on electrophysiological recordings, several computational models have tackled the problem using dedicated and explicit mechanisms. We propose instead to consider an implicit mechanism based on a random recurrent neural network. We introduce a robust yet simple reservoir model of gated working memory with instantaneous updates [11]. The model is able to store an arbitrary real value at random time over an extended period of time. The dynamics of the model is a line attractor that learns to exploit reentry and a non-linearity during the training phase using only a few representative values. A deeper study of the model shows that there is actually a large range of hyper parameters for which the results hold (number of neurons, sparsity, global weight scaling, etc.) such that any large enough population, mixing excitatory and inhibitory neurons can quickly learn to realize such gated working memory. This suggests this property could be an implicit property of any random population, that can be acquired through learning. Furthermore, considering working memory to be a physically open but functionally closed system, we give account on some counter-intuitive electrophysiological recordings.

We also developed a model of working memory combining short-term and long-term components [24]. For the long-term component, we used Conceptors in order to store constant temporal patterns. For the short-term component , we used the Gated-Reservoir model [11]. We combined both components in order to obtain a model in which information can go from long-term memory to short-term memory and vice-versa.

The prefrontal cortex is also known to be the place where complex and abstract behavioral rules are implemented. In order to study the mechanisms related to the manipulation of such rules, we have begun the study of networks able to build rules to manipulate such framework as the Wisconsin Card Sorting Test, widely used in the clinical domain [3].

7.4. The motor loop

Sensorimotor learning represents a challenging problem for artificial and natural systems. Several computational models try to explain the neural mechanisms at play in the brain to implement such learning. These models have several common components: a motor control model, a sensory system and a learning architecture. In S. Pagliarini's PhD, our challenge is to build a biologically plausible model for song learning in birds including neuro-anatomical and developmental constraints.

We made a review on a specific type of sensorimotor learning referred to as imitative vocal learning and examplified by song learning in birds or human complex vocalizations[35]. Sensorimotor learning represents a challenging problem for natural and artificial systems. Several computational models have been proposed to explain the neural and cognitive mechanisms at play in the brain [34]. In general, these models can be decomposed in three common components: a sensory system, a motor control device and a learning framework. The latter includes the architecture, the learning rule or optimisation method, and the exploration strategy used to guide learning. In this review, we focus on imitative vocal learning, that is exemplified in song learning in birds and speech acquisition in humans. We aim to synthesise, analyse and compare the various models of vocal learning that have been proposed, highlighting their common points and differences. We first introduce the biological context, including the behavioural and physiological hallmarks of vocal learning and sketch the neural circuits involved. Then, we detail the different components of a vocal learning model and how they are implemented in the reviewed models.

On this topic, X. Hinaut is also collaborating with Catherine del Negro's team (CNRS, NeuroPSI, Orsay) on the representation of syntax in songbird brains. In particular, the project aims at (1) linking the neural activity of a sensori-motor area (HVC) to syntax elements in the songs of domestic canaries ; (2) analysing the audio files and transcripts of canary songs in order to find syntax cues and higher order representations (graph properties of songs, evaluate Markovian forward and backward transition probabilities of various orders). The song transcription and analyses has been done by M1 intern (in Neuroscience) Juliette Giraudon, and preliminary work on song segmentation and classification has been done by L3 intern (ENS) Pierre Marcus. In December, Aurore Cazala (student in the NeuroPSI collaborator team since 2014) defended her PhD at the University of Paris-Saclay on "Codage neuronal de l'ordre des signaux acoustiques dans le chant des oiseaux chanteurs"; X. Hinaut participated in studies done in this PhD.

7.5. Systemic integration

Several global approaches corresponding to the systemic integration of several loops have been studied this year. The PhD work [1] evoked in section § 7.2 for its contributions to modeling the limbic loop, has also been partly devoted to the definition of a global cognitive model and its embodiment in an agent in the Minecraft game, in order to illustrate the performances of autonomous behavior of a system endowed by such a limbic loop [33].

7.6. Association to other scientific domains

Concerning Machine Learning and our work on reservoir computing, X. Hinaut is collaborating with Michael Spranger (Sony Lab, Tokyo, Japan) on grounding of language, adapting Hinaut's previous Reservoir parser (ResPars) with the representational system of Spranger: IRL (Incremental Recruitment Language) [17]. He is also collaborating with Hamburg on the use of reservoir models for robotic tasks (*cf.* § 9.3). In this work, we have shown that the RLM can successfully learn to parse sentences related to home scenarios in fifteen languages [5]. This demonstrates that (1) the learning principle of our model is not limited to a particular language (or particular sentence structures), and (2) it can deal with various kinds of representations (not only predicates), which enable users to adapt it to their own needs. Some people can mix two languages within the same sentence: this is known as intra-sentential code-switching. With M1 intern Pauline Detraz, we collected data from human subjects that were required to mix pairs of given sentences in French and English. The corpus obtained have some very complex mixed sentences: there can be until eleven language switches within the same sentence. Then, we trained our Reservoir-based sentence Parsing model, with the collected corpus. Surprisingly the model is able to learn and generalize on the mixed corpus with performances nearly as good as the unmixed French-English corpus [16]. A post-doc joined the team in Nov 2019 to work on the project HuRRiCane ("Hierarchical Reservoir Computing for Language Comprehension") project founded by Inria. This project aims at extending the ResPars model to work from speech inputs to sentence comprehension including coherancy checking. In other words, the objective is to experiment how a sentence comprehension model, based on reservoir computing, can learn to understand sentences by exploring which meanings can have the sentences, implying several steps from stream of phonemes to words and from stream of words to sentence comprehension. The model will be implemented on a virtual agent first and then on the Nao humanoid robot.

This project is linked to other projects in the team on the hierarchical organization of the prefrontal cortex (including Broca's area, involved in language). This hierarchy corresponds to an increasingly higher abstraction, which is made by different sub-areas. We will therefore be able to link this post-doc project to existing projects of the team, where different levels of abstractions are necessary for sentence comprehension.

As explained in § 7.6, song segmentation and classification has been done by L3 intern (ENS) Pierre Marcus.

The on-going work on an original prototype based approach of deep-learning considering not so big data sets, and targeting also interpretability of the result, has been finalized [4], including a fine study on metaparameter adjustment in this context, while both standard learning and meta-learning paradigms have been considered. The capability to easily the "how it works" mechanism to no specialist of the field is an important outcome of the paper.

Co-leaded by Margarida Romero scientific director of the LINE laboratory of the UCA and researchers of our team, a preliminary work regarding artificial intelligence devoted to education (AIDE) was developed to study applications to educational science. This first year has been devoted to study to which extents the existing collaboration between Inria science outreach regarding computational thinking initiation and educational science research in order to be understand the underlying cognitive processes of the former actions and evaluate them, could be enlarged to multi-disciplinary research in both fields. The first outcome of this collaboration has been an analysis of a computational thinking unplugged activity under the perspective of embodied cognition [9] and deep and large review in the field, analyzing how computational thinking in K-12 education could be developed [22], within the scope of studies regarding co-creativity, robotics and maker education. [20], while a qualitative analysis one very large audience (more then 18000 inscriptions) on-line course outcomes has been published [18], with some operational outcomes regarding enlarging comptational thinking training from teachers to all citizens [12].

Software is a fundamental pillar of modern scientific research, across all fields and disciplines. However, there is a lack of adequate means to cite and reference software due to the complexity of the problem in terms of authorship, roles and credits. This complexity is further increased when it is considered over the lifetime of a software that can span up to several decades. Building upon the internal experience of Inria, the French research institute for digital sciences, we provide in this paper a contribution to the ongoing efforts in order to develop proper guidelines and recommendations for software citation and reference. Namely, we recommend: (1) a richer taxonomy for software contributions with a qualitative scale; (2) to put humans at the heart of the evaluation; and (3) to distinguish citation from reference.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

8.1.1. Contract with CEA Cesta

Participants: Frédéric Alexandre, Guillaume Padiolleau.

In the context of the PhD of Guillaume Padiolleau, we are working with the CEA on possible interactions between model-based and model-free approaches of reinforcement learning, based on cognitive consideration. Particularly, to decrease the complexity of exploration of a large data space in model-free approaches, we aim at considering introducing a priori knowledge coming from a model and we also propose to consider motivation as another way to orient the search in the learning space. This is applied in the robotic domain to manipulations by a robotic arm.

8.1.2. Contract with Ubisoft

Participants: Frédéric Alexandre, Pramod Kaushik.

Together with the Inria Project-team Flowers, we are working with the video game editor Ubisoft to define original bio-inspired learning methods, to qualify the behavior of human players observed during runs of games. Such learning algorithms will be specifically considered in the PhD of Pramod Kaushik.

9. Partnerships and Cooperations

9.1. Regional Initiatives

9.1.1. EcoMob

Participants: Frédéric Alexandre, Snigdha Dagar, Nicolas Rougier.

Project gathering researchers from: University of La Rochelle (Cerege lab in social sciences and L3I lab in computer science); University of Bordeaux (IRGO lab in organisation management); Town and suburbs of La Rochelle.

The goal of this project is to study and model user urban mobility behaviours in an eco-responsibility context. Interactive mobile applications are used to measure the effective evolution of behaviour. Our team is in charge of studying models of decision in such complex contexts, in interaction with teams in social sciences aiming at influencing user behaviours.

9.1.2. PsyPhINe

Participant: Nicolas Rougier.

Project gathering researchers from: MSH Lorraine (USR3261), InterPsy (EA 4432), APEMAC, EPSaM (EA4360), Archives Henri-Poincaré (UMR7117), Loria (UMR7503) & Mnemosyne.

PsyPhiNe is a pluridisciplinary and exploratory project between philosophers, psychologists, neuroscientists and computer scientists. The goal of the project is to explore cognition and behavior from different perspectives. The project aims at exploring the idea of assignments of intelligence or intentionality, assuming that our intersubjectivity and our natural tendency to anthropomorphize play a central role: we project onto others parts of our own cognition. To test these hypotheses, we ran a series of experiments with human subject confronted to a motorized lamp that can or cannot interact with them while they're doing a specific task. We've organized our third national conference in Nancy gathering speakers from philosophy, robotics, art and psychology and closed a three years cycle. The group now aims at publishing a book gathering text from all the invited speakers.

9.2. National Initiatives

9.2.1. FUI Sumatra

Participants: Frédéric Alexandre, Thalita Firmo Drumond, Xavier Hinaut, Nicolas Rougier, Thierry Viéville.

This FUI project, supported by the Aerospace Valley Innovation Pole, gathers two industrial groups (Safran Helicopter and SPIE), three research labs and four SME. Its goal is to provide contextualized information to maintenance operators by the online analysis of the operating scene. We are concerned in this project with the analysis of visual scenes, in industrial contexts, and the extraction of visual primitives, categories and pertinent features, best decribing the scenes, with biologically inspired neuronal models.

Firstly, this is an opportunity for us to revisit the principles of deep network architectures by adapting principles that we will elaborate from the context of the hierarchical architecture of the temporal visual cortex. Secondly, we intend to exploit and adapt our model of hippocampus to extract more heterogenous features. This project is an excellent opportunity to associate and combine our models and also to evaluate the robustness of our models in real-world applications.

9.2.2. ANR SOMA (PRCI)

Participants: Nicolas Rougier, Remya Sankar.

This project is a convergence point between past research approaches toward new computational paradigms: adaptive reconfigurable architecture, cellular computing, computational neuroscience, and neuromorphic hardware:

1. SOMA is an adaptive reconfigurable architecture to the extent that it will dynamically re-organize both its computation and its communication by adapting itself to the data to process.
2. SOMA is based on cellular computing since it targets a massively parallel, distributed and decentralized neuromorphic architecture.
3. SOMA is based on computational neuroscience since its self-organization capabilities are inspired from neural mechanisms.
4. SOMA is a neuromorphic hardware system since its organization emerges from the interactions between neural maps transposed into hardware from brain observation.

This project represents a significant step toward the definition of a true fine-grained distributed, adaptive and decentralized neural computation framework. Using self-organized neural populations onto a cellular machine where local routing resources are not separated from computational resources, it will ensure natural scalability and adaptability as well as a better performance/power consumption tradeoff compared to other conventional embedded solutions.

9.2.3. ANR MACAQUE40

Participant: Nicolas Rougier.

Most of the theoretical models in economics proposed so far to describe money emergence are based on three intangible assumptions: the omniscience of economic agents, an infinite time and an extremely large number of agents (not bounded). The goal of this interdisciplinary study is to investigate the condition of apparition of a monetary economy in a more ecological framework provided with the assumption that the market is made up of a finite number of agents having a bounded rationality and facing a time constraint.

In this study, we propose a generic model and environment of monetary prospecting. Our first objective is to artificially identify structural (trading organisation, agents specialisation) and cognitive conditions (learning skills, memory and strategic anticipation abilities, tradeoff exploration/exploitation) that allowed money emergence. This will provide relevant environmental constraints that we will use during our manipulations in the laboratory. The agents that will be involved in these manipulations will be of two types: non-human primates (rhesus macaques) and humans.

9.3. International Initiatives

9.3.1. Participation in Other International Programs

9.3.1.1. Project LingoRob with Germany

LingoRob - Learning Language in Developmental Robots - is a project of the Programme Hubert Curien PHC Procope with Germany (University of Hamburg). The scientific objective of the collaboration is to better understand the mechanisms underlying language acquisition and enable more natural interaction between humans and robots in different languages, while modelling how the brain processes sentences and integrates semantic information of scenes. Models developed in both labs involve artificial neural networks, and in particular Echo State Networks (ESN), also known as pertaining to the Reservoir Computing framework.

These neural models allow insights on high-level processes of the human brain, and at the same time are well suited as robot control platform, because they can be trained and executed online with low computational resources. The collaborators will also combine Deep Learning networks to the reservoir models already used in order to benefit from their very good feature extraction abilities.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events: Selection

10.1.1.1. Chair of Conference Program Committees

X. Hinaut: Co-organizer of the workshop on language learning at IEEE ICDL-EPIROB 2019, Oslo, Norway, August 2019; of the "Day of the NeuroRobotics Working Group", Nov 2019, Bordeaux, France; Session chair at the CogSci conference, Montréal, Canada. Jul 2019.

N.Rougier: co-chair for the track on Neuroscience and Cognitive science during the SciPy conference (Austin, Texas, USA)

10.1.1.2. Member of the Conference Program Committees

X. Hinaut: IROS Workshop on Deep Probabilistic Generative Models for Cognitive Architecture in Robotics, Macau, China. Nov 2019. International Workshop on Cognitive and Neural Systems, Granada, Spain. Oct 2019.

10.1.1.3. Reviewer

X. Hinaut: CogSci'19, ICANN'19, ICDL-Epirob'19, IWANN'19; S. Pagliarini: ICDL-Epirob'19;

10.1.2. Journal

10.1.2.1. Member of the Editorial Boards

- Frédéric Alexandre: Academic Editor for PLOS ONE; Review Editor for Frontiers in Neurorobotics;
- Nicolas Rougier: Editor in chief for ReScience, Academic editor for PeerJ, review editor for Frontiers in Neurorobotics.
- Xavier Hinaut: guest editor in the Journal Advanced Robotics of a special issue on "Machine Learning Methods for High-Level Cognitive-Capabilities-in-Robotics"; guest editor for Frontiers Robotics and AI special issue on "Language and Robotics" https://www.frontiersin.org/research-topics/8861/language-and-robotics ; Member of the Editorial Board of Frontiers in Neurorobotics as Review Editor.

10.1.2.2. Reviewer - Reviewing Activities

- F. Alexandre: Elife; EMBC; Frontiers in Neurobotics; Cognitive Computation; PLoS ONE
- Xavier Hinaut: Cognitive Computation, Entropy, Front. in Neurorobotics, Neural Networks, PeerJ, ReScience, IEEE Transactions in Cognitive Developmental Systems (TCDS).
- N.Rougier: Current Biology, PLoS Computational Biology, Journal of Open Science Software, PeerJ

10.1.3. Invited Talks

F. Alexandre:

- Invited speaker at the joint workshop between Inria and LIAMA (The Sino-European Laboratory of Computer Science, Automation and Applied Mathematics), Paris, April 3rd, for the talk: “Setting the basis of a bio-inspired Reinforcement Learning”;

- talk to the Interdisciplinary and Translational Neuroscience research network (IT-Neuro) of the University of Lorraine, Nancy, April 25th: “Modeling the frontal cortex for motivated decision making”;
- Invited talk “A computational model to study the dynamics of representations of rewards in the orbital and medial frontal cortex”, on October 2nd to the 2019 Bordeaux Neurocampus Conference on Reward http://brainconf.u-bordeaux.fr/;
- Invited talk “Trusted AI in medicine” and participation to a round table on december 11th in Merignac at MediSpace congress on transfers of technologies and best practices between space, aeronautical and medical industries https://www.medispace2019.com/en/presentation-2/

X. Hinaut:

- “How to ground sensorimotor sequence of symbols ? From robot learning languages to songbirds”, ICDL- Epirob workshop on Language Learning (M. Spranger), Olso, NW. Aug 2019.
- “Random recurrent networks for language and bird song learning”, B. Golosio, Physics dept., University of Cagliari, IT.
- “Modélisation de l’encodage neuronal pour l’apprentissage de séquences complexes : applications à l’interaction homme-robot et aux chants des oiseaux”. LIRIS, Lyon, June 2019.
- “Modèles Neuronaux Récurrents pour le Traitement de Séquences Complexes”, Journée GT-ACAI-Neurorobotique: Neuroscience et multimodalité dans les interactions humain-humain, humain-agent ou humain-robot, ACAI-GT8 common working group day, Telecom ParisTech, Paris, FR.
- “Modélisation de l’encodage neuronal pour l’apprentissage de séquences complexes”, “Acoustic Perception” seminar from ETIS lab, University of Cergy-Pontoise, FR. March 2019.
- “Little Mechanisms of AI: from Ants to Language”, PhD Retreat of Center for Research and Interdisciplinarity of Paris. Arcachon, June 2019.
- “How to ground sensorimotor sequences of symbols? From robot learning languages to songbirds”, ICDL-epirob workshop on Language learning, Oslo, Aug. 2019.
- Symposium organised by regional chair on technological systems for human augmentation, March 28—29, 2019, Bordeaux, France.
- “Echo State Networks”, invited lecture at the International MSc “Intelligent Adaptive Systems”, KT lab, University of Hamburg, Germany, June 2019.

N.Rougier: Invited talk at the “Robotics, development and neurosciences” conference (Cergy, France)

10.1.4. Leadership within the Scientific Community

X. Hinaut:

- Co-Head of the "NeuroRobotics" CNRS Working Group Organisation of several workshops throughout the year
- IEEE Task Force (TF) member: "Reservoir Computing", "Cognitive and Developmental Systems Technical Committee": "Language and Cognition" TF and "Action and Perception" TF.
- President of the association MindLaBDX: “open citizen lab” in Cognitive Sciences and Artificial Intelligence in Bordeaux.

Nicolas Rougier: Editor in chief for ReScience

10.1.5. Scientific Expertise

F. Alexandre is the french expert for Mathematics and Computer Science of the PHC (Hubert Curien Program) Utique for scientific cooperation between France and Tunisia.

Thierry Vieville has been required as expert to review a large neuroscience lab by the HCERES agency. He has also contributed to a large audience report on « AI in the media and creative industries » [25].

10.1.6. Research Administration

- F. Alexandre is member of the steering committee of Inria Bordeaux Sud-Ouest Project Committee; Corresponding scientist for Bordeaux Sud-Ouest of the Inria COERLE ethical committee; Member of the national Inria committee for international chairs; Member of the steering committee of the regional Cluster on Information Technology and Health; of the regional Cluster on Robotics; Expert of the ITMO 'Neurosciences, Sciences Cognitive, Neurologie, Psychiatrie'
- X. Hinaut: Member of the "Committee for Technological Development" of Inria, Bordeaux, FR
- N. Rougier is vice-head of the Mnemosyne team-project; elected member of the Inria Evaluation Committee; IES referent for Inria Bordeaux Sud-Ouest; Member of the commitee for researcher recruitment; Member of the steering committee for the BioComp CNRS consortium; Editor in chief and co-founder of ReScience.
- Thierry Viéville is involved in the http://classcode.fr project and in charge, for Inria of the MSc SmartEdTech at Univ. Cote d'Azur (UCA).

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

Many courses are given in french universities and schools of engineers at different levels (LMD) by most team members, in computer science, in applied mathematics, in neuroscience and in cognitive science. Thierry Viéville is teaching computational thinking in the Msc #CreaSmartEdtech ("Digital Expertise", "Educational Informatics" including Artificial Intelligence and Ontologies, "Digital Intedisciplinary Project ") and is co-orgazning this Master of Science. He has been involved in the production of the "Science Numérique et Technologie" (SNT) new high-school course teacher formation, via the creation of a MOOC, with more than 18000 inscriptions, and has collaborated to the qualitative analysis of the course outcomes [18].

In addition, this year, F. Alexandre gave a lecture at the Barcelona Cognition, Brain and Technology Summer School https://bcbt.specs-lab.com/bcbt19/.

10.2.2. Juries

In addition to several juries in France, we can note this year a reviewing and participation to a PhD defense in Germany (F. Alexandre)

10.3. Popularization

10.3.1. Articles and contents

- F. Alexandre published an article about AI and neuroscience in The Conversation https://theconversation.com/de-quelles-facons-lintelligence-artificielle-se-sert-elle-des-neurosciences-124402
- N. Rougier published article: Pourquoi votre chat est nul aux échecs et pourtant plus intelligent qu'une IA, The Conversation (FR); article: Why your cat is lousy at chess yet way smarter than even the most advanced AI, The Conversation (US); Interview: Et le cerveau dans tout ça ? U magazine (Univ. Bordeaux)

10.3.2. Education

F. Alexandre: A lesson about AI (2 hours) and an unplugged activity about learning and memory (1 hour) given to a high-school class of 2nd on november 14th in Dax for the "1 scientist 1 class : Chiche !" MENJ program.

N. Rougier: Science outreach day at the Montendre high-school on unplugged AI (Montendre, France)

Several people in the team (F. Alexandre, T. Firmo-Drumond, N. Rougier, T. Vieville) participated (talks and demonstrations) to the Day “Activities for teaching AI” organized between Inria Bordeaux and LINE laboratory in Sciences of Education in Nice, June 21st;

10.3.3. Interventions

F. Alexandre:

- Intervention at the annual conference of the Bishops of France (Lourdes, April 2nd), with a conference (“What can medicine expect from AI”) and the organization of a workshop on Robotics for AI;
- Participation to a round table discussion at the Robot Makers Day Festival, Talence, April 12th: “AI: threats and opportunities for our companies: what training for tomorrow’s engineers?”
- conference to the ESME-Sudria School of Engineers, Bordeaux, May 21st: “Is the brain a good model of intelligence ?”
- Conference “Should we be afraid of artificial intelligence?”, at the “Université de tous les savoirs” in Saint Jean de Luz on November 13th http://www.utl-luz.fr/index_002.htm
- Conference: “What can we expect from AI ?”, in the special day “AI and me” organized on November 15-16 by the city of Pontonx-sur-Adour https://www.pontonx.fr/Pontonx-sur-l-Adour/Agenda-et-actualites/Toutes-les-actus-de-Pontonx/L-intelligence-artificielle

A. Garenne: intervention about “Artificial Neural Networks and Machine Learning” at a club of companies, Pessac, decembre 12

X. Hinaut:

- "Pint of Science" invited talk, Bordeaux, FR, May 2019.
- "Les petits mécanismes de l’IA", invited talk at the Library of "Le Haillan", FR, April 2019.
- Invited jury member of the world scale hackathon "Créathon", Poitiers, FR, May 2019.
- Invited talk at the Science Fest Day, Cap Sciences, Bordeaux, FR, Oct 2019.

N. Rougier:

- Reboot conference “Will robots dominate us ?” (Bordeaux, France)
- Discussion with the general public about science, fiction and AI at Cap-Sciences (Bordeaux, France)

Thierry Viéville is an active member of Femmes et Sciences, has been invited speaker at Un rêve pour les filles et les garçons : LA SCIENCE and is involved in dedicated science outreach actions [15].

Several people in the team (F. Alexandre, T. Firmo-Drumond, N. Rougier) participated to the “Trial of AI” on november 20, in the project “The controversy of Bordeaux Macropole” during the festival Facts, program Arts and Sciences of University of Bordeaux. https://www.youtube.com/watch?v=UI4B4TteRmA and https://twitter.com/bdxmacropole

Intervention by A. Garenne and T. Firmo-Drumond at the inter-university seminar "artificial intelligence and clinical sense", Bordeaux, march 11-12

10.3.4. Creation of media or tools for science outreach

Thanks to fundings from the Bordeaux Museum of Science Cap Sciences (http://www.cap-sciences.net/) and from the Foundation Blaise Pascal (https://www.fondation-blaise-pascal.org/), we have designed a software tool to run small demonstrative scenarios, to help everyone discover the brain functions at the origin of our sensorimotor and vital cognitive behaviors (instinctive and motivated behavior, selection of embodied action, emotional decision-making, seat of self-awareness, etc.). This resource is for a wide audience to whom we can show scenarios, but also co-build multi-media resources to share methods and knowledge (participatory scientific mediation approach) and to discuss these topics. It is also at the disposal of scientific mediators (researchers and beyond) who wish to co-construct such resources, or to present research results involving the animation of anatomy of the nervous system as well as of users or authors of computer code who want to reuse shared technologies to derive other applications, in particular become familiar with the specification languages (here JSON and markdown).

11. Bibliography

Publications of the year

Doctoral Dissertations and Habilitation Theses

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Articles in International Peer-Reviewed Journal

[2] P. ALLIEZ, R. DI COSMO, B. GUEDJ, A. GIRAULT, M.-S. HACID, A. LEGRAND, N. P. ROUGIER.*Attributing and Referencing (Research) Software: Best Practices and Outlook from Inria*, in "Computing in Science & Engineering", 2019, p. 1-14, https://arxiv.org/abs/1905.11123 [*DOI :* 10.1109/MCSE.2019.2949413], https://hal.archives-ouvertes.fr/hal-02135891

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[5] X. HINAUT, J. TWIEFEL.*Teach Your Robot Your Language! Trainable Neural Parser for Modelling Human Sentence Processing: Examples for 15 Languages*, in "IEEE Transactions on Cognitive and Developmental Systems", December 2019 [*DOI :* 10.1109/TCDS.2019.2957006], https://hal.inria.fr/hal-01964541

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Articles in National Peer-Reviewed Journal

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Invited Conferences

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International Conferences with Proceedings

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Project-Team MONC

Mathematical modeling for Oncology

IN COLLABORATION WITH: Institut de Mathématiques de Bordeaux (IMB)

IN PARTNERSHIP WITH:
CNRS

Institut Polytechnique de Bordeaux

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Modeling and Control for Life Sciences

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Project-Team MONC

Creation of the Team: 2015 January 01, updated into Project-Team: 2016 November 01

Keywords:

Computer Science and Digital Science:

A6.1. - Methods in mathematical modeling
A6.1.1. - Continuous Modeling (PDE, ODE)
A6.1.4. - Multiscale modeling
A6.2.1. - Numerical analysis of PDE and ODE
A6.2.4. - Statistical methods
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B1.1.7. - Bioinformatics
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B1.1.10. - Systems and synthetic biology
B2.2.3. - Cancer
B2.4.2. - Drug resistance
B2.6.1. - Brain imaging
B2.6.3. - Biological Imaging

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2. Overall Objectives

2.1. Objectives

The MONC project-team aims at developing new mathematical models from partial differential equations and statistical methods and based on biological and medical knowledge. Our goal is ultimately to be able to help clinicians and/or biologists to better understand, predict or control the evolution of the disease and possibly evaluate the therapeutic response, in a clinical context or for pre-clinical studies. We develop patient-specific approaches (mainly based on medical images) as well as population-type approaches in order to take advantage of large databases.

In vivo modeling of tumors is limited by the amount of information available. However, recently, there have been dramatic increases in the scope and quality of patient-specific data from non-invasive imaging methods, so that several potentially valuable measurements are now available to quantitatively measure tumor evolution, assess tumor status as well as anatomical or functional details. Using different techniques from biology or imaging - such as CT scan, magnetic resonance imaging (MRI), or positron emission tomography (PET) - it is now possible to evaluate and define tumor status at different levels or scales: physiological, molecular and cellular.

In the meantime, the understanding of the biological mechanisms of tumor growth, including the influence of the micro-environment, has greatly increased. Medical doctors now have access to a wide spectrum of therapies (surgery, mini-invasive techniques, radiotherapies, chemotherapies, targeted therapies, immunotherapies...).

Our project aims at helping oncologists in their followup of patients via the development of novel quantitative methods for evaluation cancer progression. The idea is to build phenomenological mathematical models based on data obtained in the clinical imaging routine like CT scans, MRIs and PET scans. We therefore want to offer medical doctors patient-specific tumor evolution models, which are able to evaluate – on the basis of previously collected data and within the limits of phenomenological models – the time evolution of the pathology at subsequent times and the response to therapies. More precisely, our goal is to help clinicians answer the following questions thanks to our numerical tools:

1. When is it necessary to start a treatment?

2. What is the best time to change a treatment?
3. When to stop a treatment?

We also intend to incorporate real-time model information for improving the accuracy and efficacy of non invasive or micro-invasive tumor ablation techniques like acoustic hyperthermia, electroporation, radio-frequency, cryo-ablation and of course radiotherapies.

There is therefore a dire need of integrating biological knowledge into mathematical models based on clinical or experimental data. A major purpose of our project is also to create new mathematical models and new paradigms for data assimilation that are adapted to the biological nature of the disease and to the amount of multi-modal data available.

2.2. General strategy

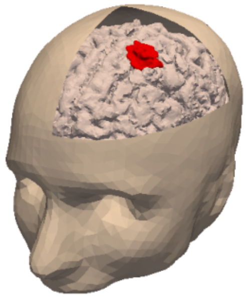

Figure 1. 3D numerical simulation of a meningioma. The tumor is shown in red.

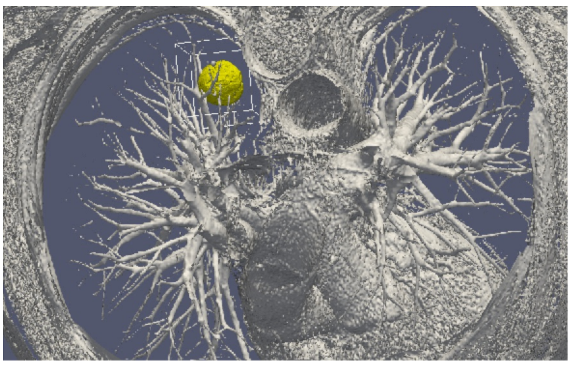

Figure 2. 3D numerical simulation of a lung tumor. The tumor is shown in yellow.

Our general strategy may be described with the following sequence:

- Stage 1: *Derivation of mechanistic models based on the biological knowledge and the available observations.* The construction of such models relies on the up-to-date biological knowledge at the cellular level including description of the cell-cycle, interaction with the microenvironement (angiogenesis, interaction with the stroma). Such models also include a "macroscopic" description of specific molecular pathways that are known to have a critical role in carcinogenesis or that are targeted by new drugs. We emphasize that for this purpose, close interactions with biologists are crucial. Lots of works devoted to modeling at the cellular level are available in the literature. However, in order to be able to use these models in a clinical context, the tumor is also to be described at the tissue level. The *in vitro* mechanical characterization of tumor tissues has been widely studied. Yet no description that could be patient specific or even tumor specific is available. It is therefore necessary to build adapted phenomenological models, according to the biological and clinical reality.
- Stage 2: *Data collection.* In the clinical context, data may come from medical imaging (MRI, CT-Scan, PET scan) at different time points. We need *longitudinal* data in time in order to be able to understand or describe the evolution of the disease. Data may also be obtained from analyses of blood samples, biopsies or other quantitative biomarkers. A close collaboration with clinicians is required for selecting the specific cases to focus on, the understanding of the key points and data, the classification of the grades of the tumors, the understanding of the treatment,...In the preclinical context, data may for instance be macroscopic measurements of the tumor volume for subcutaneous cases, green fluorescence protein (GFP) quantifications for total number of living cells, non-invasive bioluminescence signals or even imaging obtained with devices adapted to small animals.
  - *Data processing:* Besides selection of representative cases by our collaborators, most of the time, data has to be processed before being used in our models. We develop novel methods for semi-automatic (implemented in SegmentIt) as well as supervized approaches (machine learning or deep learning) for segmentation, non-rigid registration and extraction of image texture information (radiomics, deep learning).
- Stage 3: *Adaptation of the model to data.* The model has to be adapted to data: it is useless to have a model considering many biological features of the disease if it cannot be reliably parameterized with available data. For example, very detailed descriptions of the angiogenesis process found in the literature cannot be used, as they have too much parameters to determine for the information available. A pragmatic approach has to be developed for this purpose. On the other hand, one has to try to model any element that can be useful to exploit the image. Parameterizing must be performed carefully in order to achieve an optimal trade-off between the accuracy of the model, its complexity, identifiability and predictive power. Parameter estimation is a critical issue in mathematical biology: if there are too many parameters, it will be impossible to estimate them but if the model is too simple, it will be too far from reality.
- Stage 4: *Data assimilation.* Because of data complexity and scarcity - for example multimodal, longitudinal medical imaging - data assimilation is a major challenge. Such a process is a combination of methods for solving inverse problems and statistical methods including machine learning strategies.
  - *Personalized models:* Currently, most of the inverse problems developed in the team are solved using a gradient method coupled with some MCMC type algorithm. We are now trying to use more efficient methods as Kalman type filters or so-called Luenberger filter (nudging). Using sequential methods could also simplify Stage 3 because they can be used even with complex models. Of course, the strategy used by the team depends on the quantity and the quality of data. It is not the same if we have an homogeneous population of cases or if it is a very specific isolated case.
  - *Statistical learning:* In some clinical cases, there is no longitudinal data available to build a mathematical model describing the evolution of the disease. In these cases (*e.g.* in our

collaboration with Humanitas Research Hospital on low grade gliomas or Institut Bergonié on soft-tissue sarcoma), we use machine learning techniques to correlate clinical and imaging features with clinical outcome of patients (radiomics). When longitudinal data and a sufficient number of patients are available, we combine this approach and mathematical modeling by adding the personalized model parameters for each patient as features in the statistical algorithm. Our goal is then to have a better description of the evolution of the disease over time (as compared to only taking temporal variations of features into account as in delta-radiomics approaches). We also plan to use statistical algorithms to build reduced-order models, more efficient to run or calibrate than the original models.

  – *Data assimilation of gene expression.* "Omics" data become more and more important in oncology and we aim at developing our models using this information as well. For example, in our work on GIST, we have taken the effect of a Ckit mutation on resistance to treatment into account. However, it is still not clear how to use in general gene expression data in our macroscopic models, and particularly how to connect the genotype to the phenotype and the macroscopic growth. We expect to use statistical learning techniques on populations of patients in order to move towards this direction, but we emphasize that this task is very prospective and is a scientific challenge in itself.

- Stage 5: *Patient-specific Simulation and prediction, Stratification*. Once the mechanistic models have been parametrized, they can be used to run patient-specific simulations and predictions. The statistical models offer new stratifications of patients (*i.t.* an algorithm that tells from images and clinical information wheter a patient with soft-tissue sarcoma is more likely to be a good or bad responder to neoadjuvant chemotherapy). Building robust algorithms (*e.g.* that can be deployed over multiple clinical centers) also requires working on quantifying uncertainties.

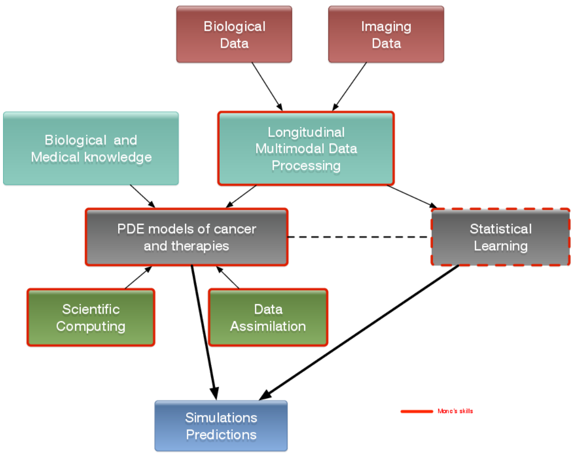

Figure 3. General strategy of the team to build meaningful models in oncology.

3. Research Program

3.1. Introduction

We are working in the context of data-driven medicine against cancer. We aim at coupling mathematical models with data to address relevant challenges for biologists and clinicians in order for instance to improve our understanding in cancer biology and pharmacology, assist the development of novel therapeutic approaches or develop personalized decision-helping tools for monitoring the disease and evaluating therapies.

More precisely, our research on mathematical oncology is three-fold:

- Axis 1: Tumor modeling for patient-specific simulations: *Clinical monitoring. Numerical markers from imaging data. Radiomics*.
- Axis 2: Bio-physical modeling for personalized therapies: *Electroporation from cells to tissue. Radiotherapy*.
- Axis 3: Quantitative cancer modeling for biological, clinical and preclinical studies: *Biological mechanisms. Metastatic dissemination. Pharmacometrics*.

In the first axis, we aim at producing patient-specific simulations of the growth of a tumor or its response to treatment starting from a series of images. We hope to be able to offer a valuable insight on the disease to the clinicians in order to improve the decision process. This would be particularly useful in the cases of relapses or for metastatic diseases.

The second axis aims at modeling biophysical therapies like electroporation, but also radiotherapy, thermo-ablations, radio-frequency ablations or electroporation that play a crucial role for a local treatment of the disease if possible limiting the metastatic dissemination, which is precisely the clinical context where the techniques of axis 1 will be applied.

The third axis is essential since it is a way to better understand and model the biological reality of cancer growth and the (possibly complex) effects of therapeutic intervention. Modeling in this case also helps to interpret the experimental results and improve the accuracy of the models used in Axis 1. Technically speaking, some of the computing tools are similar to those of Axis 1.

3.2. Axis 1: Tumor modeling for patient-specific simulations

The gold standard treatment for most cancers is surgery. In the case where total resection of the tumor is possible, the patient often benefits from an adjuvant therapy (radiotherapy, chemotherapy, targeted therapy or a combination of them) in order to eliminate the potentially remaining cells that may not be visible. In this case personalized modeling of tumor growth is useless and statistical modeling will be able to quantify the risk of relapse, the mean progression-free survival time...However if total resection is not possible or if metastases emerge from distant sites, clinicians will try to control the disease for as long as possible. A wide set of tools are available. Clinicians may treat the disease by physical interventions (radiofrequency ablation, cryoablation, radiotherapy, electroporation, focalized ultrasound,...) or chemical agents (chemotherapies, targeted therapies, antiangiogenic drugs, immunotherapies, hormonotherapies). One can also decide to monitor the patient without any treatment (this is the case for slowly growing tumors like some metastases to the lung, some lymphomas or for some low grade glioma). A reliable patient-specific model of tumor evolution with or without therapy may have different uses:

- Case without treatment: the evaluation of the growth of the tumor would offer a useful indication for the time at which the tumor may reach a critical size. For example, radiofrequency ablation of pulmonary lesion is very efficient as long as the diameter of the lesion is smaller than 3 cm. Thus, the prediction can help the clinician plan the intervention. For slowly growing tumors, quantitative modeling can also help to decide at what time interval the patient has to undergo a CT-scan. CT-scans are irradiative exams and there is a challenge for decreasing their occurrence for each patient. It has also an economical impact. And if the disease evolution starts to differ from the prediction, this might mean that some events have occurred at the biological level. For instance, it could be the rise of an aggressive phenotype or cells that leave a dormancy state. This kind of events cannot be predicted, but some mismatch with respect to the prediction can be an indirect proof of their existence. It could be an indication for the clinician to start a treatment.
- Case with treatment: a model can help to understand and to quantify the final outcome of a treatment using the early response. It can help for a redefinition of the treatment planning. Modeling can also help to anticipate the relapse by analyzing some functional aspects of the tumor. Again, a deviation

with respect to reference curves can mean a lack of efficiency of the therapy or a relapse. Moreover, for a long time, the response to a treatment has been quantified by the RECIST criteria which consists in (roughly speaking) measuring the diameters of the largest tumor of the patient, as it is seen on a CT-scan. This criteria is still widely used and was quite efficient for chemotherapies and radiotherapies that induce a decrease of the size of the lesion. However, with the systematic use of targeted therapies and anti-angiogenic drugs that modify the physiology of the tumor, the size may remain unchanged even if the drug is efficient and deeply modifies the tumor behavior. One better way to estimate this effect could be to use functional imaging (Pet-scan, perfusion or diffusion MRI, ...), a model can then be used to exploit the data and to understand in what extent the therapy is efficient.

- Optimization: currently, we do not believe that we can optimize a particular treatment in terms of distribution of doses, number, planning with the model that we will develop in a medium term perspective.

The scientific challenge is therefore as follows: given the history of the patient, the nature of the primitive tumor, its histopathology, knowing the treatments that patients have undergone, some biological facts on the tumor and having a sequence of images (CT-scan, MRI, PET or a mix of them), are we able to provide a numerical simulation of the extension of the tumor and of its metabolism that fits as best as possible with the data (CT-scans or functional data) and that is predictive in order to address the clinical cases described above?

Our approach relies on the elaboration of PDE models and their parametrization with images by coupling deterministic and stochastic methods. The PDE models rely on the description of the dynamics of cell populations. The number of populations depends on the pathology. For example, for glioblastoma, one needs to use proliferative cells, invasive cells, quiescent cells as well as necrotic tissues to be able to reproduce realistic behaviors of the disease. In order to describe the relapse for hepatic metastases of gastro-intestinal stromal tumor (gist), one needs three cell populations: proliferative cells, healthy tissue and necrotic tissue.

The law of proliferation is often coupled with a model for the angiogenesis. However such models of angiogenesis involve too many non measurable parameters to be used with real clinical data and therefore one has to use simplified or even simplistic versions. The law of proliferation often mimics the existence of an hypoxia threshold, it consists of an ODE. or a PDE that describes the evolution of the growth rate as a combination of sigmoid functions of nutrients or roughly speaking oxygen concentration. Usually, several laws are available for a given pathology since at this level, there are no quantitative argument to choose a particular one.

The velocity of the tumor growth differs depending on the nature of the tumor. For metastases, we will derive the velocity thanks to Darcy's law in order to express that the extension of the tumor is basically due to the increase of volume. This gives a sharp interface between the metastasis and the surrounding healthy tissues, as observed by anatomopathologists. For primitive tumors like glioma or lung cancer, we use reaction-diffusion equations in order to describe the invasive aspects of such primitive tumors.

The modeling of the drugs depends on the nature of the drug: for chemotherapies, a death term can be added into the equations of the population of cells, while antiangiogenic drugs have to be introduced in a angiogenic model. Resistance to treatment can be described either by several populations of cells or with non-constant growth or death rates. As said before, it is still currently difficult to model the changes of phenotype or mutations, we therefore propose to investigate this kind of phenomena by looking at deviations of the numerical simulations compared to the medical observations.

The calibration of the model is achieved by using a series (at least 2) of images of the same patient and by minimizing a cost function. The cost function contains at least the difference between the volume of the tumor that is measured on the images with the computed one. It also contains elements on the geometry, on the necrosis and any information that can be obtained through the medical images. We will pay special attention to functional imaging (PET, perfusion and diffusion MRI). The inverse problem is solved using a gradient method coupled with some Monte-Carlo type algorithm. If a large number of similar cases is available, one can imagine to use statistical algorithms like random forests to use some non quantitative data like the gender, the age, the origin of the primitive tumor...for example for choosing the model for the growth rate for a patient using this population knowledge (and then to fully adapt the model to the patient by calibrating this particular model on patient data) or for having a better initial estimation of the modeling parameters. We have obtained several preliminary results concerning lung metastases including treatments and for metastases to the liver.

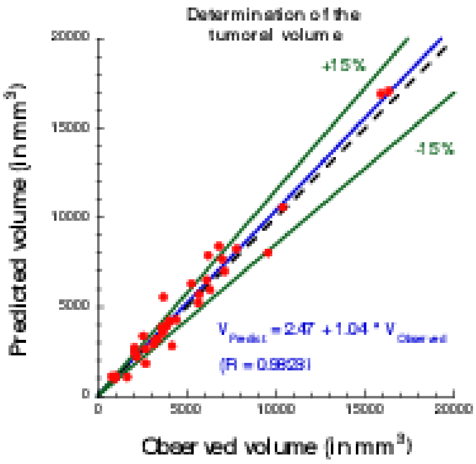

Figure 4. Plot showing the accuracy of our prediction on meningioma volume. Each point corresponds to a patient whose two first exams were used to calibrate our model. A patient-specific prediction was made with this calibrated model and compared with the actual volume as measured on a third time by clinicians. A perfect prediction would be on the black dashed line. Medical data was obtained from Prof. Loiseau, CHU Pellegrin.

3.3. Axis 2: Bio-physical modeling for personalized therapies

In this axis, we investigate locoregional therapies such as radiotherapy, irreversible electroporation. Electroporation consists in increasing the membrane permeability of cells by the delivery of high voltage pulses. This non-thermal phenomenon can be transient (reversible) or irreversible (IRE). IRE or electro-chemotherapy – which is a combination of reversible electroporation with a cytotoxic drug – are essential tools for the treatment of a metastatic disease. Numerical modeling of these therapies is a clear scientific challenge. Clinical applications of the modeling are the main target, which thus drives the scientific approach, even though theoretical studies in order to improve the knowledge of the biological phenomena, in particular for electroporation, should also be addressed. However, this subject is quite wide and we focus on two particular approaches: some aspects of radiotherapies and electro-chemotherapy. This choice is motivated partly by pragmatic reasons: we already have collaborations with physicians on these therapies. Other treatments could be probably treated with the same approach, but we do not plan to work on this subject on a medium term.

- Radiotherapy (RT) is a common therapy for cancer. Typically, using a CT scan of the patient with the structures of interest (tumor, organs at risk) delineated, the clinicians optimize the dose delivery to treat the tumor while preserving healthy tissues. The RT is then delivered every day using low resolution scans (CBCT) to position the beams. Under treatment the patient may lose weight and the tumor shrinks. These changes may affect the propagation of the beams and subsequently change the dose that is effectively delivered. It could be harmful for the patient especially if sensitive organs are concerned. In such cases, a replanification of the RT could be done to adjust the therapeutical protocol. Unfortunately, this process takes too much time to be performed routinely. The challenges faced by clinicians are numerous, we focus on two of them:

- *Detecting the need of replanification:* we are using the positioning scans to evaluate the movement and deformation of the various structures of interest. Thus we can detect whether or not a structure has moved out of the safe margins (fixed by clinicians) and thus if a replanification may be necessary. In a retrospective study, our work can also be used to determine RT margins when there are no standard ones. A collaboration with the RT department of Institut Bergonié is underway on the treatment of retroperitoneal sarcoma and ENT tumors (head and neck cancers). A retrospective study was performed on 11 patients with retro-peritoneal sarcoma. The results have shown that the safety margins (on the RT) that clinicians are currently using are probably not large enough. The tool used in this study was developed by an engineer funded by Inria (Cynthia Périer, ADT Sesar). We used well validated methods from a level-set approach and segmentation / registration methods. The originality and difficulty lie in the fact that we are dealing with real data in a clinical setup. Clinicians have currently no way to perform complex measurements with their clinical tools. This prevents them from investigating the replanification. Our work and the tools developed pave the way for easier studies on evaluation of RT plans in collaboration with Institut Bergonié. *There was no modeling involved in this work that arose during discussions with our collaborators.* The main purpose of the team is to have meaningful outcomes of our research for clinicians, sometimes it implies leaving a bit our area of expertise.
- *Evaluating RT efficacy and finding correlation between the radiological responses and the clinical outcome:* our goal is to help doctors to identify correlation between the response to RT (as seen on images) and the longer term clinical outcome of the patient. Typically, we aim at helping them to decide when to plan the next exam after the RT. For patients whose response has been linked to worse prognosis, this exam would have to be planned earlier. This is the subject of collaborations with Institut Bergonié and CHU Bordeaux on different cancers (head and neck, pancreas). The response is evaluated from image markers (*e.g.* using texture information) or with a mathematical model developed in Axis 1. The other challenges are either out of reach or not in the domain of expertise of the team. Yet our works may tackle some important issues for adaptive radiotherapy.

• Both IRE and electrochemotherapy are anticancerous treatments based on the same phenomenon: the electroporation of cell membranes. This phenomenon is known for a few decades but it is still not well understood, therefore our interest is two fold:

1. We want to use mathematical models in order to better understand the biological behavior and the effect of the treatment. We work in tight collaboration with biologists and bioeletromagneticians to derive precise models of cell and tissue electroporation, in the continuity of the research program of the Inria team-project MC2. These studies lead to complex non-linear mathematical models involving some parameters (as less as possible). Numerical methods to compute precisely such models and the calibration of the parameters with the experimental data are then addressed. Tight collaborations with the Vectorology and Anticancerous Therapies (VAT) of IGR at Villejuif, Laboratoire Ampère of Ecole Centrale Lyon and the Karlsruhe Institute of technology will continue, and we aim at developing new collaborations with Institute of Pharmacology and Structural Biology (IPBS) of Toulouse and the Laboratory of Molecular Pathology and Experimental Oncology (LMPEO) at CNR Rome, in order to understand differences of the electroporation of healthy cells and cancer cells in spheroids and tissues.
2. This basic research aims at providing new understanding of electroporation, however it is necessary to address, particular questions raised by radio-oncologists that apply such treatments. One crucial question is "What pulse or what train of pulses should I apply to electroporate the tumor if the electrodes are located as given by the medical images"?

Even if the real-time optimization of the placement of the electrodes for deep tumors may seem quite utopian since the clinicians face too many medical constraints that cannot be taken into account (like the position of some organs, arteries, nerves...), one can expect to produce real-time information of the validity of the placement done by the clinician. Indeed, once the placement is performed by the radiologists, medical images are usually used to visualize the localization of the electrodes. Using these medical data, a crucial goal is to provide a tool in order to compute in real-time and visualize the electric field and the electroporated region directly on theses medical images, to give the doctors a precise knowledge of the region affected by the electric field. In the long run, this research will benefit from the knowledge of the theoretical electroporation modeling, but it seems important to use the current knowledge of tissue electroporation – even quite rough –, in order to rapidly address the specific difficulty of such a goal (real-time computing of non-linear model, image segmentation and visualization). Tight collaborations with CHU Pellegrin at Bordeaux, and CHU J. Verdier at Bondy are crucial.

- Radiofrequency ablation. In a collaboration with Hopital Haut Leveque, CHU Bordeaux we are trying to determine the efficacy and risk of relapse of hepatocellular carcinoma treated by radiofrequency ablation. For this matter we are using geometrical measurements on images (margins of the RFA, distance to the boundary of the organ) as well as texture information to statistically evaluate the clinical outcome of patients.
- Intensity focused ultrasound. In collaboration with Utrecht Medical center, we aim at tackling several challenges in clinical applications of IFU: target tracking, dose delivery...

3.4. Axis 3: Quantitative cancer modeling for biological and preclinical studies

With the emergence and improvement of a plethora of experimental techniques, the molecular, cellular and tissue biology has operated a shift toward a more quantitative science, in particular in the domain of cancer biology. These quantitative assays generate a large amount of data that call for theoretical formalism in order to better understand and predict the complex phenomena involved. Indeed, due to the huge complexity underlying the development of a cancer disease that involves multiple scales (from the genetic, intra-cellular scale to the scale of the whole organism), and a large number of interacting physiological processes (see the so-called "hallmarks of cancer"), several questions are not fully understood. Among these, we want to focus on the most clinically relevant ones, such as the general laws governing tumor growth and the development of metastases (secondary tumors, responsible of 90% of the deaths from a solid cancer). In this context, it is thus challenging to exploit the diversity of the data available in experimental settings (such as *in vitro* tumor spheroids or *in vivo* mice experiments) in order to improve our understanding of the disease and its dynamics, which in turn lead to validation, refinement and better tuning of the macroscopic models used in the axes 1 and 2 for clinical applications.

In recent years, several new findings challenged the classical vision of the metastatic development biology, in particular by the discovery of organism-scale phenomena that are amenable to a dynamical description in terms of mathematical models based on differential equations. These include the angiogenesis-mediated distant inhibition of secondary tumors by a primary tumor the pre-metastatic niche or the self-seeding phenomenon Building a general, cancer type specific, comprehensive theory that would integrate these dynamical processes remains an open challenge. On the therapeutic side, recent studies demonstrated that some drugs (such as the Sunitinib), while having a positive effect on the primary tumor (reduction of the growth), could *accelerate* the growth of the metastases. Moreover, this effect was found to be scheduling-dependent. Designing better ways to use this drug in order to control these phenomena is another challenge. In the context of combination therapies, the question of the *sequence* of administration between the two drugs is also particularly relevant.

One of the technical challenge that we need to overcome when dealing with biological data is the presence of potentially very large inter-animal (or inter-individual) variability.

Starting from the available multi-modal data and relevant biological or therapeutic questions, our purpose is to develop adapted mathematical models (*i.e.* identifiable from the data) that recapitulate the existing knowledge and reduce it to its more fundamental components, with two main purposes:

1. to generate quantitative and empirically testable predictions that allow to assess biological hypotheses or
2. to investigate the therapeutic management of the disease and assist preclinical studies of anti-cancerous drug development.

We believe that the feedback loop between theoretical modeling and experimental studies can help to generate new knowledge and improve our predictive abilities for clinical diagnosis, prognosis, and therapeutic decision. Let us note that the first point is in direct link with the axes 1 and 2 of the team since it allows us to experimentally validate the models at the biological scale (*in vitro* and *in vivo* experiments) for further clinical applications.

More precisely, we first base ourselves on a thorough exploration of the biological literature of the biological phenomena we want to model: growth of tumor spheroids, *in vivo* tumor growth in mice, initiation and development of the metastases, effect of anti-cancerous drugs. Then we investigate, using basic statistical tools, the data we dispose, which can range from: spatial distribution of heterogeneous cell population within tumor spheroids, expression of cell markers (such as green fluorescent protein for cancer cells or specific antibodies for other cell types), bioluminescence, direct volume measurement or even intra-vital images obtained with specific imaging devices. According to the data type, we further build dedicated mathematical models that are based either on PDEs (when spatial data is available, or when time evolution of a structured density can be inferred from the data, for instance for a population of tumors) or ODEs (for scalar longitudinal data). These models are confronted to the data by two principal means:

1. when possible, experimental assays can give a direct measurement of some parameters (such as the proliferation rate or the migration speed) or
2. statistical tools to infer the parameters from observables of the model.

This last point is of particular relevance to tackle the problem of the large inter-animal variability and we use adapted statistical tools such as the mixed-effects modeling framework.

Once the models are shown able to describe the data and are properly calibrated, we use them to test or simulate biological hypotheses. Based on our simulations, we then aim at proposing to our biological collaborators new experiments to confirm or infirm newly generated hypotheses, or to test different administration protocols of the drugs. For instance, in a collaboration with the team of the professor Andreas Bikfalvi (Laboratoire de l'Angiogénèse et du Micro-environnement des Cancers, Inserm, Bordeaux), based on confrontation of a mathematical model to multi-modal biological data (total number of cells in the primary and distant sites and MRI), we could demonstrate that the classical view of metastatic dissemination and development (one metastasis is born from one cell) was probably inaccurate, in mice grafted with metastatic kidney tumors. We then proposed that metastatic germs could merge or attract circulating cells. Experiments involving cells tagged with two different colors are currently performed in order to confirm or infirm this hypothesis.

Eventually, we use the large amount of temporal data generated in preclinical experiments for the effect of anti-cancerous drugs in order to design and validate mathematical formalisms translating the biological mechanisms of action of these drugs for application to clinical cases, in direct connection with the axis 1. We have a special focus on targeted therapies (designed to specifically attack the cancer cells while sparing the healthy tissue) such as the Sunitinib. This drug is indeed indicated as a first line treatment for metastatic renal cancer and we plan to conduct a translational study coupled between A. Bikfalvi's laboratory and medical doctors, F. Cornelis (radiologist) and A. Ravaud (head of the medical oncology department).

4. Application Domains

4.1. Tumor growth monitoring and therapeutic evaluation

Each type of cancer is different and requires an adequate model. More specifically, we are currently working on the following diseases:

- Glioma (brain tumors) of various grades,
- Metastases to the lung, liver and brain from various organs,
- Soft-tissue sarcoma,
- Kidney cancer and its metastases,
- non small cell lung carcinoma.

In this context our application domains are

- Image-driven patient-specific simulations of tumor growth and treatments,
- Parameter estimation and data assimilation of medical images.
- Machine and deep learning methods for delineating the lesions and stratifying patients according to their responses to treatment or risks of relapse.

4.2. Biophysical therapies

- Modeling of electrochemotherapy on biological and clinical scales.
- Evaluation of radiotherapy and radiofrequency ablation.

4.3. In-vitro and animals experimentations in oncology

- Theoretical biology of the metastatic process: dynamics of a population of tumors in mutual interactions, dormancy, pre-metastatic and metastatic niche, quantification of metastatic potential and differential effects of anti-angiogenic therapies on primary tumor and metastases.
- Mathematical models for preclinical cancer research: description and prediction of tumor growth and metastatic development, effect of anti-cancerous therapies.

5. Highlights of the Year

5.1. Highlights of the Year

- 2 abstracts accepted as oral communications at the PAGE meeting (main international conference in population modeling) (C. Nicolò and S. Benzekry)

5.1.1. Awards

- Floriane Gildel is French Young Talent 2019 - L'Oréal-UNESCO for Women in Science.

6. New Software and Platforms

6.1. August

Antibody Drug Uptake Simulator

KEYWORD: Mechanistic modeling

FUNCTIONAL DESCRIPTION: Numerical code to compute the uptake of an antibody drug at the scale of an histopathology blade. The computation domain (reconstructed from segmented images) is completely meshed and sub-divided accross computational nodes to distribute the load efficiently. The model (based on reaction-diffusion equations) is then solved in parallel using a domain decomposition method. C ++

- Contact: Olivier Saut

7. New Results

7.1. Machine learning and mechanistic modeling for prediction of metastatic relapse in early-stage breast cancer

Authors: *C. Nicolò; C. Périer*; M. Prague; C. Bellera; G. MacGrogan; *O.Saut; S. Benzekry*. Accepted for publication in the Journal of Clinical Oncology: Clinical Cancer Informatics.

Purpose: For patients with early-stage breast cancer, prediction of the risk of metastatic relapse is of crucial importance. Existing predictive models rely on agnostic survival analysis statistical tools (e.g. Cox regression). Here we define and evaluate the predictive ability of a mechanistic model for the time to metastatic relapse.

Methods: The data consisted of 642 patients with 21 clinicopathological variables. A mechanistic model was developed on the basis of two intrinsic mechanisms of metastatic progression: growth (parameter α) and dissemination (parameter μ). Population statistical distributions of the parameters were inferred using mixed-effects modeling. A random survival forest analysis was used to select a minimal set of 5 covariates with best predictive power. These were further considered to individually predict the model parameters, by using a backward selection approach. Predictive performances were compared to classical Cox regression and machine learning algorithms.

Results: The mechanistic model was able to accurately fit the data. Covariate analysis revealed statistically significant association of Ki67 expression with α (p=0.001) and EGFR with μ (p=0.009). Achieving a c-index of 0.65 (0.60-0.71), the model had similar predictive performance as the random survival forest (c-index 0.66-0.69) and Cox regression (c-index 0.62 - 0.67), as well as machine learning classification algorithms.

Conclusion: By providing informative estimates of the invisible metastatic burden at the time of diagnosis and forward simulations of metastatic growth, the proposed model could be used as a personalized prediction tool of help for routine management of breast cancer patients.

7.2. Numerical workflow for clinical electroporation ablation

Authors: *Olivier Gallinato*, *Baudouin Denis de Senneville*, Olivier Seror, *Clair Poignard*. Published in Physics in Medicine and Biology. https://hal.inria.fr/hal-02063020/file/paperIRE_workflow_R3.pdf.

The paper describes a numerical workflow, based on the "real-life" clinical workflow ofirreversible electroporation (IRE) performed for the treatment of deep-seated liver tumors. Thanksto a combination of numerical modeling, image registration algorithm and clinical data, our numerical workflow enables to provide the distribution of the electric field as effectively delivered by theclinical IRE procedure. As a proof of concept, we show on a specific clinical case of IRE ablation ofliver tumor that clinical data could be advantageously combined to numerical simulations in a nearfuture , in order to give to the interventional radiologists information on the effective IRE ablation.We also corroborate the simulated treated region with the post-treatment MRI performed 3 days after treatment.

7.3. A reduced Gompertz model for predicting tumor age using a population approach

Authors: *C. Vaghi*, A. Rodallec, R. Fanciullino, J. Ciccolini, J. Mochel, M. Mastri, *C. Poignard*, J. ML Ebos, *S. Benzekry*. Accepted for publication in PLoS Computational Biology. https://www.biorxiv.org/content/10.1101/670869v2

Tumor growth curves are classically modeled by means of ordinary differential equations. In analyzing the Gompertz model several studies have reported a striking correlation between the two parameters of the model, which could be used to reduce the dimensionality and improve predictive power.

We analyzed tumor growth kinetics within the statistical framework of nonlinear mixed-effects (population approach). This allowed the simultaneous modeling of tumor dynamics and inter-animal variability. Experimental data comprised three animal models of breast and lung cancers, with 833 measurements in 94 animals. Candidate models of tumor growth included the exponential, logistic and Gompertz. The exponential and – more notably – logistic models failed to describe the experimental data whereas the Gompertz model generated very good fits. The previously reported population-level correlation between the Gompertz parameters was further confirmed in our analysis ($R^2 > 0.92$ in all groups). Combining this structural correlation with rigorous population parameter estimation, we propose a reduced Gompertz function consisting of a single individual parameter (and one population parameter). Leveraging the population approach using Bayesian inference, we estimated times of tumor initiation using three late measurement timepoints. The reduced Gompertz model was found to exhibit the best results, with drastic improvements when using Bayesian inference as compared to likelihood maximization alone, for both accuracy and precision. Specifically, mean accuracy was 12.2% versus 78% and mean precision was 15.6 days versus 210 days, for the breast cancer cell line.

These results offer promising clinical perspectives for the personalized prediction of tumor age from limited data at diagnosis. In turn, such predictions could be helpful for assessing the extent of invisible metastasis at the time of diagnosis.

The code and the data used in our analysis are available at https://github.com/cristinavaghi/plumky.

7.4. T2-based MRI Delta-Radiomics Improve Response Prediction in Soft-Tissue Sarcomas Treated by Neoadjuvant Chemotherapy

Authors: *Amandine Crombé*, *Cynthia Perier*, Michèle Kind, *Baudouin Denis de Senneville*, Francois Le Loarer, Antoine Italiano, Xavier Buy, *Olivier Saut*. Published in Journal of Magnetic Reasonance Imaging https://hal.inria.fr/hal-01929807v2

Background: Standard of care for patients with high-grade soft-tissue sarcoma (STS) are being redefined since neoadjuvant chemotherapy (NAC) has demonstrated a positive effect on patients' outcome. Yet, response evaluation in clinical trials still remains on RECIST criteria.

Purpose: To investigate the added value of a Delta-radiomics approach for early response prediction in patients with STS undergoing NAC Study type: Retrospective Population: 65 adult patients with newly-diagnosed, locally-advanced, histologically proven high-grade STS of trunk and extremities. All were treated by anthracycline-based NAC followed by surgery and had available MRI at baseline and after 2 cycles. Field strength/Sequence: Pre- and post-contrast enhanced T1-weighted imaging (T1-WI), turbo spin echo T2-WI at 1.5T.

Assessment: A threshold of <10% viable cells on surgical specimen defined good response (Good-HR). Two senior radiologists performed a semantic analysis of the MRI. After 3D manual segmentation of tumors at baseline and early evaluation, and standardization of voxelsizes and intensities, absolute changes in 33 texture and shape features were calculated. Statistical tests: Classification models based on logistic regression, support vector machine, k-nearest neighbors and random forests were elaborated using cross-validation (training and validation) on 50 patients ('training cohort') and was validated on 15 other patients ('test cohort').

Results: 16 patients were good-HR. Neither RECIST status, nor semantic radiological variables were associated with response except an edema decrease (p=0.003) although 14 shape and texture features were (range of p-values: 0.002-0.037). On the training cohort, the highest diagnostic performances were obtained with random forests built on 3 features, which provided: AUROC=0.86, accuracy=88.1%, sensitivity=94.1%, specificity=66.3%. On the test cohort, this model provided an accuracy of 74.6% but 3/5 good-HR were systematically ill-classified.

Data conclusions: A T2-based Delta-Radiomics approach can improve early response prediction in STS patients with a limited number of features.

7.5. Quantitative mathematical modeling of clinical brain metastasis dynamics in non-small cell lung cancer

Authors: *M. Bilous*, C. Serdjebi, A. Boyer, P. Tomasini, *C. Pouypoudat*, D. Barbolosi, F. Barlesi, F. Chomy, *S. Benzekry*. Published in Scientific Reports. https://hal.inria.fr/hal-01928442v2

Brain metastases (BMs) are associated with poor prognosis in non-small cell lung cancer (NSCLC), but are only visible when large enough. Therapeutic decisions such as whole brain radiation therapy would benefit from patient-specific predictions of radiologically undetectable BMs. Here, we propose a mathematical modeling approach and use it to analyze clinical data of BM from NSCLC. Primary tumor growth was best described by a gompertzian model for the pre-diagnosis history, followed by a tumor growth inhibition model during treatment. Growth parameters were estimated only from the size at diagnosis and histology, but predicted plausible individual estimates of the tumor age (2.1–5.3 years). Multiple metastatic models were further assessed from fitting either literature data of BM probability (n = 183 patients) or longitudinal measurements of visible BMs in two patients. Among the tested models, the one featuring dormancy was best able to describe the data. It predicted latency phases of 4.4–5.7 months and onset of BMs 14–19 months before diagnosis. This quantitative model paves the way for a computational tool of potential help during therapeutic management.

7.6. Optimizing 4D abdominal MRI: Image denoisingusing an iterative back-projection approach

Authors: *B Denis de Senneville*, C R Cardiet, A J Trotier, E J Ribot, L Lafitte, L Facq, S Miraux. Published in Physics in Medicine and Biology. https://hal.archives-ouvertes.fr/hal-02367839/file/2019_4D_reconstruction_revision2_final.pdf

4D-MRI is a promising tool for organ exploration, target delineationand treatmentplanning. Intra-scan motion artifacts may be greatly reduced by increasing the imagingframe rate. However, poor signal-to-noise ratios (SNR) are observed when increasingspatial and/or frame number per physiological cycle, in particular inthe abdomen.In the current work, the proposed 4D-MRI method favored spatial resolution, framenumber, isotropic voxels and large field-of-view (FOV) during MR-acquisition. Theconsequential SNR penalty in the reconstructed data is addressed retrospectively usingan iterative back-projection (IBP) algorithm. Practically, after computing individualspatial 3D deformations present in the images using a deformable image registration(DIR) algorithm, each 3D image is individually enhanced by fusing several successiveframes in its local temporal neighborood, these latter being likely tocover commonindependent informations. A tuning parameter allows one to freely readjust the balancebetween temporal resolution and precision of the 4D-MRI.The benefit of the method was quantitatively evaluated on the thorax of 6 miceunder free breathing using a clinically acceptable duration. Improved 4D cardiacimaging was also shown in the heart of 1 mice. Obtained results are comparedto theoretical expectations and discussed. The proposed implementation is easilyparallelizable and optimized 4D-MRI could thereby be obtained with a clinicallyacceptable duration.

7.7. Optimal Scheduling of Bevacizumab and Pemetrexed/cisplatin Dosing in Non-Small Cell Lung Cancer

Authors: Benjamin Schneider, Arnaud Boyer, Joseph Ciccolini, Fabrice Barlési, Kenneth Wang, *Sébastien Benzekry**, Jonathan Mochel*. * = co-senior authors. Published in CPT: Pharmacometrics and Systems Pharmacology. https://hal.inria.fr/hal-02109335

Bevacizumab-pemetrexed/cisplatin (BEV-PEM/CIS) is a first line therapeutic for advanced non-squamous non-small cell lung cancer (NSCLC). Bevacizumab potentiates PEM/CIS cytotoxicity by inducing transient tumor vasculature normalization. BE V- PEM/CIS has a narrow therapeutic window. Therefore, it is an attractive target for administration schedule optimization. The present study leverages our previous work on BEV-PEM/CIS pharmacodynamic modeling in NSCLC-bearing mice to estimate the optimal gap in the scheduling of sequential BEV-PEM/CIS. We predicted the optimal gap in BEV-PEM/CIS dosing to be 2.0 days in mice and 1.2 days in humans. Our simulationssuggest that the efficacy loss in scheduling BEV-PEM/CIS at too great of a gap is much less than the efficacy loss in scheduling BEV-PEM/CIS at too short of a gap.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

- Research contract between Roche and the MONC team.
- Collaboration contract with Sophia Genetics in the context of the Pimiento project.

8.2. Bilateral Grants with Industry

Pimiento project from MSDAvenir (http://www.msdavenir.fr/) through Inria Foundation.

9. Partnerships and Cooperations

9.1. National Initiatives

9.1.1. Plan Cancer

9.1.1.1. NUMEP

Plan Cancer NUMEP: 2016–2019. Numerics for Clinical Electroporation

Funding: 460 kE.

Partners: Institut de Pharmacologie de Toulouse, CHU J. Verdier de Bondy.

Duration: Octobre 2016—Septembre 2019.

Project leader: C. Poignard

Co-PI: M-P. Rols (IPBS), O. Séror (CHU J. Verdier)

9.1.1.2. Moglimaging

Project acronym - Moglimaging: Modeling of Glioblastoma treatment-induced resistance and heterogeneity by multi-modal imaging.

Partners - Inria Monc, IUCT, Institut Pasteur, Univ. Grenoble, INSERM, Inria Mamba.

Duration - from Nov. 2016 to May 2020.

Coordinator - E. Cohen-Jonathan Moyal, Institut Universitaire du Cancer Toulouse / Local coordinator - O. Saut.

Team participants - S. Benzekry, A. Collin, C. Poignard, O. Saut.

9.1.1.3. Systems Biology of Renal Carcinoma

Title: Plan Cancer Systems Biology of Renal Carcinoma using a Mouse RCC model

Partners : LAMC, INSERM-Univ. Bordeaux.

Duration - June 2018 to June 2021

Team participants: O. Saut, S. Benzekry (co-PI)

Funding: 116.64k€

9.1.1.4. QUANTIC

Plan Cancer QUANTIC: 2020–2022. QUANTitative modeling combined to statistical learning to understand and predict resistance to Immune-checkpoint inhibition in non-small cell lung Cancer.

Funding: 338 k€

Partners: Inria Team MONC, SMARTc (Centre de Recherche sur le Cancer de Marseille, Inserm, CNRS), Assistance Publique Hôpitaux de Marseille

Duration: Décembre 2019 — Décembre 2022

Project leader: S. Benzekry

Co-PI: D. Barbolosi (SMARTc), F. Barlési (AP-HM)

9.1.2. Transnation call: INCA/ARC

Title: Minimally and non-invasive methods for early detection and/or progression of low grade glioma

Partners: Inria Monc, Inria SISTM, INSERM, Humanitas Research Hostital, Univ. Bergen

Acronym: Glioma PRD

Team participants: A. Collin, C. Poignard, O. Saut (local PI)

Total funds: 1M150, Monc's share 275k€.

9.1.3. Competitivity Clusters

Labex TRAIL (http://trail.labex.u-bordeaux.fr): MOD Project Consolidation. 1 2-years post-doc position (100k€), led by A. Collin, 1 PhD funding (100k€) led by O. Saut.

9.2. International Initiatives

9.2.1. Inria International Labs

Inria@SiliconValley
Associate Team involved in the International Lab:

9.2.1.1. Num4SEP

Title: Numerics for Spherical Electroporation

International Partner (Institution - Laboratory - Researcher):

University of California, Santa Barbara (United States) Frederic Gibou

Start year: 2017

See also: http://num4sep.bordeaux.inria.fr/

Electroporation-based therapies (EPTs) consist in applying high voltage short pulses to cells in order to create defects in the plasma membrane. They provide interesting alternatives to standard ablative techniques, for instance for deep seated badly located tumors. However their use is still limited due to a lack of knowledge of tissue electroporation. The goal of the associate team is to focus on the multiscale numerical modeling of spheroid electroporation, in order to provide new insights in electroporation at the mesoscopic scales (spheroids provide interesting tumor-like biological models). Benefiting from the expertise of F. Gibou's team in HPC for multiphysics, and the expertise of the team MONC in tumor growth and cell electroporation modeling, the goal of the associate team Num4SEP is to obtain accurate and efficient numerical tools for the quantitative evaluation of the EPTs at the mesoscopic scale.

9.2.2. Inria Associate Teams Not Involved in an Inria International Labs

9.2.2.1. METAMATS

Title: Modeling ExperimenTAl MetAsTasiS

International Partner (Institution - Laboratory - Researcher):

Roswell Park Cancer Institute (United States) - Department of Cancer Genetics Department of Medicine Department of Pharmacology and Therapeutics (Graduate Program) - John Ebos

Start year: 2017

See also: http://metamats.bordeaux.inria.fr/

The aim of the METAMATS associate team is to bring together a cancer biology experimental laboratory led by John ML Ebos (Roswell Park Cancer Institute) and the inria MONC team composed of applied mathematicians. The Ebos laboratory is specialized in the study of anti-cancer therapeutics (in particular, novel biologically targeted therapeutics such as anti-angiogenics and immunotherapies) on the development of metastases and produces unique, hard-to-obtain data sets on this process' dynamics. The MONC team is specialized in mathematical models in oncology, with a dedicated axis about modeling support and methodological development for analysis of data from preclinical studies. In particular, the work of S. Benzekry puts emphasis on proposing, studying and validating mathematical models of metastatic development under the action of various therapeutic modalities. Indeed, metastatic expansion remains the main challenge in the treatment of cancer and integrative studies combining experiments, mathematical models and clinical data have the potential to yield predictive computational tools of help to assist both the design of clinical trials and clinical oncologists in therapeutic decisions such as the control of the toxicity/efficacy balance or the optimal combination of treatment modalities.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events: Organisation

10.1.1.1. General Chair, Scientific Chair

- C. Poignard: Organization of the Core-to-Core meeting March 21st-22nd at Bordeaux. This is the annual meeting of the JSPS Consortium « Establishing networks in mathematical medicine », which gathers Osaka University (Suzuki's lab), Vanderbilt University (Quaranta's lab), St Andrews Univ. (Chaplain's lab), and Inria Bordeaux team MONC.

10.1.2. Scientific Events: Selection

10.1.2.1. Reviewer

S. Benzekry served as a reviewer for the IEEE Control Systems Society Conference and for the International Symposium on Mathematical and Computational Oncology (Lake Tahoe, NV, USA).

10.1.3. Journal

10.1.3.1. Member of the Editorial Boards

- S. Benzekry is a member of the Editorial Board of "Mathematical Biosciences and Engineering"
- C. Poignard is a member of the editorial board of DCDS-S.

10.1.3.2. Reviewer - Reviewing Activities

- S. Benzekry served as a reviewer for Nature Communications, Cancer Research, Clinical Pharmacology and Therapeutics, Scientific Reports and ESAIM: Proc.
- A. Collin: Reviewer for Plos One.
- C. Etchegaray: ESAIM: Mathematical Modelling and Numerical Analysis, Royal Society Open Sciences.
- O. Saut: Mathematical Modelling of Natural Phenomena, PLOS One, Journal of Theoretical Biology, EBioMedicine, Nature Communications, Medical Image Analysis.

10.1.4. Invited Talks

- S. Benzekry: May 2019, RITS conference (Recherche en Imagerie et Technologies pour la Sante) of the French Society of Biomedical Engineering (SFGBM), Tours, France.
- S. Benzekry: May 2019, Seminaire phases I en oncologie, Marseille, France. Old concept, new name? l'intelligence artificielle en oncologie.
- S. Benzekry: May 2019, Masterclass Mathematiques appliquees CEPS Mathematiques Des Sciences du Vivant, CIRM, Marseille, France.
- S. Benzekry: May 2019, NCI Mathematical Oncology Meeting, Portland, USA.
- S. Benzekry: May 2019, Biomedicum Helsinki Seminar (Invitation by Sampsa Hautaniemi), Faculty of Medicine, Helsinki, Finland.
- S. Benzekry: June 2019, Seminar in the Novartis pharmacometrics department. Basel, Switwerland. Artificial intelligence and machine learning in oncology: myths and reality.
- S. Benzekry: July 2019, International Society of Pharmacometrics (ISoP) workshop. Paris, France.
- C. Etchegaray: Equadiff conference, Leiden.
- O. Saut: July 2019, Mathematical models in Biology and Medicine, Vienna, Austria.

10.1.5. Scientific Expertise

- S. Benzekry is expert within the scientific board of the national multi-thematic institute (ITMO) Cancer of the French alliance for health sciences (AVIESAN).
- A. Collin, Steering Committee Axe 5, Cancéropole Grand Sud Ouest
- C. Poignard: Member of the INCA committee on pediatric cancer data structuration
- C. Poignard: Member of the GAMNI prize committee.
- O. Saut: expert in the "Single Cell" call at ITMO Cancer / Plan Cancer.
- O. Saut: expert for the French Ministry of Research (for various programs including PHC and EGIDE programs).
- O. Saut: reviewer for SIRIC CURAMUS projects.

10.1.6. Research Administration

- S. Benzekry is a member of the local Inria commission of informatical tools users (CUMI)
- Annabelle Collin, member of "conseil de Laboratoire", Institut Mathématique de Bordeaux.
- Annabelle Collin, "chargée de mission parité", Institut Mathématique de Bordeaux.
- Annabelle Collin, member of "commission ADT", Inria Bordeaux Sud-Ouest.
- Annabelle Collin, "chargée de mission Développement Durable et Responsabilité Sociétale", ENSEIRB-MATMECA.
- Annabelle Collin, elected member of "comité de centre", Inria Bordeaux Sud-Ouest.
- C. Poignard is a member of the Inria Evaluation Committee
- Clair Poignard, member of "conseil scientifique", Institut Mathématique de Bordeaux.
- Olivier Saut: member of the steering committee of ITMO consortium HTE (on tumor heterogeneity) and coordinator of work package Model and Data.
- Olivier Saut: member of the steering committee of Labex TRAIL (Translational Imaging) http://trail.labex.u-bordeaux.fr.
- Olivier Saut: in charge of "Interdisciplinarité" at Institut de Mathématiques du CNRS http://www.cnrs.fr/insmi.
- Olivier Saut: member of the steering committee of the MITI at CNRS http://www.cnrs.fr/mi.
- Olivier Saut: member of the steering committee of the Oncosphere Project https://siric-brio.com/oncosphere/.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

Master : S. Benzekry, Cours "Modélisation de la croissance tumorale", 3h, niveau M2, Université de Tours, France.

Master : S. Benzekry, Cours "Mathematical tools for pharmacometrics", 10h, niveau M2, Aix-Marseille Université, France.

Master : S. Benzekry, TP "Introduction to Monolix", 2 x 3h, EUR "Modeling Life Sciences" (Université de Bordeaux) and DESU “Pharmacokinetics modeling" (Aix-Marseille Université), France.

Master: A. Collin, Pratical C++ programming, 96h, niveau M1, INP Bordeaux, France.

Master: A. Collin, Mesh theory, 36h, niveau M2, INP Bordeaux, France.

Master: A. Collin, Machine Learning, niveau M2, INP Bordeaux, France.

PHD: A. Collin, Modeling Life Science Module, Digital Public Health, Graduate Program.

Licence : C. Poignard, Undergraduate teaching in Numerical and Applied Mathematics, 80h, L3-M1, INP Bordeaux, ENSAM, France.

Master: O. Saut, Mathematical modeling in Oncology, 2h, niveau M2, Univ. Bordeaux, France.

10.2.2. Supervision

PhD: C. Nicolò, *Mathematical modeling of systemic aspects of cancer and cancer therapy*, 2016 - 2019, supervision S. Benzekry and O. Saut. Defended October 14th, 2019.

PhD in progress: C. Vaghi, Improving intra-tumor drug distribution of anti-cancer nanoparticles by data-informed mathematical modeling, Nov 2017 - Nov 2020, supervision S. Benzekry and C. Poignard.

PhD in progress: Sergio Corridore, 2016-..., supervision A. Collin and C. Poignard

PhD in progress: Pedro Jaramillo-Aguayo, 2019-..., supervision A. Collin and C. Poignard

PhD: C. Perier, *Analyse quantitative des données de routine clinique pour le pronostic précoce en oncologie*, 2016-2019, supervision B. Denis de Senneville and O. Saut. Defended November 14th, 2019.

PhD in progress: A. Crombé, 2017-..., supervision O. Saut

10.2.3. Juries

- S. Benzekry: Reviewer of the PhD thesis of E. Kozlowska (University of Helsinki, Finland)
- S. Benzekry: Reviewer of the PhD thesis of A. Alvarez-Arenas Alcami (Universidad de Castilla La Mancha, Ciudad Real, Spain)
- S. Benzekry: Reviewer of the PhD thesis of A-S Giaccobi (Université Picardie Jules Verne)
- S. Benzekry: Reviewer of the PhD thesis of J Goya-Outi (Paris Saclay University)
- A. Collin, Phd defense committee, Antoine Gérard, Inria Bordeaux Sud-Ouest, Modèles numériques personnalisés de la fibrillation auriculaire, 10 juillet 2019
- A. Collin, Phd defense committee, Thibaut Hirschler, INSA Lyon, IsoGeometric Modeling for the Optimal Design of Aerostructures, 13 nov. 2019
- A. Collin, Jury member, agrégation de Mathématiques
- O. Saut: Reviewer of the HdR thesis of A. Decoene, Univ. Paris Sud, France.
- O. Saut: Reviewer of the PhD thesis of A. Perrillat-Mercerot, Univ. Poitiers, France.
- O. Saut: PhD defense committee, A. Hocquelet, Univ. Bordeaux, France
- O. Saut: PhD defense committee, G. Birindelli, Univ. Bordeaux, France

10.3. Popularization

10.3.1. Internal or external Inria responsibilities

10.3.2. Interventions

- A. Collin, intervention "midi-rencontre sur les femmes dans les sciences", association TousEn-Sciences
- A. Collin, intervention "place de la femme dans les métiers scientifiques", Robot makers' days
- C. Etchegaray: Fête de la science.
- O. Saut: Journée Scientifique Institut Bergonié.

10.3.3. Internal action

- O. Saut: Café des Sciences.

11. Bibliography

Major publications by the team in recent years

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[2] S. BENZEKRY, C. LAMONT, A. BEHESHTI, A. TRACZ, J. M. EBOS, L. HALTKY, P. HAHNFELDT.*Classical Mathematical Models for Description and Forecast of Experimental Tumor Growth*, in "PLoS Computational Biology", August 2014, vol. 10, n^o 8, e1003800 [*DOI :* 10.1371/JOURNAL.PCBI.1003800], https://hal.inria.fr/hal-00922553

[3] S. BENZEKRY, A. TRACZ, M. MASTRI, R. CORBELLI, D. BARBOLOSI, J. M. EBOS.*Modeling Spontaneous Metastasis following Surgery: An In Vivo-In Silico Approach*, in "Cancer Research", February 2016, vol. 76, n^o 3, p. 535 - 547 [*DOI :* 10.1158/0008-5472.CAN-15-1389], https://hal.inria.fr/hal-01222046

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[5] T. COLIN, F. CORNELIS, J. JOUGANOUS, J. PALUSSIÈRE, O. SAUT.*Patient specific simulation of tumor growth, response to the treatment and relapse of a lung metastasis: a clinical case*, in "Journal of Computational Surgery", 2015, 18 [*DOI :* 10.1186/S40244-014-0014-1], https://hal.inria.fr/hal-01102586

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[7] D.-C. IMBS, R. EL CHEIKH, A. BOYER, J. CICCOLINI, C. MASCAUX, B. LACARELLE, F. BARLESI, D. BARBOLOSI, S. BENZEKRY.*Revisiting bevacizumab + cytotoxics scheduling using mathematical modeling: proof of concept study in experimental non-small cell lung carcinoma*, in "CPT: Pharmacometrics and Systems Pharmacology", 2018, p. 1-9 [*DOI :* 10.1002/PSP4.12265], https://hal.inria.fr/hal-01624423

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[9] M. LEGUEBE, A. SILVE, L. M. MIR, C. POIGNARD.*Conducting and permeable states of cell membrane submitted to high voltage pulses: Mathematical and numerical studies validated by the experiments*, in "Journal of Theoretical Biology", November 2014, vol. 360, p. 83-94 [*DOI :* 10.1016/J.JTBI.2014.06.027], https://hal.inria.fr/hal-01027477

[10] F. RAMAN, E. SCRIBNER, O. SAUT, C. WENGER, T. COLIN, H. M. FATHALLAH-SHAYKH.*Computational Trials: Unraveling Motility Phenotypes, Progression Patterns, and Treatment Options for Glioblastoma Multiforme*, in "PLoS ONE", January 2016, vol. 11, n^{o} 1 [*DOI :* 10.1371/JOURNAL.PONE.0146617], https://hal.inria.fr/hal-01396271

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Articles in International Peer-Reviewed Journal

[11] M. BILOUS, C. SERDJEBI, A. BOYER, P. TOMASINI, C. POUYPOUDAT, D. BARBOLOSI, F. BARLESI, F. CHOMY, S. BENZEKRY.*Quantitative mathematical modeling of clinical brain metastasis dynamics in non-small cell lung cancer*, in "Scientific Reports", September 2019, vol. 9, n^{o} 1 [*DOI :* 10.1038/S41598-019-49407-3], https://hal.inria.fr/hal-01928442

[12] V. BONNAILLIE-NOËL, C. POIGNARD, G. VIAL.*Asymptotic expansions for the conductivity problem with nearly touching inclusions with corner*, in "Annales Henri Lebesgue", 2019, https://hal.archives-ouvertes.fr/hal-01766052

[13] C. BRONNIMANN, A. HUCHET, J. BENECH-FAURE, C. DUTRIAUX, O. SAUT, E. BLAIS, O. MOLLIER, R. TROUETTE, V. VENDRELY.*Interval between planning and frameless stereotactic radiotherapy for brain metastases: are our margins still accurate?*, in "Neuro-Oncology Practice", October 2019 [*DOI :* 10.1093/NOP/NPZ048], https://hal.inria.fr/hal-02406540

[14] J. CICCOLINI, D. BARBOLOSI, N. ANDRE, S. BENZEKRY, F. BARLESI.*Combinatorial immunotherapy strategies : most gods throw dice, but fate plays chess : Editorial*, in "Annals of Oncology", September 2019 [*DOI :* 10.1093/ANNONC/MDZ297], https://hal.inria.fr/hal-02383826

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[16] Y. COUDIÈRE, A. DAVIDOVIĆ, C. POIGNARD.*Modified bidomain model with passive periodic heterogeneities*, in "Discrete and Continuous Dynamical Systems - Series S", October 2019 [*DOI :* 10.3934/DCDSS.2020126], https://hal.inria.fr/hal-02363470

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[18] A. CROMBÉ, O. SAUT, J. GUIGUI, A. ITALIANO, X. BUY, M. KIND.*Influence of Temporal Parameters of DCE-MRI on the Quantification of Heterogeneity in Tumor Vascularization*, in "Journal of Magnetic Resonance Imaging", May 2019, vol. 50, n^o 6, p. 1773-1788 [*DOI :* 10.1002/JMRI.26753], https://hal.inria.fr/hal-02406497

[19] B. DENIS DE SENNEVILLE, C. R. CARDIET, A. TROTIER, E. RIBOT, L. LAFITTE, L. FACQ, S. MIRAUX.*Optimizing 4D abdominal MRI: image denoising using an iterative back-projection approach*, in "Physics in Medicine and Biology", November 2019, forthcoming [*DOI :* 10.1088/1361-6560/AB563E], https://hal.archives-ouvertes.fr/hal-02367839

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[37] S. BENZEKRY.*Machine learning versus mechanistic modeling for prediction of metastatic relapse in breast cancer*, in "2019 CSBC-PSON Mathematical Oncology Meeting", Portland, United States, May 2019, https://hal.inria.fr/hal-02424419

[38] S. BENZEKRY.*Mechanistic modeling of metastasis: cancer at the organism scale*, in "International Society of Pharmacometrics (ISoP) workshop", Paris, France, July 2019, https://hal.inria.fr/hal-02424424

[39] C. VAGHI.*Combining Population Modeling and Bayesian Inference for Tumor Growth Prediction*, in "SMB 2019 annual meeting", Montreal, Canada, July 2019, https://hal.archives-ouvertes.fr/hal-02424592

International Conferences with Proceedings

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Conferences without Proceedings

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Project-Team PLEIADE

Patterns of diversity and networks of function

IN COLLABORATION WITH: Laboratoire Bordelais de Recherche en Informatique (LaBRI)

IN PARTNERSHIP WITH:
CNRS

INRA

Institut national de recherche pour l'agriculture, l'alimentation et l'environnement

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Computational Biology

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Project-Team PLEIADE

Creation of the Team: 2015 January 01, updated into Project-Team: 2019 March 01

Keywords:

Computer Science and Digital Science:

A3.1. - Data
A3.2. - Knowledge
A3.3.2. - Data mining
A3.3.3. - Big data analysis
A3.4. - Machine learning and statistics
A6.2.8. - Computational geometry and meshes

Other Research Topics and Application Domains:

B1.1.7. - Bioinformatics
B1.1.10. - Systems and synthetic biology
B3. - Environment and planet

1. Team, Visitors, External Collaborators

Research Scientists

David Sherman [Team leader, Inria, Senior Researcher, HDR]
Pascal Durrens [CNRS, Researcher, HDR]
Alain Franc [INRA, Senior Researcher, HDR]

Technical Staff

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Franck Salin [INRA, Engineer]

PhD Student

Mohamed Anwar Abouabdallah [Inria, PhD Student, from Oct 2019]

Post-Doctoral Fellow

Swarna Kanchan [Inria, Post-Doctoral Fellow]

Administrative Assistant

Catherine Cattaert Megrat [Inria, Administrative Assistant]

2. Overall Objectives

2.1. Overall Objectives

Diversity, evolution, and inheritance form the heart of modern biological thought. Modeling the complexity of biological systems has been a challenge of theoretical biology for over a century [29] and flourished with the evolution of data for describing biological diversity, most recently with the transformative development of high-throughput sequencing. However, most concepts and tools in ecology and population genetics for capitalizing on this wealth of data are still not adapted to high throughput data production. A better connection between high-throughput data production and tool evolution is highly needed: *computational biodiversity*.

Paradoxically, diversity emphasizes differences between biological objects, while modeling aims at unifying them under a common framework. This means that there is a limit beyond which some components of diversity cannot be mastered by modeling. We need efficient methods for recognizing patterns in diversity, and linking them to patterns in function. It is important to realize that diversity in function is not the same as coupling observed diversity with function. Diversity informs both the study of traits, and the study of biological functions (Figure 1). The double challenge is to measure these links quickly and precisely with pattern recognition, and to explore the relations between diversity in traits and diversity in function through modeling

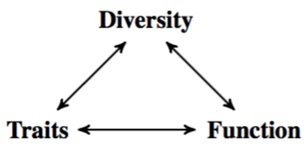

Figure 1. Diversity informs both the study of traits, and the study of biological functions

PLEIADE links recognition of patterns, classes, and interactions with applications in biodiversity studies and biotechnology. We develop distance methods for NGS datasets at different levels of organization: between genomes, between individual organisms, and between communities; and develop high-performance pattern recognition and statistical learning techniques for analyzing the resulting point clouds. We refine inferential methods for building hierarchical models of networks of cellular functions, exploiting the mathematical relations that are revealed by large-scale comparison of related genomes and their models. We combine these methods into integrated e-Science solutions to place these tools directly in the hands of biologists.

Our methodology (Figure 2) is designed pragmatically to advance the state of the art in applications from biodiversity and biotechnology: molecular based systematics and community ecology, annotation and modeling for biotechnology.

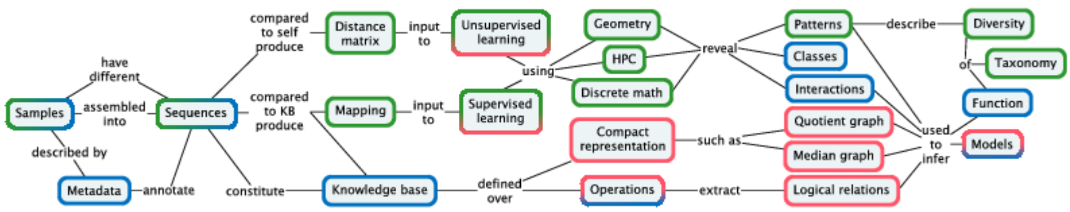

Figure 2. PLEIADE *is a pluridisciplinary team. Each application in biodiversity and biotechnology follows a path calling on methods from biology (blue), mathematics (green), and computer science (red).*

3. Research Program

3.1. A Geometric View of Diversity

Diversity may be studied as a set of dissimilarities between objects. The underlying mathematical construction is the notion of distance. Knowing a set of objects, it is possible, after computation of pairwise distances, or sometimes dissimilarities, to build a Euclidean image of it as a point cloud in a space of relevant dimension. Then, diversity can be associated with the shape of the point cloud. The human eye is often far better than an algorithm at recognizing a pattern or shape. One objective of our project is to narrow the gap between the story that a human eye can tell, and that an algorithm can tell. Several directions will be explored. First, this requires mastering classical tools in dimension reduction, mainly algebraic tools (PCA, NGS, Isomap, eigenmaps, etc ...). Second, neighborhoods in point clouds naturally lead to graphs describing the neighborhood networks. There is a natural link between modular structures in distance arrays and communities on graphs. Third, points (representing, say, DNA sequences) are samples of diversity. Dimension reduction may show that they live on a given manifold. This leads to geometry (differential or Riemannian geometry). It is expected that some properties of the manifold can tell something of the constraints on the space where measured individuals live. The connection between Riemannian geometry and graphs, where weighted graphs are seen as mesh embedded in a manifold, is currently an active field of research [28], [27]. See as well [30] for a link between geometric structure, linear and nonlinear dimensionality reduction.

Biodiversity and high-performance computing: Most methods and tools for characterizing diversity have been designed for datasets that can be analyzed on a laptop, but NGS datasets produced for metabarcoding are far too large. Data analysis algorithms and tools must be revisited and scaled up. We will mobilize both distributed algorithms like the Arnoldi method and new algorithms, like random projection or column selection methods, to build point clouds in Euclidean spaces from massive data sets, and thus to overcome the cubic complexity of computation of eigenvectors and eigenvalues of very large dense matrices. We will also link distance geometry [22] with convex optimization procedures through matrix completion [15], [17].

Intercalibration: There is a considerable difference between supervised and unsupervised clustering: in supervised clustering, the result for an item i is independent from the result for an item $j \neq i$, whereas in unsupervised clustering, the result for an item i (e.g. the cluster it belongs to, and its composition) depends on nearby items $j \neq i$. Which means that the result may change if some items are added to or subtracted from the sample. This raises the more global problem of how to merge two studies to yield a more comprehensive view of biodiversity?

3.2. Knowledge Management for Biology

The heterogenous data generated in computational molecular biology and ecology are distinguished not only by their volume, but by the richness of the many levels of interpretation that biologists create. The same nucleic acid sequence can be seen as a molecule with a structure, a sequence of base pairs, a collection of genes, an allele, or a molecular fingerprint. To extract the maximum benefit from this treasure trove we must organize the knowledge in ways that facilitate extraction, analysis, and inference. Our focus has been on the efficient representation of relations between biological objects and operations on those representations, in particular heuristic analyses and logical inference.

PLEIADE will develop applications in comparative genomics of related organisms, using new mathematical tools for representing compactly, at different scales of difference, comparisons between related genomes. New methods based on distance geometry will refine these comparisons. Compact representations can be stored, exchanged, and combined. They will form the basis of new simultaneous genome annotation methods, linked directly to abductive inference methods for building functional models of the organisms and their communities.

Since a goal of PLEIADE is to integrate diversity throughout the analysis process, it is necessary to incorporate **diversity as a form of knowledge** that can be stored in a knowledge base. Diversity can be represented using various compact representations, such as trees and quotient graphs storing nested sets of relations. Extracting structured representations and logical relations from integrated knowledge bases (Figure 2) will require domain-specific query methods that can express forms of diversity.

3.3. Modeling by successive refinement

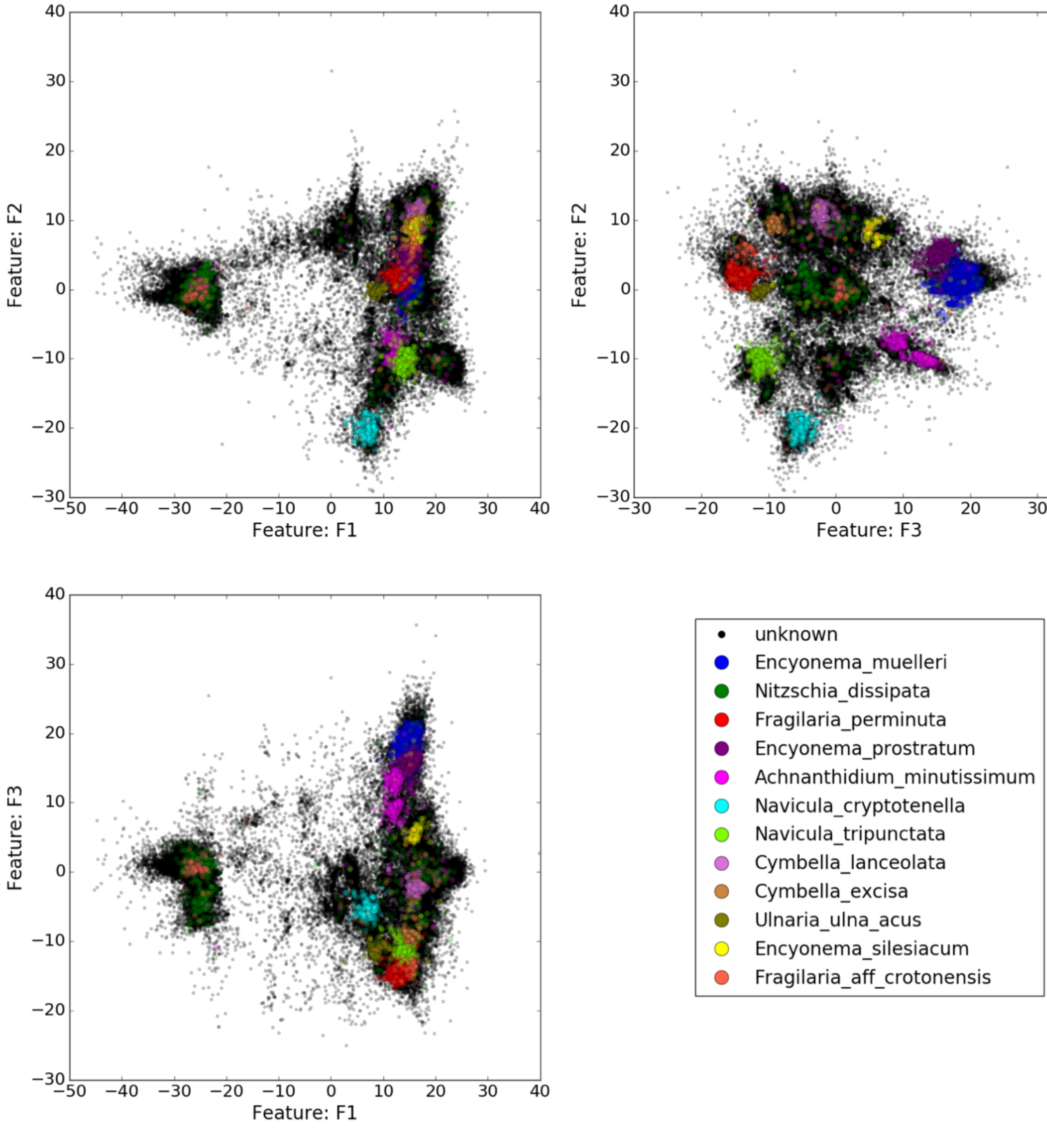

Figure 3. Validation of high density islands using supervised classification. Metagenomic reads from diatoms in Lake Geneva [26] were analyzed by the method from [16] and colored by species according to a reference database.

Describing the links between diversity in traits and diversity in function will require comprehensive models, assembled from and refining existing models. A recurring difficulty in building comprehensive models of biological systems is that accurate models for subsystems are built using different formalisms and simulation techniques, and hand-tuned models tend to be so focused in scope that it is difficult to repurpose them [13]. Our belief is that a sustainable effort in building efficient behavioral models must proceed incrementally, rather than by modeling individual processes *de novo*. *Hierarchical modeling* [10] is one way of combining specific models into networks. Effective use of hierarchical models requires both formal definition of the semantics of such composition, and efficient simulation tools for exploring the large space of complex behaviors. We have previously shown that this approach can be effective for certains kinds of systems in biotechnology [2], [14] and medicine [12]. Our challenge is to adapt incremental, hierarchical refinement to modeling organisms and communities in metagenomic and comparative genomic applications.

4. Application Domains

4.1. Genome and transcriptome annotation, to model function

Sequencing genomes and transcriptomes provides a picture of how a biological system can function, or does function under a given physiological condition. Simultaneous sequencing of a group of related organisms is now a routine procedure in biological laboratories for studying a behavior of interest, and provides a marvelous opportunity for building a comprehensive knowledge base of the relations between genomes. Key elements in mining these relations are: classifying the genes in related organisms and the reactions in their metabolic networks, recognizing the patterns that describe shared features, and highlighting specific differences.

PLEIADE will develops applications in comparative genomics of related organisms, using new mathematical tools for representing compactly, at different scales of difference, comparisons between related genomes. New methods based on computational geometry refine these comparisons. Compact representations can be stored, exchanged, and combined. They will form the basis of new simultaneous genome annotation methods, linked directly to abductive inference methods for building functional models of the organisms and their communities.

Our ambition in biotechnology is to permit the design of synthetic or genetically selected organisms at an abstract level, and guide the modification or assembly of a new genome. Our effort is focused on two main applications: genetic engineering and synthetic biology of oil-producing organisms (biofuels in CAER, palm oils), and improving and selecting starter microorganisms used in winemaking (collaboration with the ISVV and the BioLaffort company).

4.1.1. Oil Palm lipid synthesis

The largest source of vegetable oil [0] is the fruit mesocarp of the oil palm *Elaeis guineensis*, a remarkable tissue that can accumulate up to 90% oil, the highest level observed in the plant kingdom. The market share of oil palm is expected to increase in order to meet increased demand for vegetable oil, predicted to double by 2030 [18], be it as food or as a source of biofuels in Africa. A significant proportion of palm oil is produced on small estates that do not have access to efficient milling facilities, and run a great risk of spoilage through oil acidification. Improving palm oil quality through genetics and selection will result in economic gains [24] by addressing several targets such as improvement of oil yield, tuning of oil quality through the rate of unsaturated fatty acids or impairment of degradation processes. Furthermore, as genome biodiversity resides mostly in Africa, oil from African oil palms can vary greatly in fatty acid composition according to cultivar genetic differences and to weather conditions, and the precise mechanisms regulating this variability are not yet understood.

[0] 32% of the world market share [24]

A growing body of molecular resources for studying oil palm fruit are making it possible to study and improve the quality and quantity of oil produced by oil palms. In particular, these oils can vary greatly in fatty acid composition, and while the precise mechanisms regulating this variability are not completely understood, establishing a link between oil palm genotype and phenotype appears increasingly feasible. PLEIADE will work with the CNRS/UB UMR 5200 (LBM), a laboratory with an established reputation in studying fatty acid metabolism in *E. guineensis*, to improve understanding of the links between genetic diversity and oil production, and participate in developing applications.

4.1.2. Engineering pico-algae

Figure 4. Phylogenetic structure of long-chain polyunsaturated fatty acid desaturase specificity. Highlighted are thirteen desaturases from Ostreococcus tauri

Docosahexaenoic acid (DHA) is an essential nutriment for human brain tissue and can only be obtained from marine or riverine fish that live on phytoplankton and zooplankton, since human neurons lack the delta desaturase required for *de novo* synthesis of DHA. [21] Unfortunately, fishing is become less and less a sustainable resource. Since phytoplankton and zooplankton are the ultimate source of DHA consumed, there is considerable interest in obtaining DHA directly rather than through the intermediary of fish. A very promising approach is through the bio-engineering of pico-algae.

In order to produce the long-chain polyunsaturated fatty acids (LC-PUFA) needed for human nutrition, it is necessary to precisely engineer the desaturases that produce them. Desaturases are enzymes responsible for the introduction of double bonds into fatty acids. Desaturases are specific in recognizing their substrates and in placing the double bond in the proper place. The desaturases that produce the LC-PUFA necessary for human nutrition are present only in some species.

Our goal is to design methods to predict the substrate and region specificities for desaturases in algal species, particularly *Ostreococcus tauri*, the smallest photosynthetic eukaryote that can be cultivated. Thirteen desaturases are known in *O. tauri* and can be placed in the phylogeny of the desaturase family (figure 4). The biochemical and structural characterization of these enzymes is as yet very incomplete. This work is ongoing (see section 8.2.2) and requires close collaboration between biologists and computer scientists.

4.2. Molecular based systematics and taxonomy

Defining and recognizing myriads of species in biosphere has taken phenomenal energy over the past centuries and remains a major goal of Natural History. It is an iconic paradigm in pattern recognition (clustering has coevolved with numerical taxonomy many decades ago). Developments in evolution and molecular biology, as well as in data analysis, have over the past decades enabled a profound revolution, where species can be delimited and recognized by data analysis of sequences. We aim at proposing new tools, in the framework of E-science, which make possible (i) better exploration of the diversity in a given clade, and (ii) assignment of a place in these patterns for new, unknown organisms, using information provided by sets of sequences. This will require investment in data analysis, machine learning, and pattern recognition to deal with the volumes of data and their complexity.

One example of this project is about the diversity of trees in Amazonian forest, in collaboration with botanists in French Guiana. Protists (unicellular Eukaryots) are by far more diverse than plants, and far less known. Molecular exploration of Eukaryotes diversity is nowadays a standard in biodiversity studies. Data are available, through metagenomics, as an avalanche and make molecular diversity enter the domain of Big Data. Hence, an effort will be invested, in collaboration with other Inria teams (GenScale, HiePACS) for porting to HPC algorithms of pattern recognition and machine learning, or distance geometry, for these tools to be available as well in metagenomics. This will be developed first on diatoms (unicellular algae) in collaboration with INRA team at Thonon and University of Uppsala), on pathogens of tomato and grapewine, within an existing network, and on bacterial communities, in collaboration with University of Pau. For the latter, the studies will extend to correlations between molecular diversity and sets of traits and functions in the ecosystem.

4.3. Community ecology and population genetics

Community assembly models how species can assemble or diassemble to build stable or metastable communities. It has grown out of inventories of countable organisms. Using *metagenomics* one can produce molecular based inventories at rates never reached before. Most communities can be understood as pathways of carbon exchange, mostly in the form of sugar, between species. Even a plant cannot exist without carbon exchange with its rhizosphere. Two main routes for carbon exchange have been recognized: predation and parasitism. In predation, interactions–even if sometimes dramatic–may be loose and infrequent, whereas parasitism requires what Claude Combes has called intimate and sustainable interactions [19]. About one decade ago, some works [25] have proposed a comprehensive framework to link the studies of biodiversity with community assembly. This is still incipient research, connecting community ecology and biogeography.

We aim at developping graph-based models of co-occurence between species from NGS inventories in metagenomics, i.e. recognition of patterns in community assembly, and as a further layer to study links, if any, between diversity at different scales and community assemblies, starting from current, but oversimplified theories, where species assemble from a regional pool either randomly, as in neutral models, or by environmental filtering, as in niche modeling. We propose to study community assembly as a multiscale process between nested pools, both in tree communities in Amazonia, and diatom communities in freshwaters. This will be a step towards community genomics, which adds an ecological flavour to metagenomics.

Convergence between the processes that shape genetic diversity and community diversity–drift, selection, mutation/speciation and migration–has been noted for decades and is now a paradigm, establishing a continuous scale between levels of diversity patterns, beyond classical approaches based on iconic levels like species and populations. We will aim at deciphering diversity pattern along these gradients, connecting population and community genetics. Therefore, some key points must be adressed on reliability of tools.

Next-generation sequencing technologies are now an essential tool in population and community genomics, either for making evolutionary inferences or for developing SNPs for population genotyping analyses. Two problems are highlighted in the literature related to the use of those technologies for population genomics: variable sequence coverage and higher sequencing error in comparison to the Sanger sequencing technology. Methods are developed to develop unbiased estimates of key parameters, especially integrating sequencing errors [23]. An additional problem can be created when sequences are mapped on a reference sequence, either the sequenced species or an heterologous one, since paralogous genes are then considered to be the same physical position, creating a false signal of diversity [20]. Several approaches were proposed to correct for paralogy, either by working directly on the sequences issued from mapped reads [20] or by filtering detected SNPs. Finally, an increasingly popular method (RADseq) is used to develop SNP markers, but it was shown that using RADseq data to estimate diversity directly biases estimates [11]. Workflows to implement statistical methods that correct for diversity biases estimates now need an implementation for biologists.

5. Highlights of the Year

5.1. Highlights of the Year

5.1.1. Genomic determinants:

The study [7] appearing in *BMC Genomics* resolves a longstanding enigma in winemaking. While the *fact* of resistant strains of wine yeasts has been known for many years, the actual mechanism underlying the phenomena have only now been elucidated by a combined genetic and bioinformatic analysis.

5.1.2. INRAE-Inria PhD:

PLEIADE was succesful in applying for a PhD in 2019 INRA-Inria call for PhD. The submitted topic is: “Statistical Learning for OTU identification and Biodiversty characterizaton.” This PhD is a collaboration between PLEIADE (INRAE-Inria, supervision), HiePACS (Inria) and MIAT Toulouse (INRAE).

6. New Software and Platforms

6.1. magecal

KEYWORD: Genomics

SCIENTIFIC DESCRIPTION: Magecal independently runs training and prediction steps for Augustus, Conrad, GeneID, GeneMark, and Snap. The results are cleaned and integrated into a common format. Jigsaw is trained and used for model reconciliation. Consistency constraints are applied to ensure that phase and intron structure are biologically plausible.

FUNCTIONAL DESCRIPTION: Magecal predicts a set of protein coding genes in fungal genomic sequences, using different de novo prediction algorithms, and reconciling the predictions with the aid of comparative data. Magecal applies consistency constraints to guarantee that the predicted genes are biologically valid.

RELEASE FUNCTIONAL DESCRIPTION: Dockerization and compatibility with Alcyone

- Participants: Pascal Durrens and David James Sherman
- Contact: David James Sherman
- URL: https://gitlab.inria.fr/magecal/magecal

6.2. Declic

KEYWORDS: Data analysis - Machine learning - Taxonomies

FUNCTIONAL DESCRIPTION: Declic is a Python library that provides several tools for data analysis in the domains of multivariate data analysis, machine learning, and graph based methods. It can be used to study in-depth the accuracy of the dictionary between molecular based and morphological based taxonomy.

Declic includes an interpreter for a Domain Specific Language (DSL) to make its Python library easy to use for scientists familiar with environments such as R.

- Partner: INRA
- Contact: Alain Franc
- URL: https://gitlab.inria.fr/pleiade/declic

6.3. Magus

KEYWORDS: Bioinformatics - Genomic sequence - Knowledge database

SCIENTIFIC DESCRIPTION: MAGUS can be used on small installations with a web server and a relational database on a single machine, or scaled out in clusters or elastic clouds using Apache Cassandra for NoSQL data storage and Apache Hadoop for Map-Reduce.

FUNCTIONAL DESCRIPTION: The MAGUS genome annotation system integrates genome sequences and sequences features, in silico analyses, and views of external data resources into a familiar user interface requiring only a Web navigator. MAGUS implements annotation workflows and enforces curation standards to guarantee consistency and integrity. As a novel feature the system provides a workflow for simultaneous annotation of related genomes through the use of protein families identified by in silico analyses this has resulted in a three-fold increase in curation speed, compared to one-at-a-time curation of individual genes. This allows us to maintain standards of high-quality manual annotation while efficiently using the time of volunteer curators.

NEWS OF THE YEAR: Magus is now available as a Docker image, and can be integrated with other containerized services using Pleiade's Alcyone system.

- Participants: David James Sherman, Florian Lajus, Natalia Golenetskaya, Pascal Durrens and Xavier Calcas
- Partners: Université de Bordeaux - CNRS - INRA
- Contact: David James Sherman
- Publication: High-performance comparative annotation
- URL: http://magus.gforge.inria.fr

6.4. Mimoza

KEYWORDS: Systems Biology - Bioinformatics - Biotechnology

FUNCTIONAL DESCRIPTION: Mimoza uses metabolic model generalization and cartographic paradigms to allow human experts to explore a metabolic model in a hierarchical manner. Mimoza generalizes genome-scale metabolic models, by factoring equivalent reactions and metabolites while preserving reaction consistency. The software creates an zoomable representation of a model submitted by the user in SBML format. The most general view represents the compartments of the model, the next view shows the visualization of generalized versions of reactions and metabolites in each compartment , and the most detailed view visualizes the initial model with the generalization-based layout (where similar metabolites and reactions are placed next to each other). The resulting map can be explored on-line, or downloaded in a COMBINE archive. The zoomable representation is implemented using the Leaflet JavaScript library for mobile-friendly interactive maps. Users can click on reactions and compounds to see the information about their annotations.

NEWS OF THE YEAR: Mimoza is now available as a Docker image, and can be integrated with other containerized services using Pleiade's Alcyone system.

- Participants: Anna Zhukova and David James Sherman
- Contact: David James Sherman
- Publications: Knowledge-based generalization of metabolic models - Knowledge-based zooming for metabolic models - Knowledge-based generalization of metabolic networks: a practical study
- URL: http://mimoza.bordeaux.inria.fr/

6.5. Diagno-Syst

diagno-syst: a tool for accurate inventories in metabarcoding

KEYWORDS: Biodiversity - Clustering - Ecology

FUNCTIONAL DESCRIPTION: Diagno-syst builds accurate inventories for biodiversity. It performs supervised clustering of reads obtained from a next-generation sequencing experiment, mapping onto an existing reference database, and assignment of taxonomic annotations.

- Participants: Alain Franc, Jean-Marc Frigerio, Philippe Chaumeil and Franck Salin
- Partner: INRA
- Contact: Alain Franc
- Publication: diagno-syst: a tool for accurate inventories in metabarcoding

6.6. Alcyone

Alcyone instantiates bioinformatics environments from specifications committed to a Git repository

KEYWORDS: Docker - Orchestration - Bioinformatics - Microservices - Versioning

SCIENTIFIC DESCRIPTION: Alcyone conceives the user's computing environment as a microservices architecture, where each bioinformatics tool in the specification is a separate containerized Docker service. Alcyone builds a master container for the specified environment that is responsible for building, updating, deploying and stopping these containers, as well as recording and sharing the environment in a Git repository. The master container can be manipulated using a command-line interface.

FUNCTIONAL DESCRIPTION: Alcyone defines a file structure for the specifying bioinformatics analysis environments, including tool choice, interoperability, and sources of raw data. These specifications are recorded in a Git repository. Alcyone compiles a specification into a master Docker container that deploys and orchestrates containers for each of the component tools. Alcyone can restore any version of an environment recorded in the Git repository.

NEWS OF THE YEAR: Alcyone was designed and implemented this year.

- Participants: Louise-Amelie Schmitt and David James Sherman
- Contact: David James Sherman
- URL: https://team.inria.fr/pleiade/alcyone/

6.7. family-3d

KEYWORDS: Biodiversity - Point cloud - 3D modeling

SCIENTIFIC DESCRIPTION: The method statistically selects a subset of pairwise distances between proteins in the family, constructs a weighted graph, and lays it out using an adaptation of the three-dimensional extension of the Kamada-Kawai force-directed layout.

FUNCTIONAL DESCRIPTION: Family-3D lays out high-dimension protein family point clouds in 3D space. The resulting lower-dimension forms can be printed, so that they can be explored and compared manually. They can also be explored interactively or stereographically.

Comparison of the 3D forms reveals classes of structurally similar families, whose characteristic shapes correspond to different evolutionary scenarios. Some of these scenarios are: neofunctionalization, subfunctionalization, founder gene effect, ancestral family.

To facilitate curator training, Family-3D includes an interactive terminal containing a microcontroller, an RFID reader, and an LED ring. A set of shapes that fall in predetermined classes is printed, with a unique RFID tag in each shape. Trainees classify family shapes by manual inspection and submit their classes to the terminal, which evaluates the proposed class and provides visual feedback.

- Participant: David James Sherman
- Contact: David James Sherman
- URL: https://gitlab.inria.fr/pleiade/family-3d

6.8. Yapotu

Yet Another Pipeline for OTU building

KEYWORDS: Taxonomies - Distance matrices - Clustering - Metagenomics

FUNCTIONAL DESCRIPTION: OTU building is one of the key operation in metabarcoding: how to delimit Operational Taxonomic Units in the "soup" where all amplicons of thousands of unicellular organisms have been lumped together (from visible plankton to nano- and picoplankton, for example). Yapotu is a software tool that enables approaches to unsupervised clustering on very large matrices of distances: each element is a distance between two reads produced by a sequencer. It permits one to select one method among several, like building MultiDimensional Scaling to produce an Euclidean image, and clustering within the point cloud, or building a graph where a node is a sequence and there is an edge if both sequences are at a distance smaller than a given threshold, and then after build connected components or communities on this graph. Other functions visualize the OTUs as clusters or subgraphs.

- Contact: Alain Franc
- URL: https://gitlab.inria.fr/afranc/diodon/tree/master/yapotu

6.9. Diodon

KEYWORDS: Dimensionality reduction - Data analysis

FUNCTIONAL DESCRIPTION: Most of dimension reduction methods inherited from Multivariate Data Analysis, and currently implemented as element in statistical learning for handling very large datasets (the dimension of spaces is the number of features) rely on a chain of pretreatments, a core with a SVD for low rank approximation of a given matrix, and a post-treatment for interpreting results. The costly part in computations is the SVD, which is in cubic complexity. Diodon is a list of functions and drivers which implement (i) pre-treatments, SVD and post-treatments on a large diversity of methods, (ii) random projection methods for running the SVD which permits to bypass the time limit in computing the SVD, and (iii) an implementation in C++ of the SVD with random projection at prescribed rank or precision, connected to MDS.

- Contact: Alain Franc
- URL: https://gitlab.inria.fr/afranc/diodon

7. New Results

7.1. Genetic Determinisms of Aborted Fermentation in Winemaking

This study contributes to the understanding of the mechanisms leading to stuck fermentation in winemaking, an economic prejudice [7]. A number of factors can trigger stuck or aborted fermentation such as high temperature, high ethanol concentration, low pH. The biodiversity of natural yeast strains used in winemaking starters has as a consequence that some of them are more prone to abort fermentation than others, indicating a genetic determinism. Crosses between strains called "sensitive" or "resistant" to stuck fermentation occurrence, followed by back-crosses with the "sensitive" parent while selecting for the "resistant" phenotype, allowed us to reduce the amount of genetic material inherited from the "resistant" parent in the progeny, ending to 3 small introgression areas after 4 generations. Quantitative Trait Locus (QTL) detection in this progeny (77 strains) involved characterization of SNP inheritence (circa 1200 validated SNPs) from either parent, through micro-array hybridization, mapping of the SNP on the reference genome and phenotypic measurements on the progeny. This analysis made it possible to detect two genes which, when inactivated by naturally occurring mutations, act as major perturbators of several fermentation parameters in winemaking physiological conditions. Consequently, our industrial partner incorporated into its catalogue of winemaking starters, strains carrying the functional forms of these genes.

7.2. Characterization of Molecular Biodiversity

In 2019 PLEIADE developed new methods for characterizing molecular biodiversity (see [4], [5] for applications). This point itself has been developed with two approaches in 2019, each with the beginning of a PhD.

- Building OTUs from a pairwise distance matrix typically is an unsupervised clustering issue. In this new development, the PhD student (PLEIADE) tests whether SBM (Stochastic Block Model) approach yields relevant results for a global characterization of biodiversity beyond a summary by a scalar index. This is done in collaboration with MIAT INRAE research unit in Toulouse and EPC HiePACS. It represents a connection between metabarcoding and statistical modeling, a topic which deserves investigation and is expanding. (Figure 5 from [8])
- A major goal of PLEIADE is to develop a geometric view on biodiversity. The tool selected up to now is to associate a point cloud to a dataset (pairwise distances between sequences) and study its shape. In 2019, PLEIADE has been associated in a collaboration with HiePACS to begin a new topic: comparison between point clouds, each cloud being associated to a data set. Indeed, the development of metabarcoding leads to the new issue of comparison between OTUs built from different dataset. This approach is part of the issues raised in a PhD supervized by HiePACS, in collaboration with PLEIADE.

7.3. Scaling Metabarcoding Programs

Metabarcoding is a series of technical procedures to build molecular based inventories from large datasets of amplicons. We derived new methods and tools to scale metabarcoding programs in collaboration with EPC HiePACS. This has been realized through following participation in research projects:

- Contribution to ADT Gordon project in Inria BSO. The objective of this project (partners: Tadaam (coordinator), STORM, HiePACS, PLEIADE) is to integrate SVD as an available tool in Chameleon, starPU and new Madeleine. The contribution of Pleiade is to bring metabarcoding as a use case, and random projection ([6]) as a method for scaling Multidimensional Scaling (which requires an SVD) in collaboration with HiePACS with a template implemented in Diodon. In 2019, PLEIADE has bought to the project a series of 55 matrices with size about 10^5 rows/column which, assembled, yield a full pairwise distance matrix between one million of sequences. The objective is to reach the million in 2020.
- Contribution to Region Nouvelle Aquitaine project "HPC Scalable Ecosystem." This project is chaired by HiePACS. In collaboration with this EPC, PLEIADE is involved in developing a new approach for comparing OTUs built from different datasets.

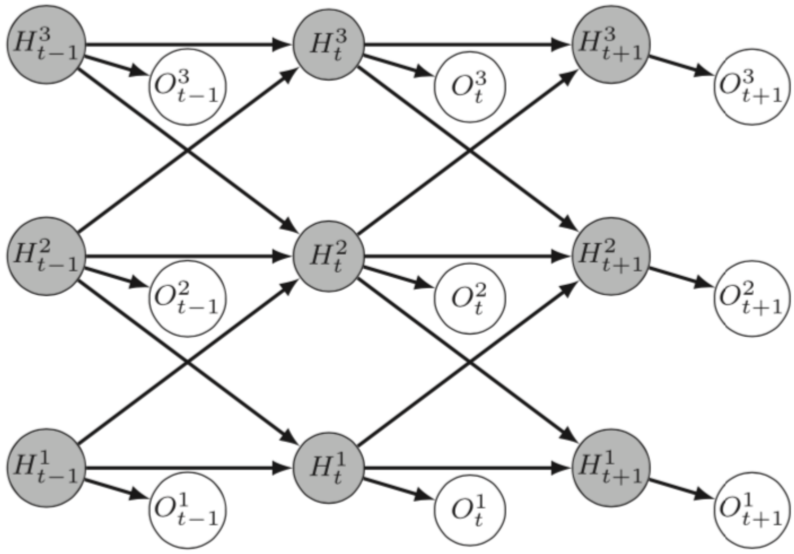

Figure 5. Graphical representation of a coupled HMM with three hidden chains (from [8])

7.4. Linking Homology and Function for Algal Desaturases

Polyunsaturated fatty acids (PUFA) such as Omega-3 that are essential for human health cannot be synthesized by the human body and must be acquired through the consumption of certains foods, such as oily fish, that are becoming increasing difficult to produce sustainably. However, fish do not produce them either: their role is to concentrate PUFA through the food chain. There is consequently considerable interest in producing these essential nutriments directly, through the cultivation of domesticated strains of naturally occurring or of engineered strains of green algae.

Ultimately, polyunsaturated fatty acids are produced by molecular machines called **desaturases**. While desaturases are abundant in all branches of life, the link between gene sequence and the precise activity of the corresponding enzyme is poorly understood. The particular challenge is that, while the catalytic active site is well conserved, the features that recognize the substrate and that determine the regiospecificity of the enzyme are not. In order to produce specific PUFA at industrial scale, it is necessary to develop efficient tools for high-throughput identification of candidate genes in algal species, and precise models for designing desaturases through synthetic biology.

In collaboration with the LBM (UMR 5200 CNRS) and with the support of the Inria Project Lab *In silico algae*, we used a core collection of thirteen desaturases from *Osteococcus tauri* to explore the link between homology and function in 23 species ([9]). The study reinforced our understanding of the evolutionary conservation of desaturases and confirmed the identification of substrate and regio- specificity through graph neighborhoods. We were further able to extend the identification of PPR motifs correlated with specificity. This work is ongoing. Since most of the pertinent desaturases are membrane bound, the prediction of protein structure has proved perilous, but we are hopeful that future work will allow us to use structure-inspired prediction to narrow in on the sites responsible for specificity despite their poor sequence conservation.

8. Partnerships and Cooperations

8.1. Regional Initiatives

8.1.1. Malabar

This is a project funded by labex COTE (University of Bordeaux) as a collaboration with IFREMER at Arcachon, EPOC (Talence), and ETI chair of the labex. The guideline of the project is to build models in statistical ecology on a series of molecular based invetories (300 samples) from occurence matrices of OTUs in samples, with environmental variables. The samples have been collected in 2018-2019, the sequences produced by BioGeCo in 2019, and data analysis will begin in 2020.

8.1.2. High-performance computing and metabarcoding

PLEIADE is member of two projects, one funded by the Région Nouvelle Aquitaine and one funded as Inria ADT Gordon, connecting Chameleon, StartPU and NewMadeleine, where the use case of metabarcoding (questions, data sets) hase been selected to link these layers together. This will permit us to address unsupervised clustering of one million reads next year. These projects are in collaboration with the HiePACS, TADAAM, and STORM project-teams.

8.1.3. COTE – Continental to Coastal Ecosystems

The Labex cluster of excellence COTE (Continental To coastal Ecosystems: evolution, adaptability and governance) develops tools to understand and predict ecosystem responses to human-induced changes as well as methods of adaptative management and governance to ensure their sustainability. The LabEx includes nine laboratories of the University of Bordeaux and major national research institutes involved in research on terrestrial and aquatic ecosystems (INRA, CNRS, IFREMER and IRSTEA).

8.2. National Initiatives

8.2.1. Agence Française pour la Biodiversité

The AFB is a public law agency of the French Ministry of Ecology that supports public policy in the domains of knowledge, preservation, management, and restoration of biodiversity in terrestrial, aquatic, and marine environments. PLEIADE is a partner in two AFB projects developed with the former ONEMA: one funded by ONEMA, the second by labex COTE, where BioGeCo/Pleiade is responsible for data analysis, with implementaton of the tools recently developed for scaling MDS. Calculations have been made on CURTA at MCIA and PlaFRIM at Inria.

8.2.2. Inria Projet Lab in silico Algae

In 2017 PLEIADE joined the IPL “In silico Algae” coordinated by Olivier Bernard. The IPL addresses challenges in modeling and optimizing microalgae growth for industrial applications. PLEIADE worked this year on comparative genomic analysis of genes implicated in lipid production by the picoalgae *Ostreococcus tauri*, in collaboration with Florence Corellou of the CNRS UMR 5200 (Laboratoire de Biogénèse Membranaire). The goal of this work is the production of long-chain polyunsaturated fatty acids, developed as nutritional additives. Mercia Ngoma Komb’s two-month internship in PLEIADE contributed to this work.

8.3. European Initiatives

8.3.1. Collaborations in European Programs, Except FP7 & H2020

Program: COST

Project title: COST Action DNAqua.net

Abstract: PLEIADE is responsible for the WG "Data Analysis and storage" in this action. As such, we have organized with CNR Verbana (Italy) two Europeanwide workshops: one in Lyon in February 2019, and one in Limassol (Cyprus) in October 2019. As a follow up of these workshops, Pleiade and BioGeCo will be responsible for taking in charge data analysis of OTU picking in two European wide projects:

- a benchmark for different tools for OTU picking, with datasets from different European teams
- a comparison between different organisms (metabarcoding inventories) for assessing the quality of the water of Danube river, in collaboration with raparian countries

Program: EOSC

Project title: EOSC-Pillar

Abstract: This is a follow up of our former participation in EOSC-Pilot. In collaboration with HiePACS, PLEIADE is involved in task 7.4, for bringing use cases in metabarcoding as testbeds for circulation of codes between different infrastructures, including PlaFRIM.

8.4. International Initiatives

8.4.1. Vitapalm – Food and nutrition security and sustainable agriculture in Africa

PLEIADE participates in the Vitapalm program financed by LEAP-Agri [0], the joint Europe Africa Research and Innovation (R&I) initiative related to Food and Nutrition Security and Sustainable Agriculture. Vitapalm uses genomics and selection to improve the nutritional quality and the stability of palm oil produced by Africa smallholdings for local consumption. Project partners are from Cameroon, France, Germany, and Ghana.

8.4.2. Simulation of metacommunities

In collaboration with the Pasteur Institute in Cayenne and the INRA MIA Research Team in Toulouse, PLEIADE is developing a stochastic model for simulation of metacommunities, in the framework of patch occupancy models. The objective is a better understanding of zoonose propagation, namely rabies through bat hosts in connection with disturbances of pristine forests in French Guiana, which have an impact on the exposure of human populations to wildlife that act as reservoirs of zoonoses.

8.4.3. CEBA – Center for the study of biodiversity in Amazonia

The Laboratoire of excellence CEBA promotes innovation in research on tropical biodiversity. It brings together a network of internationally-recognized French research teams, contributes to university education, and encourages scientific collaboration with South American countries. PLEIADE participates in three current international projects funded by CEBA:

- *MicroBIOMES: Microbial Biodiversities*. 2017-19.
- *Neutrophyl: Inferring the drivers of Neotropical diversification*. 2017-19.
- *Phyloguianas: Biogeography and pace of diversification in the Guiana Shield*. 2015-present

PLEIADE is involved with BioGeCo as partner of Institut Pasteur de Guyane at Cayenne for developing the domain of so-called Ecoviromics for some zoonoses in French Guiana. The spine of this collaboration is co-supervizing of a PhD student at IPG in cayenne, in bioinformatics and statistical ecology to decipher the respective roles of host phylogeny and environmetal variables in the virome of different hosts (bats, rodents, birds).

9. Dissemination

9.1. Promoting Scientific Activities

9.1.1. Journal

9.1.1.1. Member of the Editorial Boards

Alain Franc is member of the editorial board of BMC Evolutionary Biology.

[0] http://www.leap-agri.com/

Pascal Durrens is a member of the editorial board of the journal ISRN Computational Biology.

9.1.2. Scientific Expertise

David Sherman is a member of the Scientific Advisory Board of Enlightware GmbH, Zürich.

9.1.3. Research Administration

Alain Franc has been appointed “chargé de mission calcul” at INRA by INRA Delegate for Digital Transition. As such, his mission is to propose animations and solutions for the development of scientific computing at INRA, whatever the Research Department.

David Sherman is president of the Commission for Technology Development (CDT) of the Inria Bordeaux Sud-Ouest research center. The CDT has two roles. First, it evaluates funding requests for Technology Development and Technology Transfer projects, which typically involve hiring technical staff. Second, the CDT is responsible for validating and overseeing contract engineers hired by Inria project-teams.

David Sherman represents Inria in the steering committee of the Region Nouvelle Aquitaine’s regional research network “Biodiversity and Ecosystemic Services” (BIOSENA).

9.2. Popularization

9.2.1. Education

David Sherman contributed to the *Journée APEIA (Activités Pour l’Enseignement de l’IA)*
David Sherman help train teachers in programming mobile robots, in preparation for R2T2 events (http://r2t2.org) coordinated by the Mobsya association and EPFL (Switzerland).

9.2.2. Interventions

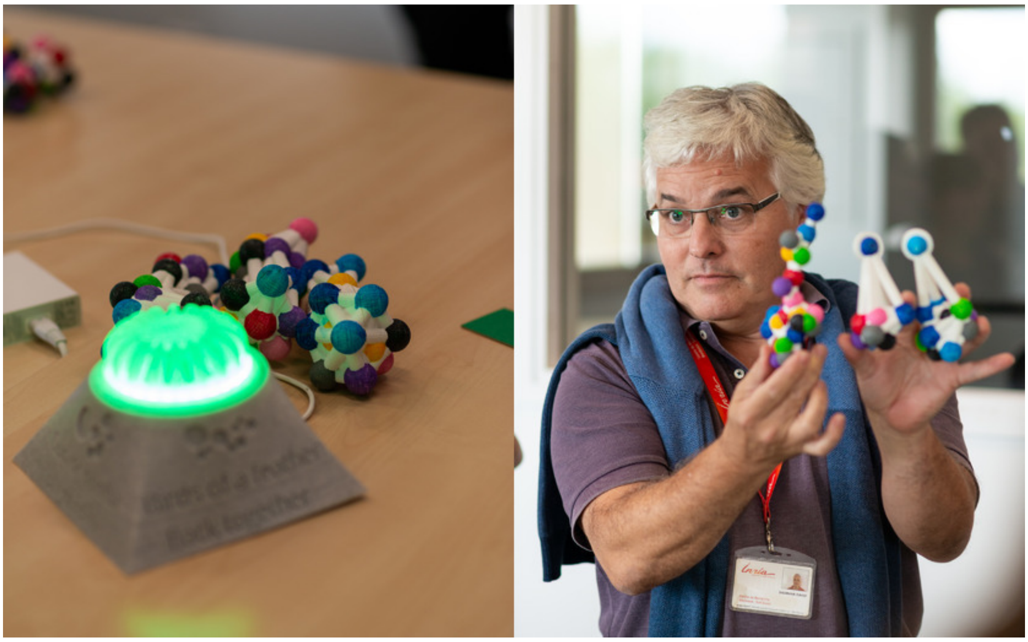

*Figure 6. **Qui se ressemble s’assemble** during the Circuit Scientifique in 2019: (left) classification oracle (right) comparing similar shapes (Photo copyright Gautier DUFAU)*

In collaboration with a local PME, David Sherman helped design an interactive exhibit on tree classification for a museum in the Region Nouvelle Aquitaine, based on a specialization of **Qui se ressemble s'assemble**.

David Sherman presented the **Qui se ressemble s'assemble** activity to 100 middle school students during the Circuit Scientifique in 2019 (Figure 6), and to 40 undergraduate students from the ENS Lyon.

9.2.3. Creation of media or tools for science outreach

David Sherman refined his design for the electronics of the **Qui se ressemble s'assemble** activity, to explain the methods and uses of pattern classification of protein families. The activity uses 20 3D-printed point clouds and 4 oracles, containing a microcontroller, an RFID reader with a custom-designed inductive coil as input, and an LED ring as output. Participants propose groups of 3D shapes that they believe belong to the same class, and the oracle evaluate the group.

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Project-Team POTIOC

Novel Multimodal Interactions for a Stimulating User Experience

IN PARTNERSHIP WITH:
CNRS

Université de Bordeaux

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Interaction and visualization

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Project-Team POTIOC

Creation of the Team: 2012 January 01, updated into Project-Team: 2014 January 01

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A3.4.1. - Supervised learning
A5.1. - Human-Computer Interaction
A5.1.1. - Engineering of interactive systems
A5.1.2. - Evaluation of interactive systems
A5.1.4. - Brain-computer interfaces, physiological computing
A5.1.5. - Body-based interfaces
A5.1.6. - Tangible interfaces
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B9.2.4. - Theater
B9.5.3. - Physics
B9.6.1. - Psychology

1. Team, Visitors, External Collaborators

Research Scientists

Martin Hachet [Team leader, Inria, Senior Researcher, HDR]
Pascal Guitton [Inria, Senior Researcher, HDR]

Fabien Lotte [Inria, Senior Researcher, HDR]

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Lauren Thevin [Univ Paul Sabatier, from Apr 2019 until Sep 2019]
Anke Brock [ENAC]

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Thibaut Monseigne [Inria, Engineer]
Erwan Normand [Univ de Bordeaux, Engineer]
Joan Odicio Vilchez [Inria, Engineer, from Dec 2019]
Nicolas Palard [Univ Paul Sabatier, Engineer, until Mar 2019]
Joan Sol Roo [Inria, Engineer, until Nov 2019]
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Camille Benaroch [Inria, PhD Student]
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Lauren Thevin [Inria, Post-Doctoral Fellow, until Mar 2019]

Administrative Assistants

Cecile Boutros [Inria, Administrative Assistant, until Apr 2019]
Audrey Plaza [Inria, Administrative Assistant, from Jul 2019]

2. Overall Objectives

2.1. Overall Objectives

The standard human-computer interaction paradigm based on mice, keyboards, and 2D screens, has shown undeniable benefits in a number of fields. It perfectly matches the requirements of a wide number of interactive applications including text editing, web browsing, or professional 3D modeling. At the same time, this paradigm shows its limits in numerous situations. This is for example the case in the following activities: i) active learning educational approaches that require numerous physical and social interactions, ii) artistic performances where both a high degree of expressivity and a high level of immersion are expected, and iii) accessible applications targeted at users with special needs including people with sensori-motor and/or cognitive disabilities.

To overcome these limitations, Potioc investigates new forms of interaction that aim at pushing the frontiers of the current interactive systems. In particular, we are interested in approaches where we vary the level of *materiality* (i.e., with or without physical reality), both in the output and the input spaces. On the output side, we explore mixed-reality environments, from fully virtual environments to very physical ones, or between both using hybrid spaces. Similarly, on the input side, we study approaches going from brain activities, that require no physical actions of the user, to tangible interactions, which emphasize physical engagement. By varying the level of materiality, we adapt the interaction to the needs of the targeted users.

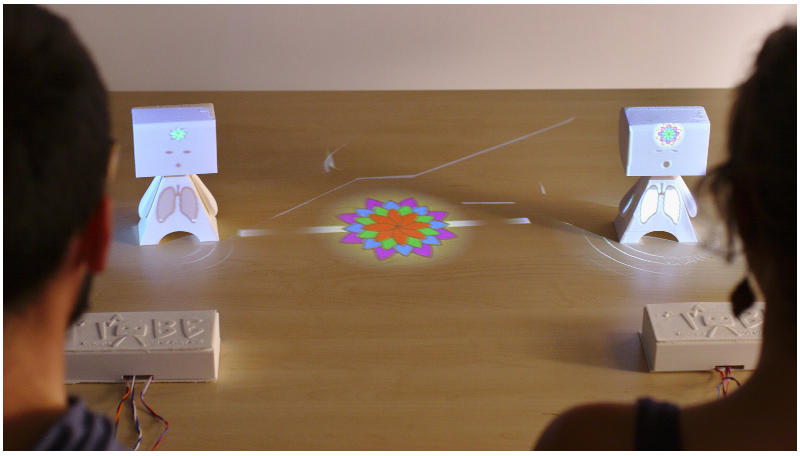

Figure 1. Tobe combines tangible interaction, spatial augmented reality, and physiological computing. It allows users to feel and explore their inner states.

The main applicative domains targeted by Potioc are Education, Art, Entertainment and Well-being. For these domains, we design, develop, and evaluate new approaches that are mainly dedicated to non-expert users. In this context, we thus emphasize approaches that stimulate curiosity, engagement, and pleasure of use.

3. Research Program

3.1. Research Program

To achieve our overall objective, we follow two main research axes, plus one transverse axis, as illustrated in Figure 2.

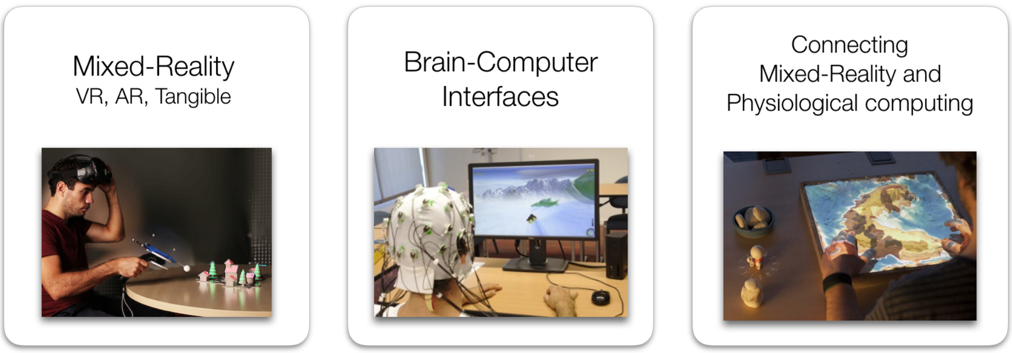

Figure 2. Main research axes of Potioc.

In the first axis dedicated to **Interaction in Mixed-Reality spaces**, we explore interaction paradigms that encompass virtual and/or physical objects. We are notably interested in hybrid environments that co-locate virtual and physical spaces, and we also explore approaches that allow one to move from one space to the other.

The second axis is dedicated to **Brain-Computer Interfaces (BCI)**, i.e., systems enabling user to interact by means of brain activity only. We target BCI systems that are reliable and accessible to a large number of people. To do so, we work on brain signal processing algorithms as well as on understanding and improving the way we train our users to control these BCIs.

Finally, in the **transverse** axis, we explore new approaches that involve both mixed-reality and neuro-physiological signals. In particular, tangible and augmented objects allow us to explore interactive physical visualizations of human inner states. Physiological signals also enable us to better assess user interaction, and consequently, to refine the proposed interaction techniques and metaphors.

From a methodological point of view, for these three axes, we work at three different interconnected levels. The first level is centered on the human sensori-motor and cognitive abilities, as well as user strategies and preferences, for completing interaction tasks. We target, in a fundamental way, a better understanding of humans interacting with interactive systems. The second level is about the creation of interactive systems. This notably includes development of hardware and software components that will allow us to explore new input and output modalities, and to propose adapted interaction techniques. Finally, in a last higher level, we are interested in specific application domains. We want to contribute to the emergence of new applications and usages, with a societal impact.

4. Application Domains

4.1. Education

Education is at the core of the motivations of the Potioc group. Indeed, we are convinced that the approaches we investigate—which target motivation, curiosity, pleasure of use and high level of interactivity—may serve education purposes. To this end, we collaborate with experts in Educational Sciences and teachers for exploring new interactive systems that enhance learning processes. We are currently investigating the fields of astronomy, optics, and neurosciences. We have also worked with special education centres for the blind on accessible augmented reality prototypes. Currently, we collaborate with teachers to enhance collaborative work for K-12 pupils. In the future, we will continue exploring new interactive approaches dedicated to education, in various fields. Popularization of Science is also a key domain for Potioc. Focusing on this subject allows us to get inspiration for the development of new interactive approaches.

4.2. Art

Art, which is strongly linked with emotions and user experiences, is also a target area for Potioc. We believe that the work conducted in Potioc may be beneficial for creation from the artist point of view, and it may open new interactive experiences from the audience point of view. As an example, we have worked with colleagues who are specialists in digital music, and with musicians. We have also worked with jugglers and we are currently working with a scenographer with the goal of enhancing interactivity of physical mockups and improve user experience.

4.3. Entertainment

Similarly, entertainment is a domain where our work may have an impact. We notably explored BCI-based gaming and non-medical applications of BCI, as well as mobile Augmented Reality games. Once again, we believe that our approaches that merge the physical and the virtual world may enhance the user experience. Exploring such a domain will raise numerous scientific and technological questions.

4.4. Well-being

Finally, well-being is a domain where the work of Potioc can have an impact. We have notably shown that spatial augmented reality and tangible interaction may favor mindfulness activities, which have been shown to be beneficial for well-being. More generally, we explore *introspectibles* objects, which are tangible and augmented objects that are connected to physiological signals and that foster introspection. We explore these directions for general public, including people with special needs.

5. Highlights of the Year

5.1. Highlights of the Year

The HOBIT system has been exported to a foreign institution (University of Jena) for the first time. The licensing of the technology is in progress for a worldwide distribution.

5.1.1. Awards

- Honorable mention award at ACM ISS 2019
- Best paper award at ACM UIST 2019
- Best presentation award at Neuroadaptive Technologies 2019 (NAT'19): "Modular biofeedback: build your own tangible experience" by Joan Sol Roo and Jeremy Frey

BEST PAPERS AWARDS :

[23]
P. GIRAUDEAU, A. OLRY, J. SOL ROO, S. FLECK, D. BERTOLO, R. VIVIAN, M. HACHET.*CARDS: A Mixed-Reality System for Collaborative Learning at School*, in "ACM ISS'19 - ACM International Conference on Interactive Surfaces and Spaces", Deajon, South Korea, November 2019 [*DOI :* 10.1145/3343055.3359721], https://hal.inria.fr/hal-02313463

[25]
A. KHAN, J. SOL ROO, T. KRAUS, J. STEIMLE.*Soft Inkjet Circuits: Rapid Multi Material Fabrication of Soft Circuits Using a Commodity Inkjet Printer*, in "UIST'19 - 32nd ACM Symposium on User interface software and technology", New Orleans, United States, October 2019, https://hal.archives-ouvertes.fr/hal-02279960

6. New Software and Platforms

6.1. Aïana

KEYWORD: Multimedia player

FUNCTIONAL DESCRIPTION: This software aims to make accessible the playing of a MOOC composed of various information flows (boards, videos, subtitles ...). It is not intended to be "reserved" for people with disabilities but rather to be open to as many as possible by allowing each user to adapt the interface, and therefore the use, to its users own capabilities and needs.

- Authors: Damien Caselli, Pierre-Antoine Cinquin, Pascal Guitton and Hélène Sauzéon
- Partner: Université de Bordeaux
- Contact: Pascal Guitton
- Publications: Towards Truly Accessible MOOCs for Persons with Cognitive Disabilities: Design and Field Assessment - Online e-learning and cognitive disabilities: A systematic review

6.2. HybridOptics : Hybrid Optical Platform

KEYWORDS: Augmented reality - Education - Tangible interface

FUNCTIONAL DESCRIPTION: The software platform - gets the values of the sensors - computes in real-time the result of the simulation - generates pedagogical supports that are directly linked to the simulation (projected on the work table) - allows the user to control several parameters from a dedicated application on a tablet

- Participants: Benoit Coulais, Lionel Canioni, Bruno Bousquet, Martin Hachet and Jean-Paul Guillet
- Contact: Martin Hachet
- URL: https://project.inria.fr/hobit/

6.3. Platforms

6.3.1. HOBIT

In 2019, we have continued working on the HOBIT platform dedicated to teaching and training of Optics at University. This has led to a version that we are able to export. A first system has been installed at University of Jena (Germany). We are currently finilizing a licensing contract to export the technology worldwide.

6.3.2. CARDS

Part of the e-Tac project, we have conceived a system composed of hardware and software components that allows us to augment pieces of papers in an interactive way (see Figure 3). 12 copies of this platform have been deployed at school. See also 7.1.

6.3.3. OpenVIBE

We have continued developing and extending the OpenViBE open-source BCI platform. As new functionalities, we have notably added the use of Riemmannian geometry for EEG classification, which includes computation of covariance matrices and covariance matrix means, projection to tangent space and various covariance matrices classifiers, both with or without supervised or unsupervised adaptation. We have also added a new visualization module which can display any number of BCI commands and associate real-time feedback. In addition to these new functionalities, we have carefully improved and clean OpenViBE code, in order to standardize / clarify / simplify / modernize it and to secure and reduce memory allocations, to reduce unnecessary function calls, type changes and casts. This aimed at facilitating the handling of the code by new contributors and to update the different dependencies of OpenViBE, thus improving its compatibility, security and stability.

7. New Results

7.1. Mixed-Reality System for Collaborative Learning at School

Participants: Philippe Giraudeau, Théo Segonds, Solène Lambert, Martin Hachet

External collaborators: Université de Lorraine

Traditional computer systems based on the WIMP paradigm (Window, Icon, Menu, Pointer) have shown potential benefits at school (e.g. for web browsing). On the other hand, they are not well suited as soon as hands-on and collaborative activities are targeted. To face this problem, we have designed and developed CARDS, a Mixed-Reality system that combines together physical and digital objects in a seamless workspace to foster active and collaborative learning (Figure 3). In [23], we describe the design process based on a participatory approach with researchers, teachers, and pupils. We then present and discuss the results of a user study that tends to show that CARDS has a good educational potential for the targeted activities.

7.2. DroneSAR: Extending Physical Spaces in Spatial Augmented Reality using Projection on a Drone

Participants: Rajkumar Darbar, Joan Sol Roo, Thibaut Lainé, Martin Hachet

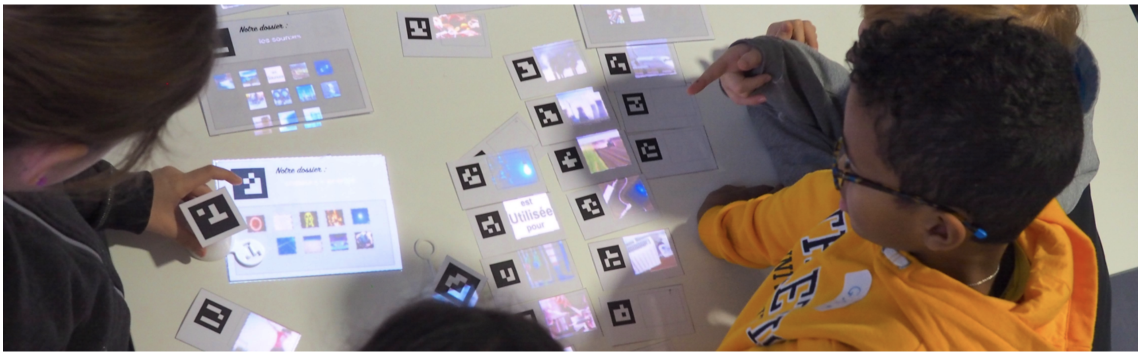

Figure 3. CARDS: Collaborative Activities based on the Real and the Digital Superimposition.

Spatial Augmented Reality (SAR) transforms real-world objects into interactive displays by projecting digital content using video projectors. SAR enables co-located collaboration immediately between multiple viewers without the need to wear any special glasses. Unfortunately, one major limitation of SAR is that visual content can only be projected onto its physical supports. As a result, displaying User Interfaces (UI) widgets such as menus and pop-up windows in SAR is very challenging. We are trying to address this limitation by extending SAR space in mid-air. We propose Drone-SAR, which extends the physical space of SAR by projecting digital information dynamically on the tracked panels mounted on a drone (see Figure 4. DroneSAR is a proof of concept of novel SAR User Interface (UI) , which provides support for 2D widgets (i.e., label, menu, interactive tools, etc.) to enrich SAR interactive experience. We describe this concept, as well as implementation details of our proposed approach in [22].

7.3. Tangible and modular devices for supporting communication

Participants: Joan Sol Roo, Pierre-Antoine Cinquin, Martin Hachet

External collaborators: Ullo

Our physiological activity reflects our inner workings. However, we are not always aware of it in full detail. Physiological devices allow us to monitor and create adaptive systems and support introspection. Given that these devices have access to sensitive data, it is vital that users have a clear understanding of the internal mechanisms (extrospection), yet the underlying processes are hard to understand and control, resulting in a loss of agency. In this work, we focus on bringing the agency back to the user, by using design guidelines based on principles of honest communication and driven by positive activities. To this end, we conceived a tangible, modular approach for the construction of physiological interfaces (see Figure 5). We are exploring the potential of such an approach with a set of examples, supporting introspection, dialog, music creation, and play.

7.4. Accessible Interactive Audio-Tactile Drawings

Participants: Lauren Thevin, Anke Brock, Martin Hachet

External collaborators: CNRS, Univesité Paul Sabatier, ENAC

Interactive tactile graphics have shown a true potential for people with visual impairments, for instance for acquiring spatial knowledge. Until today, however, they are not well adopted in real-life settings (e.g. special education schools). One obstacle consists in the creation of these media, which requires specific skills, such as the use of vector-graphic software for drawing and inserting interactive zones, which is challenging for stakeholders (social workers, teachers, families of people with visual impairments, etc.). We explored how

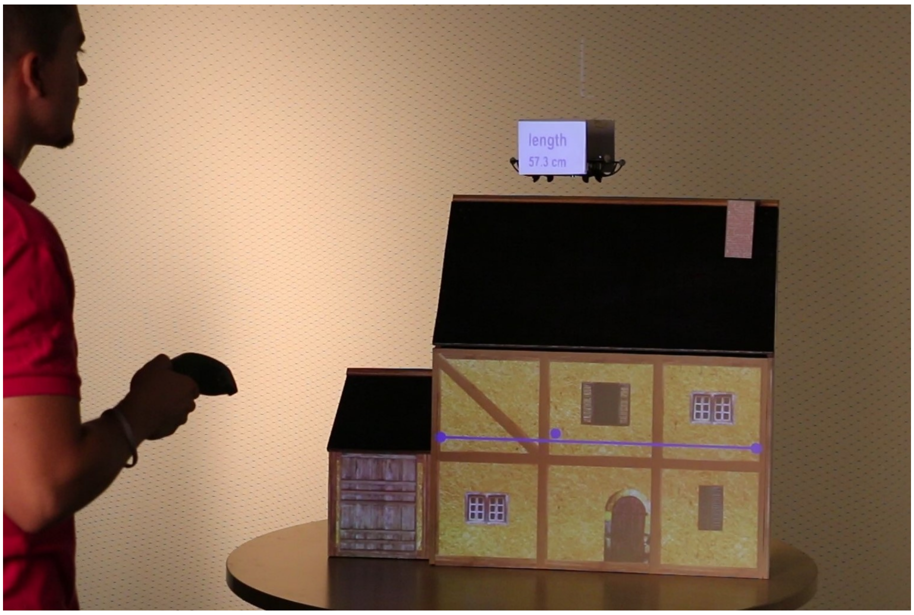

Figure 4. DroneSAR: Projection on a drone allows us to extend the physical space for interacting spatial augmented reality.

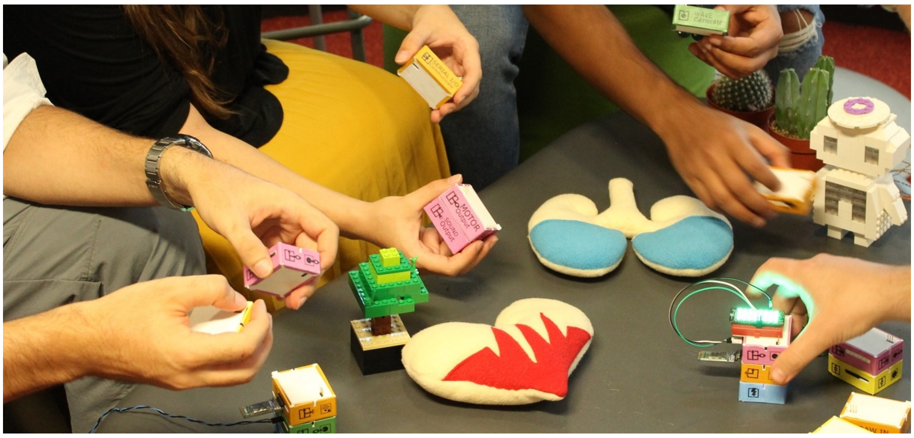

Figure 5. modular bricks that support the easy creation and interfacing with physiological applications.

a Spatial Augmented Reality approach can enhance the creation of interactive tactile graphics by sighted users. We developed the system using a participatory design method. A user study showed that the augmented reality device allowed stakeholders (N=28) to create interactive tactile graphics more efficiently than with a regular vector-drawing software (baseline), independently of their technical background. This work illustrated in Figure 6 is described in [29].

Following the same approach, we are currently exploring how physical board games can be moved into accessible ones for people with visual impairments.

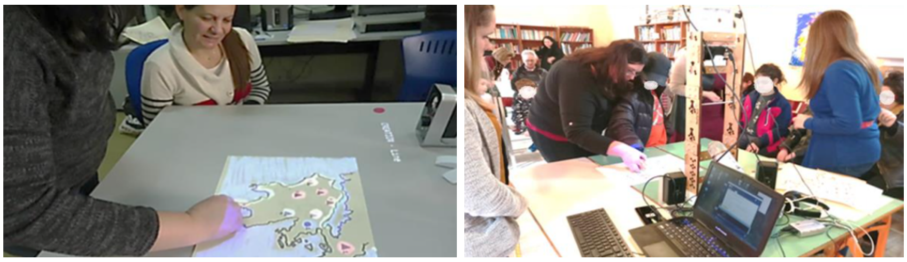

Figure 6. Combining touch and audio for accessible drawings at school.

7.5. Accessibility of e-learning systems

Participants: Pierre-Antoine Cinquin, Damien Caselli and Pascal Guitton

External collaborators: Hélène Sauzéon

In 2019, we continued to work on new digital teaching systems such as MOOCs. Unfortunately, accessibility for people with disabilities is often forgotten, which excludes them, particularly those with cognitive impairments for whom accessibility standards are fare from being established. We have shown in [12] that very few research activities deal with this issue.

In past years, we have proposed new design principles based on knowledge in the areas of accessibility (Ability-based Design and Universal Design), digital pedagogy (Instruction Design with functionalities that reduce the cognitive load : navigation by concept, slowing of the flow…), specialized pedagogy (Universal Design for Learning, eg, automatic note-taking, and Self Determination Theory, e.g., configuration of the interface according to users needs and preferences) and psychoducational interventions (eg, support the joint teacher-learner attention), but also through a participatory design approach involving students with disabilities and experts in the field of disability (Figure 7). From these framework, we have designed interaction features which have been implemented in a specific MOOC player called Aïana. Moreover, we have produced a MOOC on digital accessibility which is published on the national MOOC platform (FUN) using Aïana (4 sessions since 2016 with more than 11 000 registered participants). https://mooc-francophone.com/cours/mooc-accessibilite-numerique/. Our first field studies demonstrate the benefits of using Aïana for disabled participants [32].

7.6. A hybrid setup for an artistic experience

Participants: Vincent Da Silva Pinto, Martin Hachet

External collaborators: Léna d'azy

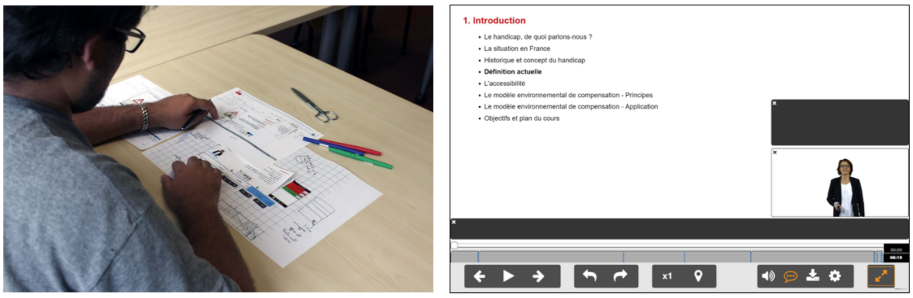

Figure 7. Design of Aïana MOOC player.

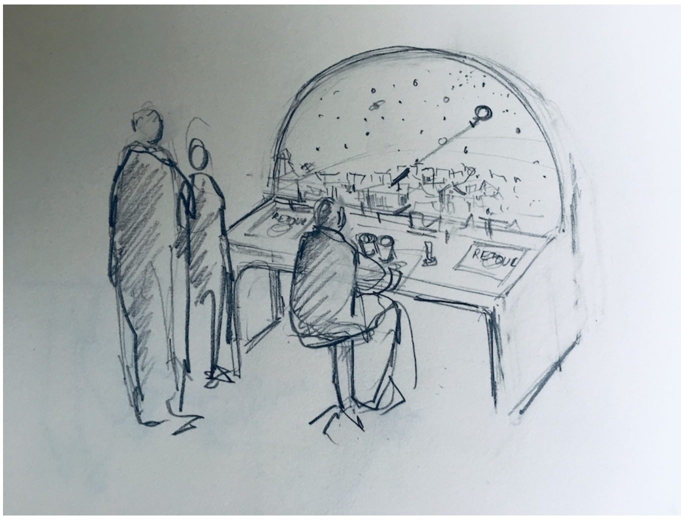

Figure 8. Echelles célestes allows the participant to explore the sky.

In 2019, we have worked with the stenographer Cécile Léna to conceive and build a hybrid setup that combines a real physical mock-up and a virtual environments. This allows the participants to explore the sky by pointing at planets with a telescope in miniature, and observing a virtual view of the pointed planet by looking through an immersive stereoscopic installation (Figure 8).

7.7. Mental state decoding from EEG signals using robust machine learning

Participants: Aurélien Appriou, Smeethy Pramij, Khadijeh Sadatnejad, Aline Roc, Léa Pillette, Thibaut Monseigne, Fabien Lotte

External collaborators: Andrzej Cichocki, Pierre-Yves Oudeyer, Edith Law, Jessie Ceha, Frédéric Dehais, Alban Duprès, Sarah Blum, Nicolas Drougard, Sébastien Scannella, Raphaëlle N. Roy

Modern machine learning algorithms to classify cognitive and affective states from electroencephalography signals: Estimating cognitive or affective states from brain signals is a key but challenging step in the creation of passive brain-computer interface (BCI) applications. So far, estimating mental workload or emotions from EEG signals is only feasible with modest classification accuracies, thus leading to unreliable neuroadaptive applications. However, recent machine learning algorithms, notably Riemannian geometry based classifiers (RGC) and convolutional neural networks (CNN), have shown to be promising for other BCI systems, e.g., motor imagery-BCIs. However, they have not been formally studied and compared together for cognitive or affective states classification. We have thus explored such machine learning algorithms, proposed new variants of them, and benchmarked them with classical methods to estimate both mental workload and affective states (Valence/Arousal) from EEG signals. We studied these approaches with both subject-specific and subject-independent calibration, to go towards calibration-free systems. Our results suggested that a CNN obtained the highest mean accuracy, although not significantly so, in both conditions for the mental workload study, followed by RGCs. However, this same CNN underperformed in both conditions for the emotion data set, a data set with little training data. On the contrary, RGCs proved to have the highest mean accuracy with the Filter Bank Tangent Space classifier (FBTSC) we introduced in this paper. Our results thus contributed to improve the reliability of cognitive and affective states classification from EEG. They also provide guidelines about when to use which machine learning algorithm. This work was just accepted for publication in the IEEE System Man and Cybernetics magazine.

Towards decoding curiosity from Brain and physiological signals: The neurophysiological mechanisms underlying curiosity and intrinsic motivation are currently not well understood. However, being able to identify objectively, from neurophysiological signals, the curiosity level of a user, would bring a very useful tool both to neuroscientists and psychologists, to understand curiosity deeper, as well as to designers of human-computer interaction, in order to trigger curiosity or to adapt an interaction to the curiosity levels of its users. A first step to do that, is to collect neurophysiological signals during known states of curiosity, in order to develop signal processing/machine learning tools to recognize those states from such signals. We designed and ran an experimental protocol to measure both brain activity through Electroencephalography (EEG) and physiological responses (heart rate, skin conductance, Electrocardiogram) when subjects were induced into different states of curiosity. During the experiment, fun facts were presented to subjects to induce different levels of curiosity. We obtained those fun facts using the Google functionality "I'm feeling curious" as well as crowdsourcing. A subject could choose a fun fact that made him curious, and push forward with a 4-to-10 questions chain on this theme. For each question on a given theme, a subject could choose to reveal the answer (interpreted as a curious state) or to skip it (interpreted as a non-curious state). Skipping an answer will automatically break the chain and will point the subject to the next fun fact. Neurophysiological signals were collected from 28 subjects, between a question and the choice of revealing the answer. Then those subjects graded the question on a 1-to-7 curiosity level scale. We are currently working on finding biological markers of curiosity by analyzing the collected signals using machine learning.

Channel Selection over Riemannian manifold with non-stationarity consideration for Brain-Computer interface applications: EEG signals are essentially non-stationary. Such non-stationarities, including cross-trial, cross-session, and cross-subject non-stationarities, are the result of various neurophysiological and extra-physiological causes. Such non-stationarities lead to variations in BCI users' performance. To handle this problem, we designed and compared multiple criteria for selecting EEG channels over the Riemannian manifold, for EEG classification. These criteria aim to promote EEG covariance matrix classifiers to generalize well by considering EEG data non-stationarity. Our approach consists of both increasing the discriminative information between classes over the manifold and reducing the dispersion within classes. We also reduce the influence of outliers in both discriminative and dispersion measures. The criteria were evaluated on EEG signals recorded from a tetraplegic subject and dataset IVa from BCI competition III. Experimental evidences confirm that considering the dispersion within each class as a measure for quantifying the effects of non-stationarity and removing the most affected channels can improve BCI performance (see Figure 9). This work was submitted to ICASSP 2020.

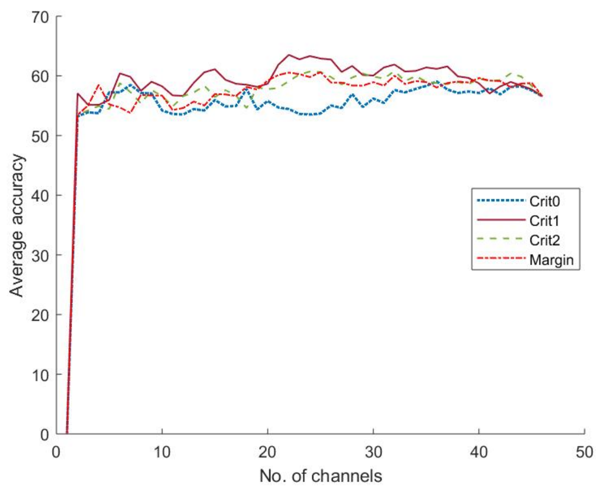

Figure 9. Results of BCI classification accuracy for various number of selected channels, for different channel selection algorithms. Our proposed algorithms - termed here Crit1, Crit2 and Margin - all improved upon the state-of-the-art (Crit0).

Monitoring Pilot's Mental Workload Using ERPs and Spectral Power with a Six-Dry-Electrode EEG System in Real Flight Conditions: Recent technological progress has allowed the development of low-cost and highly portable brain sensors such as pre-amplified dry-electrodes to measure cognitive activity out of the laboratory. This technology opens promising perspectives to monitor the "brain at work" in complex real-life situations such as while operating aircraft. However, there is a need to benchmark these sensors in real operational conditions. We therefore designed a scenario in which twenty-two pilots equipped with a six-dry-electrode EEG system had to perform one low load and one high load traffic pattern along with a passive auditory oddball. In the low load condition, the participants were monitoring the flight handled by a flight instructor, whereas they were flying the aircraft in the high load condition. At the group level, statistical analyses disclosed higher P300 amplitude for the auditory target (Pz, P4 and Oz electrodes) along with higher alpha band power (Pz electrode), and higher theta band power (Oz electrode) in the low load condition as compared to the high load one. Single trial classification accuracy using both event-related potentials and event-related frequency features at the same time did not exceed chance level to discriminate the two load conditions. However, when considering only the frequency features computed over the continuous signal, classification accuracy reached around 70% on average. This study demonstrates the potential of dry-EEG to monitor cognition in a highly ecological and noisy environment, but also reveals that hardware improvement is still needed before it can be used for everyday flight operations. This work was published in the journal Sensors in [13].

7.8. Understand and modeling Mental-Imagery BCI user training

Participants: Camille Benaroch, Aline Roc, Léa Pillette, Fabien Lotte

External collaborators: Camille Jeunet, Bernard N'Kaoua

Computational models of performance: Mental-Imagery based Brain-Computer Interfaces (MI-BCIs) make use of brain signals produced during mental imagery tasks to control a computerised system. The currently low reliability of MI-BCIs could be due, at least in part, to the use of inappropriate user-training procedures. In order to improve these procedures, it is necessary first to understand the mechanisms underlying MI-BCI user-training, notably through the identification of the factors influencing it. Thus, we first aimed at creating a statistical model that could explain/predict the performances and the progression of MI-BCI users using their traits (e.g., personality). We used the data of 42 participants (i.e., 180 MI-BCI sessions in total) collected from three different studies that were based on the same MI-BCI paradigm. We used machine learning regressions with a leave-one-subject-out cross validation to build different models. A first results showed that using the users' traits only may enable the prediction of performances for a single multiple-session experiment, but might not be sufficient to reliably predict MI-BCI performances across different experiments. A second result showed that using the users' traits and the users' past performances may enable the prediction of the progression of one user as reliable models were found for two of the three studies. Part of this work was published at the International Graz BCI conference in [21].

Would Motor-Imagery based BCI user training benefit from more women experimenters?: Throughout MI-BCI use, human supervision (e.g., experimenter or caregiver) plays a central role. While providing emotional and social feedback, people present BCIs to users and ensure smooth users' progress with BCI use. Though, very little is known about the influence experimenters might have on the results obtained. Such influence is to be expected as social and emotional feedback were shown to influence MI-BCI performances. Furthermore, literature from different fields showed an experimenter effect, and specifically of their gender, on experimental outcome. We assessed the impact of the interaction between experimenter and participant gender on MI-BCI performances and progress throughout a session. Our results revealed an interaction between participants gender, experimenter gender and progress over runs. It seems to suggest that women experimenters may positively influence participants' progress compared to men experimenters. This work was published at the International Graz BCI conference in [28].

7.9. Redefining and optimizing BCI user training tasks, stimulations and feedback

Participants: Jelena Mladenovic, Smeethy Pramij, Léa Pillette, Romain Sabau, Fabien Lotte

External collaborators: Jérémy Frey, Jérémie Mattout, Matteus Joffily, Emmanuel Maby, Bertrand Glize, Bernard N'Kaoua, Pierre-Alain Joseph, Camille Jeunet, Roger N'Kambou, Boris Mansencal

Active inference as a unifying, generic and adaptive framework for a P300-based BCI: We proposed the use of a generic, computational framework – Active (Bayesian) Inference to automatically lead the adaptation process in a P300 speller BCI. It adapts through the use of a probabilistic model of the user built upon user's reactions to flashing/spelled letters. Using such observations, at each iteration it updates its beliefs about user intentions, and converges towards a predefined goal, i.e. correctly spelled letters. Active Inference is a recent computational neuroscience approach that models learning and decision making of the brain. As such, by endowing such model to the BCI machine, it enables the machine to adapt in a similar fashion as the brain would. We demonstrate an implementation of Active Inference on a simulated P300-Speller BCI, with real EEG data from 18 subjects. Results demonstrate the ability of Active Inference to yield a significant increase in bit rate (17%) over state-of-the-art approaches. This work was published in Journal of Neural Engineering in [18].

Towards adaptive and adapted difficulty for MI-BCI user training: We investigated the relationship between the human factors and BCI performance during MI-BCI training. Additionally, we investigated the influence of user personality traits and states on learning the MI skill, i.e., evolution of performance over a session. We conducted a MI experiment in which we influence the user through task difficulty. We acquire data to build a predictive model that could unveil which kind of task is optimal for what kind of user. Moreover, depending on what we set to be predicted, be it a flow state or performance, it can serve as a guide for overall adaptation, i.e., it can serve as an optimization criteria to wager between user experience and system accuracy for instance. We then used priors on user traits and states acquired from the prediction models to perform a simple adaptive method which provides optimal task difficulty to each user. To demonstrate the usefulness of the model for maximizing performance, we perform a simulation using real data from the MI-BCI experiment mentioned above. This work was presented in the PhD thesis of Jelena Mladenovic, that was successfully defended on September 10th, 2019.

Impact of MI-BCI feedback for post-stroke and neurotypical people: We investigated how the modality of the feedback could be adapted to the learners. First, based on a review of the literature, we argued that somatosensory abilities of post-stroke patients have not, but should be, taken into account for BCI-based motor therapies. Indeed, somatosensory abilities play an important role in motor rehabilitation in general, and in BCI-based therapies in particular. It is assumed that during BCI based therapies the co-activation of ascending (i.e., somatosensory) and descending (i.e., sensorimotor) networks enables significant functional motor improvement, together with significant sensorimotor-related neurophysiological changes. Somatosensory abilities seem essential for the patients to benefit from the feedback provided by the BCI system. Yet, around half of post-stroke patients suffer from somatosensory deficits. We hypothesize that these deficits alter their ability to benefit from BCI-based therapies. Our review of the literature on BCI-based motor rehabilitation post-stroke of 14 randomized clinical trials indicates that somatosensory abilities were rarely considered and/or reported. Only two studies over the fourteen reported using them as inclusion/exclusion criteria. Though, none of these two studies reported how they assess the somatosensory abilities. We argue that assessing the somatosensory abilities of the patients is necessary to avoid any bias and enable reliable comparison between-subject and between-study. It could also be leveraged to improve our understanding of the underlying mechanisms of motor recovery and adapt the therapy to the patients' abilities.

Our review of the literature also informed us that a multimodal feedback composed of both somatosensory and visual feedback enables better performances than an unimodal visual feedback, at least in the short term. Though, the long term influence of such feedback remained unknown. Therefore, we assessed the long term effects of a multimodal feedback composed of both vibrotactile and realistic visual stimulations (presented in [43], see also Figure 10), and a unimodal feedback with only realistic visual stimulations. We found that the beneficial impact of a multimodal feedback composed of both visual and somatosensory stimulation compared to a visual feedback alone remains true even for long term training, which had not been tested before. Also, the order of presentation of the different modalities of feedback might have an influence. Using an unimodal visual feedback only seems to be better suited for untrained participants. We hypothesis that integrating information arising from two modalities of feedback while performing the task could be particularly challenging for a novice learner. Both these works were presented in the PhD thesis of Léa Pillette, that was successfully defended on December 16th, 2019.

A physical learning companion for Mental-Imagery BCI User Training: We continued our work on PEANUT, that we designed, implemented and tested, and which is the first learning companion dedicated to providing social presence and emotional feedback during MI-BCI user training. PEANUT provided social presence and emotional support, depending on the performance and progress of the user, through interventions combining both pronounced sentences and facial expressions. It was designed based on the literature, data analyses and user-studies. We notably conducted several online user surveys to identify the desired characteristics of our learning companion in terms of appearance and supporting speech content. From the results of these surveys we notably deduced which should be the characteristics (personal/non-personal, exclamatory/declarative) of the sentences to be used depending on the performance and progression of a learner. We also found that eyebrows could increase expressiveness of cartoon-like faces. Then, once this companion was implemented, we evaluated it during real online MI-BCI use. We found that non-autonomous people, who are more inclined to work in a group and are usually disadvantaged when using MI-BCI, were advantaged compared to autonomous people when PEANUT was present with an increase of 3.9% of peak performances. Furthermore, in terms of user experience, PEANUT seems to have improved how people felt

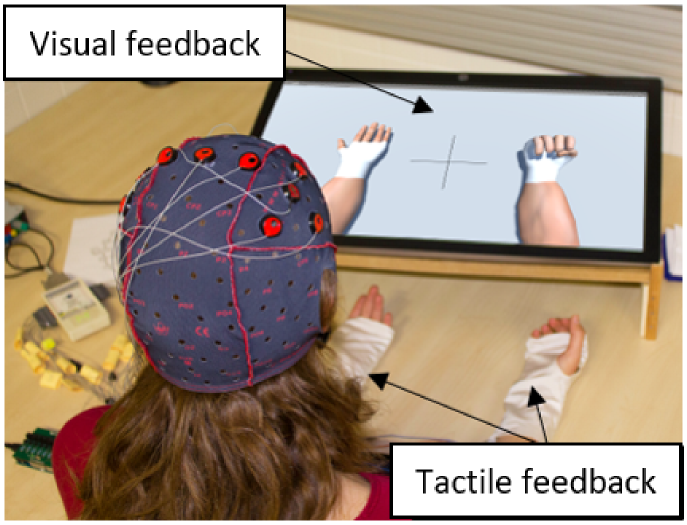

Figure 10. Our multimodal (realistic visual + vibrotactile) feedback for BCI training.

about their ability to learn and memorize how to use an MI-BCI by 7.4%, which is a dimension of the user experience we assessed. This work was published in the International Journal of Human-Computer Studies in [19].

Long-term mental imagery BCI training of a tetraplegic user: We participated to the Cybathlon BCI series 2019 competition in Graz (https://www.tugraz.at/institutes/ine/graz-bci-conferences/8th-graz-bci-conference-2019/cybathlon-bci-series-2019/), as team NITRO (Neurotechnology Inria Team Racing Odyssey), during which we trained a tetraplegic user over several months, with up to 3 training sessions per week, to learn to control a 4-class and self-paced mental imagery BCI connected to a racing video game (see Figure 11). This training and the resulting BCI design used several of our recent research and development works, notably new OpenViBE development on the feedback, progressive user training and adaptive Riemannian EEG classifiers [41].

7.10. Turning negative into positives! Exploiting "negative" results in Brain-Computer Interface research

Participants: Fabien Lotte

External collaborators: Laurent Bougrain, Ricardo Chavarriaga, Camille Jeunet, Karen Dijkstra, Andrea Kübler, Reinhold Scherer, Moritz Grosse-Wentrup, Natalie Dayan, Dave Thompson, Md Rakibul Mowla

Results that do not confirm expectations are generally referred to as "negative" results. While essential for scientific progress, they are too rarely reported in the literature - BCI research is no exception. This led us to organize a workshop on BCI negative results during the 2018 International BCI meeting. First, we demonstrated why (valid) negative results are useful, and even necessary for BCIs. These results can be used to confirm or disprove current BCI knowledge, or to refine current theories. Second, we provided concrete examples of such useful negative results, including the limits in BCI-control for complete locked-in users and predictors of motor imagery BCI performances. Finally, we suggested levers to promote the diffusion of (valid) BCI negative results, e.g., promoting hypothesis-driven research using valid statistical tools, organizing special issues dedicated to BCI negative results, or convincing institutions and editors that negative results are valuable. This work was published in the Brain-Computer Interface journal, in [16].

Figure 11. BCI-based control of a racing video game by a tetraplegic user during the Cybathlon BCI series in Graz, Austria.

7.11. Speed of rapid serial visual presentation of pictures, numbers and words affects event-related potential-based detection accuracy

Participants: Fabien Lotte

External collaborators: Stephanie Lees, Paul McCullagh, Liam Maguire, Damien Coyle

Rapid serial visual presentation (RSVP) based brain-computer interfaces (BCIs) can detect target images among a continuous stream of rapidly presented images, by classifying a viewer's event related potentials (ERPs) associated with the target and non-targets images. Whilst the majority of RSVP-BCI studies to date have concentrated on the identification of a single type of image, namely pictures, here we studied the capability of RSVP-BCI to detect three different target image types: pictures, numbers and words. The impact of presentation duration (speed) i.e., 100-200ms (5-10Hz), 200-300ms (3.3-5Hz) or 300-400ms (2.5-3.3Hz), was also investigated. 2-way repeated measure ANOVA on accuracies of detecting targets from non-target stimuli (ratio 1:9) measured via area under the receiver operator characteristics curve (AUC) for N=15 subjects revealed a significant effect of factor Stimulus-Type (pictures, numbers, words) (F (2,28) = 7.243, p = 0.003) and for Stimulus-Duration (F (2,28) = 5.591, p = 0.011). Furthermore, there was an interaction between stimulus type and duration: F (4,56) = 4.419, p = 0.004). The results indicated that when designing RSVP-BCI paradigms, the content of the images and the rate at which images are presented impact on the accuracy of detection and hence these parameters are key experimental variables in protocol design and applications, which apply RSVP for multimodal image datasets. This work was published in IEEE Transactions on Neural Systems and Rehabilitation Engineering, in [15].

7.12. Design and preliminary study of a neurofeedback protocol to self-regulate an EEG marker of drowsiness

Participants: Thibaut Monseigne, Fabien Lotte

External collaborators: Stéphanie Bioulac, Pierre Philip, Jean-Arthur Micoulaud-Franchi

Neurofeedback (NF) consists in using EEG measurements to guide users to perform a cognitive learning using information coming from their own brain activity, by means of a real-time sensory feedback (e.g., visual or auditory). Many NF approaches have been studied to improve attentional abilities, notably for attention deficit hyper activity disorder. However, to our knowledge, no NF solution has been proposed to specifically reduce drowsiness. Thus, we propose an EEG-NF solution to train users to self-regulate an EEG marker of drowsiness, and evaluate it with a preliminary study. Results with five healthy subjects showed that three of them could learn to self-regulate this EEG marker with a relatively short number of NF sessions (up to 8 sessions of 40 min). This work was published at the International Graz BCI conference in [27].

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

Ullo:

Duration: 2017-2020

Local coordinator: Martin Hachet

Following our work with the Introspectibles (Teegi, TOBE, Inner Garden), we are currently working with the ULLO company to bring these new interfaces to healthcare centers.

AKIANI:

Duration: 2019-2020

Local coordinator: Fabien Lotte

InriaTech project on physiological computing and neuroergonomics.

9. Partnerships and Cooperations

9.1. Regional Initiatives

HOBIT:

Funding: Program STEP - (Soutien à la Transformation et l'Expérimentation Pédagogiques)

Duration: 2019-2020

Local coordinator: Martin Hachet

Partners: Université de Bordeaux

The objective is to transform traditional practices for the teaching of optics in more innovative approaches based on augmented reality and tangible interaction. To this end, we continue improving and testing our HOBIT platform.

Echelles Celestes:

Funding: Idex - Université de Bordeaux - Art and Sciences program

Duration: 2019-2020

Local coordinator: Martin Hachet

Partners: Université de Bordeaux

We explore interactive artistic installations based on the combination of physical and virtual elements.

Erlen:

Funding: Université de Bordeaux - Hacketafac program

Duration: 2018-2019

Local coordinator: Pierre-Antoine Cinquin

We won a grant from Université de Bordeaux to explore awareness of power consumption by way of tangible and ambient interfaces.

Neuroperf:

Funding: Labex BRAIN / Université de Bordeaux

Duration: 2017-2019

Coordinator: Jean-Arthur Micoulaud Franchi

Local coordinator: Fabien Lotte

A project aimed at exploring EEG-based neurofeedback for improving daytime alertness.

9.2. National Initiatives

eTAC: Tangible and Augmented Interfaces for Collaborative Learning:

Funding: EFRAN

Duration: 2017-2021

Coordinator: Université de Lorraine

Local coordinator: Martin Hachet

Partners: Université de Lorraine, Inria, ESPE, Canopé, OpenEdge,

the e-TAC project proposes to investigate the potential of technologies ”beyond the mouse” in order to promote collaborative learning in a school context. In particular, we will explore augmented reality and tangible interfaces, which supports active learning and favors social interaction.

website: http://e-tac.univ-lorraine.fr/index

ANR Project EMBER:

Duration: 2020-2023

Partners: Inria/AVIZ, Sorbonne Université

Coordinator: Pierre Dragicevic (Inria Saclay)

Local coordinator: Martin Hachet

The goal of the project will be to study how embedding data into the physical world can help people get insights into their own data. While the vast majority of data analysis and visualization takes place on desktop computers located far from the objects or locations the data refers to, in situated and embedded data visualizations, the data is directly visualized near the physical space, object, or person it refers to.

website: https://ember.inria.fr

ANR Project REBEL:

Duration: 2016-2019

Partners: Potioc, Handicap Activity Cognition Health lab (Univ. Bordeaux)

Coordinator: Fabien Lotte

Brain-Computer Interfaces (BCI) are communication systems that enable their users to send commands to computers through brain activity only. While BCI are very promising for assistive technologies or human-computer interaction (HCI), they are barely used outside laboratories, due to a poor reliability. Designing a BCI requires 1) its user to learn to produce distinct brain activity patterns and 2) the machine to recognize these patterns using signal processing. Most research efforts focused on signal processing. However, BCI user training is as essential but is only scarcely studied and based on heuristics that do not satisfy human learning principles. Thus, currently poor BCI reliability is probably due to suboptimal user training. Thus, we propose to create a new generation of BCI that apply human learning principles in their design to ensure the users can learn high quality control skills, hence making BCI reliable. This could change HCI as BCI have promised but failed to do so far.

website: https://team.inria.fr/potioc/collaborative-projects/rebel/

Inria Project Lab AVATAR:

Duration: 2018-2022

Partners: Inria project-teams: GraphDeco, Hybrid, Loki, MimeTIC, Morpheo

Coordinator: Ludovic Hoyet (Inria Rennes)

Local coordinator: Martin Hachet

This project aims at designing avatars (i.e., the user's representation in virtual environments) that are better embodied, more interactive and more social, through improving all the pipeline related to avatars, from acquisition and simulation, to designing novel interaction paradigms and multi-sensory feedback.

website: https://avatar.inria.fr

9.3. European Initiatives

9.3.1. FP7 & H2020 Projects

BrainConquest:

Program: ERC Starting Grant

Project title: BrainConquest - Boosting Brain-Computer Communication with High Quality User Training

Duration: 2017-2022

Coordinator: Fabien Lotte

Abstract: Brain-Computer Interfaces (BCIs) are communication systems that enable users to send commands to computers through brain signals only, by measuring and processing these signals. Making computer control possible without any physical activity, BCIs have promised to revolutionize many application areas, notably assistive technologies, e.g., for wheelchair control, and man-machine interaction. Despite this promising potential, BCIs are still barely used outside laboratories, due to their current poor reliability. For instance, BCIs only using two imagined hand movements as mental commands decode, on average, less than 80% of these commands correctly, while 10 to 30% of users cannot control a BCI at all. A BCI should be considered a co-adaptive communication system: its users learn to encode commands in their brain signals (with mental imagery) that the machine learns to decode using signal processing. Most research efforts so far have been dedicated to decoding the commands. However, BCI control is a skill that users have to learn too. Unfortunately how BCI users learn to encode the commands is essential but is barely studied, i.e., fundamental knowledge about how users learn BCI control is lacking. Moreover standard training approaches are only based on heuristics, without satisfying human learning principles. Thus, poor BCI reliability is probably largely due to highly suboptimal user training. In order to obtain a truly reliable BCI we need to completely redefine user training approaches. To do so, I propose to study and statistically model how users learn to encode BCI commands. Then, based on human learning principles and this model, I propose to create a new generation of BCIs which ensure that users learn how to successfully encode commands with high signal-to-noise ratio in their brain signals, hence making BCIs dramatically more reliable. Such a reliable BCI could positively change man-machine interaction as BCIs have promised but failed to do so far.

9.3.2. Collaborations in European Programs, Except FP7 & H2020

VISTE:

Program: Erasmus + Key Action 2: Cooperation for Innovation and Exchange of Good Practices

Project title: VISTE: Empowering spatial thinking of students with visual impairment

Duration: 01/09/2016 - 31/08/2019

Coordinator: Professor Marinos Kavouras (Vice-Rector, National Technical University of Athens and VISTE Project Leader)

Partners: National Technical University of Athens, Inria, Intrasoft International S.A., Casa Corpului Didactic Cluj, Eidiko Dimotiko Sxolio Tiflon Kallitheas, Liceul Special pentru Deficienti de Vedere Cluj-Napoca. External collaborators : IRSA, RealityTech

Abstract: Six partners from four European countries are working together to develop strategies, educational components and an ICT toolkit towards effective spatial thinking of students with VI, facilitating inclusion. The competence of spatial thinking, usage and interpretation of maps or other spatial tools is not self-evident for all; it is a dexterity which must be cultivated. For students experiencing disabilities, such as visual impairment (VI), spatial thinking proves to be an imperative skill for perceiving the world far beyond their immediate experience. Learning functional ways to utilize spatial experiences as an entirety and realize the relationships between objects in space and themselves is vital. Maps and other spatial representations are a splendid source of information for portraying space and environment. By using tactile maps and innovative ICT technologies, children may deploy their spatial notion more effectively compared to proximate orientation experiences in accordance with verbal directions. Providing thus a concrete set of such tools would empower specific spatial thinking skills not only of those with VI but of all students. VISTE aims at empowering the spatial thinking skills of students with VI. This will be accomplished by providing an innovative methodological framework and a semantic and technical infrastructure for developing appropriate inclusive educational modules to foster spatial thinking. The project's main target groups are primary/secondary education students, as well as teachers, teachers' trainers, and staff involved in their education.

9.4. International Initiatives

9.4.1. Inria International Labs

9.4.1.1. Informal International Partners

- Univ. Ulster UK (Pr. Damien Coyle) on RSVP-BCI
- NTNU, Norway (Pr. Marta Molinas, Dr. Alejandro Torres Garcia) on colour-based BCI
- EPFL, Switzerland (Dr Ricardo Chavarriaga) on Negative Results for BCI

9.5. International Research Visitors

9.5.1. Visits of International Scientists

- Dr. Alejandro Torres Garcia, postdoc from NTNU, Norway, August 2019
- Ahmed Azab, PhD student, Univ. Sheffield, UK, August 2019
- Pr. Stephanie Enriquez-Geppert, University of Groningen, the Netherlands, April 2019
- Pr. Stephan Debener, Univ. Oldenburg, Germany, May 2019
- Pr. Jordi Solé-Casal, Univ. Vic, Spain and Pr. Feng Duan, Univ. Nankai, China, December 2019

9.5.1.1. Internships

- Sayu Yamamoto, Tokyo Univ. of Agriculture and Technology, Japan - from September 2019 to March 2020

9.5.2. Visits to International Teams

9.5.2.1. Research Stays Abroad

- Fabien Lotte was a visiting associate Professor at the Tokyo University of Agriculture and Technology (TUAT), Japan, for 2 weeks in February and for the whole month on November 2019. He worked on BCI and EEG signal processing in the lab of Pr. Toshihisa Tanaka.
- Jelena Mladenovic was a scientific visitor at the Serbian Academy of Science and Arts, Institute of Mathematics, with Dragan Urosevic, from 20th of February to 25th of March 2019.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events: Organisation

10.1.1.1. General Chair, Scientific Chair

- EduIHM workshop at IHM 2019 - Martin Hachet
- EduIHM workshop at EIAH 2019 - Martin Hachet
- "4ème conference nationale sur le Neurofeedback: le neurofeedback, un outil pour la recherche en neurosciences cognitives ?", co-chair - Fabien Lotte
- “How do we learn to use a BCI? Current state of knowledge, prospects of improvement using an interdisciplinary approach”, Workshop at the International Graz BCI conference 2019, Graz, Austria – co-chair, Fabien Lotte

10.1.1.2. Member of the Organizing Committees

- Workshops organizer and sponsors finder for the event for the French BCI/NF Society, called CORTICO days - Jelena Mladenovic

10.1.2. Scientific Events: Selection

10.1.2.1. Member of the Conference Program Committees

- International Graz BCI conference 2019, Fabien Lotte
- NeuroAdaptive Technology conference (NAT) 2019, Fabien Lotte
- Journées d’informatique théâtrale 2020, Martin Hachet, Pascal Guitton

10.1.2.2. Reviewer

- ACM UIST 2019
- ACM CHI 2019
- ACM CHI Play 2019
- HICS 2019
- TACCESS 2019

- ASSETS 2019
- IEEE SMC 2019
- ICASSP 2019
- CogSci 2019
- JJC-ICON 2019
- Int Graz BCI Conf 2019

10.1.3. Journal

10.1.3.1. Guest editor

- ERCIM News 120 - Educational Technology, Martin Hachet
- Frontiers in Human Neuroscience, Fabien Lotte
- Frontiers in Brain-Computer Interfaces, Fabien Lotte

10.1.3.2. Member of the Editorial Boards

- IEEE Computer Graphics and Applications, Martin Hachet
- Journal of Neural Engineering, Fabien Lotte
- Brain-Computer Interfaces, Fabien Lotte

10.1.3.3. Reviewer - Reviewing Activities

- Frontiers in Human Neuroscience
- Journal of Neural Engineering
- Brain-Computer Interfaces
- IEEE TBME
- Nature Communications
- ACM TOCHI
- IEEE TCYB
- IJHCS
- Scientific Report
- IEEE Trans. Games
- NeuroImage
- JMUI

10.1.4. Invited Talks

- ”Hybrid environments (real/virtual) in Education”, LIRIS, Lyon, Jan. 2019 - Martin Hachet
- ”Vers une carte multisensorielle en réalité augmentée pour les personnes aveugles et malvoyantes : une approche participative”, ARIBA Nov. 2019, Bordeaux - Lauren Thevin
- ”VISTE project”, FISAF, Nov. 2019, Paris - Lauren Thevin
- ”Example of HCI for Humas: Previous works and perspectives”, LMU Muchen, April 2019 - Lauren Thevin
- “Adaptive Riemannian Classifiers for Long-term Brain-Computer Interface training of a Tetraplegic User”, Seminar at ISAE-Supaero, December 2019 - Fabien Lotte
- “From machine learning to user learning in Brain-Computer Interaction”, Tokyo University of Agriculture and Technology (TUAT), GIR Seminar, Tokyo, Japan, November 2019 - Fabien Lotte
- “Understanding, modeling and optimizing Mental Imagery-based Brain-Computer Interface user training”, BCI: Science and Practice international conference, Keynote, Samara, Russia, October 2019 - Fabien Lotte

- “Machine learning and experimental tools towards EEG-based NeuroAdaptive Technologies”, international conference on NeuroAdaptive Technologies (NAT’19), Keynote, Liverpool, UK, July 2019 - Fabien Lotte
- “Brain-Computer Interfaces: Myths, open challenges and realistic expectations”, NICE Meeting, Ludwig Maximilian University of Munich, Germany, June 2019 - Fabien Lotte
- “Understanding and modeling user training in Mental-Imagery-based Brain-Computer Interfaces”, University of Freiburg, Germany, June 2019 - Fabien Lotte
- "ElectroEncephaloGraphic signal processing & classification for Brain-Computer Interfaces", Time Series Day, Rennes, France, March 2019 - Fabien Lotte
- "Vers une accessibilité numérique des systèmes d’éducation numérique", ESPE Angers, Rencontres académiques du numérique, Rectorat de Nantes, En visioconférence, March 2019 - Pascal Guitton & Hélène Sauzéon
- "Ethique du numérique pour la santé", Séminaire IA et sens clinique, Bordeaux, March 2019 - Pascal Guitton
- "Réalité virtuelle et handicap : étude, évaluation, réhabilitation", 20 ans d’Immersia, Rennes, November 2019 - Pascal Guitton
- "Les Sciences du Numérique au service de la pratique sportive", Colloque Sport et numérique, Bordeaux, July 2019 - Pascal Guitton
- "Interfaces Cerveau-Ordinateur (ICO) & Neurofeedback (NF): Influence des capacités somatosensorielles sur la réhabilitation motrice post-AVC", SOFMER, Bordeaux, Oct. 2019 - Léa Pillette
- "Predicting BCI performances from users’ profile using Computational Modelling", Workshop "How do we learn to use a BCI? Current state of knowledge, prospects of improvement using an interdisciplinary approach", International Graz BCI conference, Graz, Austria, September 2019 - Camille Benaroch

10.1.5. Leadership within the Scientific Community

- Co-leader of the EduIHM group dedicated to research in HCI for Education - Martin Hachet
- Member of the administrative council of CORTICO, the French national association of BCI - Fabien Lotte
- Secretary of the Bordeaux association of Doctoral Students in Computer Science (AFoDIB) - Aline Roc

10.1.6. Scientific Expertise

- Expert for ”Credit Impot Recherche” - Martin Hachet
- Committee for the creation of 2 Inria teams - Martin Hachet
- Committee for recruitment of an assistant professor at Telecom ParisTech - Martin Hachet
- Expert for Appel à projets exploratoires Institut de la cognition - Pascal Guitton

10.1.7. Research Administration

- Member of ”Bureau du comite des projets”, Martin Hachet
- Member of ”Conseil administration de l’AFIHM”, Martin Hachet
- Representative of Inria at NEM (New European Media), Fabien Lotte
- Member of ”Commission des emplois recherche Inria Bordeaux”, Fabien Lotte
- Member of Commission de recrutement des Inspecteurs Généraux de l’Education Nationale (IGEN), Pascal Guitton
- Responsable of Inria Cellule de veille et de prospective, Pascal Guitton
- Member of Inria Ethical Committee (COERLE), Pascal Guitton

- Member of Inria Comité Parité et Egalité, Pascal Guitton
- Responsable of Inria Radar Committee (new annual Activity Report), Pascal Guitton
- Member of Inria International Chairs Committee, Pascal Guitton

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

- Master: Réalité Virtuelle, 12h eqTD, M2 Cognitive science, Université de Bordeaux - Martin Hachet
- Master: Réalité Virtuelle, 6h eqTD, M2 Cognitive science, Université de Bordeaux - Fabien Lotte
- Master: Handicap et Nouvelles technologies, CM 7,5h eqtd, M2 Cognitive Science, Université de Bordeaux - Aurélien Appriou
- Master : Handicap et Nouvelles technologies, 9h eqTD, M2 Cognitive science, Université de Bordeaux - Philippe Giraudeau
- Master: Réalités Virtuelles et augmentées, 18h eqTD, M2 Computer science, Université de Bordeaux - Martin Hachet,
- Master: Réalités Virtuelles et augmentées, 6h eqTD, M2 Computer science, Université de Bordeaux - Fabien Lotte,
- Master: Réalités Virtuelles et augmentées, 18h eqTD, M2 Computer science, Université de Bordeaux - Rajkumar Darbar
- Master: Neuroergonomics & Brain-Computer Interfaces, 2h eqtd, Master Human-Computer Interaction, Ludwig-Maximilians-Universität München, Germany - Fabien Lotte
- Bachelor: Initiation to computer sciences, 31.66h eqTD, L1 Université de Bordeaux - Adélaïde Genay
- Bachelor: C programing, 14,67h eqTD, L2 Université de Bordeaux - Adélaïde Genay
- Engineering school: Ergonomie et Interaction, 15h eqTD, 3rd year, ENSEIRB, INP - Martin Hachet
- Engineering school: Réalités Virtuelles et augmentées, 1,5h eqTD, ENSC - Martin Hachet
- Engineering school: Web programming, ENSC - Lauren Thevin
- Engineering School: Aeronautical engineering and Neuroergonomics, 3h eqTD, M2 ISAE-Supaero, Toulouse - Fabien Lotte
- Engineering school: Immersion and interaction with visual worlds, 4h eqtd, Graduate Degree Artificial Intelligence, Ecole Polytechnique Palaiseau - Fabien Lotte
- Engineering school: Advanced mathematics and computer science, 2018-2019: 61.5h eqTD, Ecole Nationale Supérieure des Arts et Metiers, ENSAM, Bordeaux, France - Camille Benaroch
- Engineering school: Lecture "Interface Cerveau-Ordinateur (BCIs) Le quotidien de la recherche", UE Systèmes Cognitifs (CNU 27), 2h eqTD, ENSC, Bordeaux INP - Aline Roc and Léa Pillette

10.2.2. Supervision

- PhD in progress: Adelaïde Genay, Hybrid Avatars, 1/10/2019, Martin Hachet
- PhD in progress: Rajkumar Darbar, Actuated Tangible User Interfaces, Since 1/12/2017, Martin Hachet
- PhD in progress: Philippe Giraudeau, Collaborative learning with tangible and aumented interfaces, Since 1/10/2017, Martin Hachet
- PhD in progress: Marc Baloup, Interaction with Avatars, Since 1/10/2018, Martin Hachet (33%)
- PhD in progress: Aurélien Appriou, Estimating learning-related mental states in EEG, since 1/10/2017, Fabien Lotte

- PhD in progress: Camille Benaroch, Computational Modeling of BCI user training, since 1/10/2018, Fabien Lotte (50%)
- PhD in progress: Aline Roc, Designing, studying and optimzing training tasks and training program for BCI control, Fabien Lotte
- PhD defended: Pierre-Antoine Cinquin, Design and Experimental Validation of Accessible E-learning systems for people with cognitive disabilities, November 23th 2019, Pascal Guitton (50%)
- PhD defended: Jelena Mladenovic, User modeling for Adaptive BCI design, since 01/01/2016, Defended 10/09/2019, Fabien Lotte (50%)
- PhD defended: Léa Pillette, Formative feedback for BCI, since 01/10/2016, Defended 16/12/2019, Fabien Lotte (50%)

10.2.3. Juries

- HDR: Isabelle Pecci [president], Université de Lorraine, Martin Hachet
- HDR: Pierrick Legrand [examiner], Univ. Bordeaux, France, Fabien Lotte
- HDR: Selina Wriessnegger [with report], TU Graz, Austria, Fabien Lotte
- PhD: Grégoire Cattan [with report], Univ. Grenoble Alpes, Martin Hachet
- PhD: Sylvain Pauchet [with report], ISAE Supaero, Martin Hachet
- PhD: Flavio Camarrone [with report], KU Leuven, Belgium, Fabien Lotte
- PhD: Andreas Meinel [with report], Univ. Freiburg, Germany, Fabien Lotte
- PhD: Fanny Grosselin [with report], Sorbonne Université, France, Fabien Lotte
- PhD: Kevin Verdière [president], ISAE-Supaero, France, Fabien Lotte
- PhD: Pedro Luiz Coelho Rodrigues [examiner], Grenoble INP, France, Fabien Lotte
- PhD: Hakim Si Mohammed [guest], INSA Rennes, France, Fabien Lotte
- PhD: Leticia Seixas-Pereira [guest], Univ. Paris 8, France, Pascal Guitton
- PhD: Thomas Crespel [president], Univ. Bordeaux, France, Pascal Guitton
- MD: Andrea Ferrier [examiner], Univ. Bordeaux/CHU Bordeaux, France, Fabien Lotte
- MS: Jaime A. Riascos [examiner], Federal University of Rio Grande do Sul, Brazil, Fabien Lotte

10.3. Popularization

10.3.1. Articles and contents

- Interview - video portrait for “Dealers de Science” made by 2nd year Master’s student in Mediation of the Sciences (to be published online in 1-2 months), December 2019 - Aline Roc
- Petit binaire : les dessous du JPEG, Blog binaire – Le Monde, May 2019, Pascal Guitton, [37]
- Ethique du numérique pour la santé, Blog binaire – Le Monde, November 2019, Pascal Guitton, [38]

10.3.2. Interventions

- Computer Sciences and Art - Rencontre Mexique-France - La culture à l’ère numérique, Nov 2019 - Martin Hachet
- FACTS Festival, Art and Sciences, Bordeaux Nov. 2019 - Martin Hachet
- ”Des étoiles pleins les yeux”. Rancards du Savoir. Bordeaux Nov. 2019 - Martin Hachet
- PubHD Bordeaux, November 2019 - Philippe Giraudeau
- ”Erlen, an Ambiant Interface dedicated to the awareness of energy consumption” BootCamp #7 for Digital Vice-Presidents of french Universities, November 2019, Bordeaux - Philippe Giraudeau

- “Why and How to train to control a Brain-Computer Interfaces?”, BCI: Science and Practice international conference, outreach lecture, Samara, Russia, October 2019 - Fabien Lotte
- “One year of scientific visit on neurotechnologies at the RIKEN Brain Science Institute, Japan”, Japanese Society for the promotion of Science (JSPS) Business meeting, Bordeaux, September 2019 - Fabien Lotte
- "Progrès et applications des interfaces cerveau-ordinateur", Séminaire IRGO, Bordeaux, France, April 2019 - Fabien Lotte
- "Pourquoi et comment apprendre à contrôler une interface cerveau-ordinateur ?", conférence ’les interfaces cerveau-machine : piloter un objet par l’activité cérébrale’, cité des sciences et de l’industrie, Paris, France, February 2019 - Fabien Lotte
- "Ethique et numérique", Festival Transfo, Plongez dans l’univers du numérique, Grenoble, January 2019 - Pascal Guitton

10.3.3. Internal action

- InfoBreak Inria Bordeaux, "Une équipe de choc pour interfacer cerveaux et machines" - Fabien Lotte

11. Bibliography

Major publications by the team in recent years

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Project-Team REALOPT

Reformulations based algorithms for Combinatorial Optimization

IN COLLABORATION WITH: Institut de Mathématiques de Bordeaux (IMB), Laboratoire Bordelais de Recherche en Informatique (LaBRI)

IN PARTNERSHIP WITH:
CNRS

Université de Bordeaux

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Optimization, machine learning and statistical methods

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Project-Team REALOPT

Creation of the Project-Team: 2009 January 01

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A1.1.4. - High performance computing
A1.1.5. - Exascale
A1.3.5. - Cloud
A6.1.3. - Discrete Modeling (multi-agent, people centered)
A6.2.5. - Numerical Linear Algebra
A6.2.6. - Optimization
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A8.1. - Discrete mathematics, combinatorics
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B9.5.2. - Mathematics

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2. Overall Objectives

2.1. Overall Objectives

Keywords: Reformulation techniques in Mixed Integer Programming (MIP), Polyhedral approaches (cut generation), Robust Optimization, Approximation Algorithms, Extended formulations, Lagrangian Relaxation (Column Generation) based algorithms, Dantzig and Benders Decomposition, Primal Heuristics, Graph Theory, Constraint Programming.

Quantitative modeling is routinely used in both industry and administration to design and operate transportation, distribution, or production systems. Optimization concerns every stage of the decision-making process: long term investment budgeting and activity planning, tactical management of scarce resources, or the control of day-to-day operations. In many optimization problems that arise in decision support applications the most important decisions (control variables) are discrete in nature: such as on/off decision to buy, to invest, to hire, to send a vehicle, to allocate resources, to decide on precedence in operation planning, or to install a connection in network design. Such *combinatorial optimization* problems can be modeled as linear or nonlinear programs with integer decision variables and extra variables to deal with continuous adjustments. The most widely used modeling tool consists in defining the feasible decision set using linear inequalities with a mix of integer and continuous variables, so-called Mixed Integer Programs (MIP), which already allow a fair description of reality and are also well-suited for global optimization. The solution of such models is essentially based on enumeration techniques and is notoriously difficult given the huge size of the solution space.

Commercial solvers have made significant progress but remain quickly overwhelmed beyond a certain problem size. A key to further progress is the development of better problem formulations that provide strong continuous approximations and hence help to prune the enumerative solution scheme. Effective solution schemes are a complex blend of techniques: cutting planes to better approximate the convex hull of feasible (integer) solutions, extended reformulations (combinatorial relations can be formulated better with extra variables), constraint programming to actively reduce the solution domain through logical implications along variable fixing based on reduced cost, Lagrangian decomposition methods to produce powerful relaxations, and Bender's decomposition to project the formulation, reducing the problem to the important decision variables, and to implement multi-level programming that models a hierarchy of decision levels or recourse decision in the case of data adjustment, primal heuristics and meta-heuristics (greedy, local improvement, or randomized partial search procedures) to produce good candidates at all stage of the solution process, and branch-and-bound or dynamic programming enumeration schemes to find a global optimum, with specific strong strategies for the selection on the sequence of fixings. The real challenge is to integrate the most efficient methods in one global system so as to prune what is essentially an enumeration based solution technique. The progress are measured in terms of the large scale of input data that can now be solved, the integration of many decision levels into planning models, and not least, the account taken for random (or dynamically adjusted) data by way of modeling expectation (stochastic approaches) or worst-case behavior (robust approaches).
Building on complementary expertise, our team's overall goals are threefold:

(i) Methodologies: To design tight formulations for specific combinatorial optimization problems and generic models, relying on delayed cut and column generation, decomposition, extended formulations and projection tools for linear and nonlinear mixed integer programming models. To develop generic methods based on such strong formulations by handling their large scale dynamically. To generalize algorithmic features that have proven efficient in enhancing performance of exact optimization approaches. To develop approximation schemes with proven optimality gap and low computational complexity. More broadly, to contribute to theoretical and methodological developments of exact and approximate approaches in combinatorial optimization, while extending the scope of applications and their scale.

(ii) Problem solving: To demonstrate the strength of cooperation between complementary exact mathematical optimization techniques, dynamic programming, robust and stochastic optimization, constraint programming, combinatorial algorithms and graph theory, by developing "efficient" algorithms for specific mathematical models. To tackle large-scale real-life applications, providing provably good approximate solutions by combining exact, approximate, and heuristic methods.

(iii) Software platform & Transfer: To provide prototypes of modelers and solvers based on generic software tools that build on our research developments, writing code that serves as the proof-of-concept of the genericity and efficiency of our approaches, while transferring our research findings to internal and external users.

3. Research Program

3.1. Introduction

integer programming, graph theory, decomposition approaches, polyhedral approaches, quadratic programming approaches, constraint programming.

Combinatorial optimization is the field of discrete optimization problems. In many applications, the most important decisions (control variables) are binary (on/off decisions) or integer (indivisible quantities). Extra variables can represent continuous adjustments or amounts. This results in models known as *mixed integer programs* (MIP), where the relationships between variables and input parameters are expressed as linear constraints and the goal is defined as a linear objective function. MIPs are notoriously difficult to solve: good quality estimations of the optimal value (bounds) are required to prune enumeration-based global-optimization

algorithms whose complexity is exponential. In the standard approach to solving an MIP is so-called *branch-and-bound algorithm* : (i) one solves the linear programming (LP) relaxation using the simplex method; (ii) if the LP solution is not integer, one adds a disjunctive constraint on a factional component (rounding it up or down) that defines two sub-problems; (iii) one applies this procedure recursively, thus defining a binary enumeration tree that can be pruned by comparing the local LP bound to the best known integer solution. Commercial MIP solvers are essentially based on branch-and-bound (such IBM-CPLEX, FICO-Xpress-mp, or GUROBI). They have made tremendous progress over the last decade (with a speedup by a factor of 60). But extending their capabilities remains a continuous challenge; given the combinatorial explosion inherent to enumerative solution techniques, they remain quickly overwhelmed beyond a certain problem size or complexity.
Progress can be expected from the development of tighter formulations. Central to our field is the characterization of polyhedra defining or approximating the solution set and combinatorial algorithms to identify "efficiently" a minimum cost solution or separate an unfeasible point. With properly chosen formulations, exact optimization tools can be competitive with other methods (such as meta-heuristics) in constructing good approximate solutions within limited computational time, and of course has the important advantage of being able to provide a performance guarantee through the relaxation bounds. Decomposition techniques are implicitly leading to better problem formulation as well, while constraint propagation are tools from artificial intelligence to further improve formulation through intensive preprocessing. A new trend is robust optimization where recent progress have been made: the aim is to produce optimized solutions that remain of good quality even if the problem data has stochastic variations. In all cases, the study of specific models and challenging industrial applications is quite relevant because developments made into a specific context can become generic tools over time and see their way into commercial software.

Our project brings together researchers with expertise in mathematical programming (polyhedral approaches, decomposition and reformulation techniques in mixed integer programing, robust and stochastic programming, and dynamic programming), graph theory (characterization of graph properties, combinatorial algorithms) and constraint programming in the aim of producing better quality formulations and developing new methods to exploit these formulations. These new results are then applied to find high quality solutions for practical combinatorial problems such as routing, network design, planning, scheduling, cutting and packing problems, High Performance and Cloud Computing.

3.2. Polyhedral approaches for MIP

Adding valid inequalities to the polyhedral description of an MIP allows one to improve the resulting LP bound and hence to better prune the enumeration tree. In a cutting plane procedure, one attempt to identify valid inequalities that are violated by the LP solution of the current formulation and adds them to the formulation. This can be done at each node of the branch-and-bound tree giving rise to a so-called *branch-and-cut algorithm* [65]. The goal is to reduce the resolution of an integer program to that of a linear program by deriving a linear description of the convex hull of the feasible solutions. Polyhedral theory tells us that if X is a mixed integer program: $X = P \cap \mathbb{Z}^n \times \mathbb{R}^p$ where $P = \{x \in \mathbb{R}^{n+p} : Ax \leq b\}$ with matrix $(A, b) \in \mathbb{Q}^{m\times(n+p+1)}$, then $conv(X)$ is a polyhedron that can be described in terms of linear constraints, i.e. it writes as $conv(X) = \{x \in \mathbb{R}^{n+p} : C\,x \leq d\}$ for some matrix $(C, d) \in \mathbb{Q}^{m'\times(n+p+1)}$ although the dimension m' is typically quite large. A fundamental result in this field is the equivalence of complexity between solving the combinatorial optimization problem $\min\{cx : x \in X\}$ and solving the *separation problem* over the associated polyhedron $conv(X)$: if $\widetilde{x} \notin conv(X)$, find a linear inequality $\pi\, x \geq \pi_0$ satisfied by all points in $conv(X)$ but violated by $\widetilde{x}$. Hence, for NP-hard problems, one can not hope to get a compact description of $conv(X)$ nor a polynomial time exact separation routine. Polyhedral studies focus on identifying some of the inequalities that are involved in the polyhedral description of $conv(X)$ and derive efficient *separation procedures* (cutting plane generation). Only a subset of the inequalities $C\,x \leq d$ can offer a good approximation, that combined with a branch-and-bound enumeration techniques permits to solve the problem. Using *cutting plane algorithm* at each node of the branch-and-bound tree, gives rise to the algorithm called *branch-and-cut*.

3.3. Decomposition-and-reformulation-approaches

An hierarchical approach to tackle complex combinatorial problems consists in considering separately different substructures (subproblems). If one is able to implement relatively efficient optimization on the substructures, this can be exploited to reformulate the global problem as a selection of specific subproblem solutions that together form a global solution. If the subproblems correspond to subset of constraints in the MIP formulation, this leads to Dantzig-Wolfe decomposition. If it corresponds to isolating a subset of decision variables, this leads to Bender's decomposition. Both lead to extended formulations of the problem with either a huge number of variables or constraints. Dantzig-Wolfe approach requires specific algorithmic approaches to generate subproblem solutions and associated global decision variables dynamically in the course of the optimization. This procedure is known as *column generation*, while its combination with branch-and-bound enumeration is called *branch-and-price*. Alternatively, in Bender's approach, when dealing with exponentially many constraints in the reformulation, the *cutting plane procedures* that we defined in the previous section are well-suited tools. When optimization on a substructure is (relatively) easy, there often exists a tight reformulation of this substructure typically in an extended variable space. This gives rise powerful reformulation of the global problem, although it might be impractical given its size (typically pseudo-polynomial). It can be possible to project (part of) the extended formulation in a smaller dimensional space if not the original variable space to bring polyhedral insight (cuts derived through polyhedral studies can often be recovered through such projections).

3.4. Integration of Artificial Intelligence Techniques in Integer Programming

When one deals with combinatorial problems with a large number of integer variables, or tightly constrained problems, mixed integer programming (MIP) alone may not be able to find solutions in a reasonable amount of time. In this case, techniques from artificial intelligence can be used to improve these methods. In particular, we use variable fixing techniques, primal heuristics and constraint programming.

Primal heuristics are useful to find feasible solutions in a small amount of time. We focus on heuristics that are either based on integer programming (rounding, diving, relaxation induced neighborhood search, feasibility pump), or that are used inside our exact methods (heuristics for separation or pricing subproblem, heuristic constraint propagation, ...). Such methods are likely to produce good quality solutions only if the integer programming formulation is of top quality, i.e., if its LP relaxation provides a good approximation of the IP solution.

In the same line, variable fixing techniques, that are essential in reducing the size of large scale problems, rely on good quality approximations: either tight formulations or tight relaxation solvers (as a dynamic program combined with state space relaxation). Then if the dual bound derives when the variable is fixed to one exceeds the incubent solution value, the variable can be fixed to zero and hence removed from the problem. The process can be apply sequentially by refining the degree of relaxation.

Constraint Programming (CP) focuses on iteratively reducing the variable domains (sets of feasible values) by applying logical and problem-specific operators. The latter propagates on selected variables the restrictions that are implied by the other variable domains through the relations between variables that are defined by the constraints of the problem. Combined with enumeration, it gives rise to exact optimization algorithms. A CP approach is particularly effective for tightly constrained problems, feasibility problems and min-max problems. Mixed Integer Programming (MIP), on the other hand, is known to be effective for loosely constrained problems and for problems with an objective function defined as the weighted sum of variables. Many problems belong to the intersection of these two classes. For such problems, it is reasonable to use algorithms that exploit complementary strengths of Constraint Programming and Mixed Integer Programming.

3.5. Robust Optimization

Decision makers are usually facing several sources of uncertainty, such as the variability in time or estimation errors. A simplistic way to handle these uncertainties is to overestimate the unknown parameters. However, this results in over-conservatism and a significant waste in resource consumption. A better approach is to account for the uncertainty directly into the decision aid model by considering mixed integer programs that involve uncertain parameters. Stochastic optimization account for the expected realization of random data and optimize an expected value representing the average situation. Robust optimization on the other hand entails protecting against the worst-case behavior of unknown data. There is an analogy to game theory where one considers an oblivious adversary choosing the realization that harms the solution the most. A full worst case protection against uncertainty is too conservative and induces very high over-cost. Instead, the realization of random data are bound to belong to a restricted feasibility set, the so-called uncertainty set. Stochastic and robust optimization rely on very large scale programs where probabilistic scenarios are enumerated. There is hope of a tractable solution for realistic size problems, provided one develops very efficient ad-hoc algorithms. The techniques for dynamically handling variables and constraints (column-and-row generation and Bender's projection tools) that are at the core of our team methodological work are specially well-suited to this context.

3.6. Approximation Algorithms

In some contexts, obtaining an exact solution to an optimization problem is not feasible: when instances are too large, or when decisions need to be taken rapidly. Since most of the combinatorial optimization problems are NP-hard, another direction to obtain good quality solutions in reasonable time is to focus on **approximation algorithms**. The definition of approximation algorithms is based on the notion of input set $\mathcal{I}$ and each $I \in \mathcal{I}$ defines a solution space $\mathcal{S}_I$. For a minimization problem $\min_{x \in \mathcal{S}_I} f(x)$, an algorithm $\mathcal{A}$ is an α-approximation algorithm if it provides a solution within α of the optimal solution for all instances in the input set:

$$\forall I \in \mathcal{I}, \quad f(\mathcal{A}(I)) \leq \alpha \min_{x \in \mathcal{S}_I} f(x) = f^*(I)$$

The objective is to search for polynomial algorithms, with approximation ratios as close to 1 as possible. Such algorithms are called *worst-case* approximation algorithms, because the performance guarantee is expressed over all possible inputs of the problem. The design of these algorithms have strong links with the enumeration techniques described above: since computing $f^*(I)$ is an NP-hard problem, it is often required to derive **strong a priori bounds** on the optimal solution value which can afterward be compared to estimations of the value of the solution produced. In many cases, it is also possible to build α-approximate solutions by a careful rounding of a solution obtained from the linear relaxation of an integer formulation of the problem. Members of the team have expertise in designing and evaluating approximation algorithms for resource allocation in computer systems, using a variety of techniques, such as dual approximation (where a guess of the optimal value f^* is provided, and $\mathcal{A}$ either provides a solution within αf^*, or guarantees that no solution of value f^* or less exists), or resource augmentation (where an approximation is obtained by relaxing some of the constraints of the problem).

3.7. Polyhedral Combinatorics and Graph Theory

Many fundamental combinatorial optimization problems can be modeled as the search for a specific structure in a graph. For example, ensuring connectivity in a network amounts to building a *tree* that spans all the nodes. Inquiring about its resistance to failure amounts to searching for a minimum cardinality *cut* that partitions the graph. Selecting disjoint pairs of objects is represented by a so-called *matching*. Disjunctive choices can be modeled by edges in a so-called *conflict graph* where one searches for *stable sets* – a set of nodes that are not incident to one another. Polyhedral combinatorics is the study of combinatorial algorithms involving polyhedral considerations. Not only it leads to efficient algorithms, but also, conversely, efficient algorithms often imply polyhedral characterizations and related min-max relations. Developments of polyhedral properties of a fundamental problem will typically provide us with more interesting inequalities well suited for a branch-and-cut algorithm to more general problems. Furthermore, one can use the fundamental problems as new building bricks to decompose the more general problem at hand. For problem that let themselves easily be formulated in a graph setting, the graph theory and in particular graph decomposition theorem might help.

4. Application Domains

4.1. Network Design and Routing Problems

We are actively working on problems arising in network topology design, implementing a survivability condition of the form “at least two paths link each pair of terminals”. We have extended polyhedral approaches to problem variants with bounded length requirements and re-routing restrictions [54]. Associated to network design is the question of traffic routing in the network: one needs to check that the network capacity suffices to carry the demand for traffic. The assignment of traffic also implies the installation of specific hardware at transient or terminal nodes.

To accommodate the increase of traffic in telecommunication networks, today’s optical networks use grooming and wavelength division multiplexing technologies. Packing multiple requests together in the same optical stream requires to convert the signal in the electrical domain at each aggregation of disaggregation of traffic at an origin, a destination or a bifurcation node. Traffic grooming and routing decisions along with wavelength assignments must be optimized to reduce opto-electronics system installation cost. We developed and compared several decomposition approaches [79], [78], [77] to deal with backbone optical network with relatively few nodes (around 20) but thousands of requests for which traditional multi-commodity network flow approaches are completely overwhelmed. We also studied the impact of imposing a restriction on the number of optical hops in any request route [76]. We also developed a branch-and-cut approach to a problem that consists in placing sensors on the links of a network for a minimum cost [59], [60].

The Dial-a-Ride Problem is a variant of the pickup and delivery problem with time windows, where the user inconvenience must be taken into account. In [69], ride time and customer waiting time are modeled through both constraints and an associated penalty in the objective function. We develop a column generation approach, dynamically generating feasible vehicle routes. Handling ride time constraints explicitly in the pricing problem solver requires specific developments. Our dynamic programming approach for pricing problem makes use of a heuristic dominance rule and a heuristic enumeration procedure, which in turns implies that our overall branch-and-price procedure is a heuristic. However, in practice our heuristic solutions are experimentally very close to exact solutions and our approach is numerically competitive in terms of computation times.

In [67], [66], we consider the problem of covering an urban area with sectors under additional constraints. We adapt the aggregation method to our column generation algorithm and focus on the problem of disaggregating the dual solution returned by the aggregated master problem.

We studied several time dependent formulations for the unit demand vehicle routing problem [44], [43]. We gave new bounding flow inequalities for a single commodity flow formulation of the problem. We described their impact by projecting them on some other sets of variables, such as variables issued of the Picard and Queyranne formulation or the natural set of design variables. Some inequalities obtained by projection are facet defining for the polytope associated with the problem. We are now running more numerical experiments in order to validate in practice the efficiency of our theoretical results.

We also worked on the p-median problem, applying the matching theory to develop an efficient algorithm in Y-free graphs and to provide a simple polyhedral characterization of the problem and therefore a simple linear formulation [75] simplifying results from Baiou and Barahona.

We considered the multi-commodity transportation problem. Applications of this problem arise in, for example, rail freight service design, "less than truckload" trucking, where goods should be delivered between different locations in a transportation network using various kinds of vehicles of large capacity. A particularity here is that, to be profitable, transportation of goods should be consolidated. This means that goods are not delivered directly from the origin to the destination, but transferred from one vehicle to another in intermediate locations. We proposed an original Mixed Integer Programming formulation for this problem which is suitable for resolution by a Branch-and-Price algorithm and intelligent primal heuristics based on it.

For the problem of routing freight railcars, we proposed two algorithmes based on the column generation approach. These algorithmes have been tested on a set of real-life instances coming from a real Russian freight transportation company. Our algorithms have been faster on these instances than the current solution approach being used by the company.

4.2. Packing and Covering Problems

Realopt team has a strong experience on exact methods for cutting and packing problems. These problems occur in logistics (loading trucks), industry (wood or steel cutting), computer science (parallel processor scheduling).

We developed a branch-and-price algorithm for the Bin Packing Problem with Conflicts which improves on other approaches available in the literature [74]. The algorithm uses our methodological advances like the generic branching rule for the branch-and-price and the column based heuristic. One of the ingredients which contributes to the success of our method are fast algorithms we developed for solving the subproblem which is the Knapsack Problem with Conflicts. Two variants of the subproblem have been considered: with interval and arbitrary conflict graphs.

We also developed a branch-and-price algorithm for a variant of the bin-packing problem where the items are fragile. In [33] we studied empirically different branching schemes and different algorithms for solving the subproblems.

We studied a variant of the knapsack problem encountered in inventory routing problem [62]: we faced a multiple-class integer knapsack problem with setups [61] (items are partitioned into classes whose use implies a setup cost and associated capacity consumption). We showed the extent to which classical results for the knapsack problem can be generalized to this variant with setups and we developed a specialized branch-and-bound algorithm.

We studied the orthogonal knapsack problem, with the help of graph theory [56], [55], [58], [57]. Fekete and Schepers proposed to model multi-dimensional orthogonal placement problems by using an efficient representation of all geometrically symmetric solutions by a so called *packing class* involving one *interval graph* for each dimension. Though Fekete & Schepers' framework is very efficient, we have however identified several weaknesses in their algorithms: the most obvious one is that they do not take advantage of the different possibilities to represent interval graphs. We propose to represent these graphs by matrices with consecutive ones on each row. We proposed a branch-and-bound algorithm for the 2D knapsack problem that uses our 2D packing feasibility check. We are currently developing exact optimization tools for glass-cutting problems in a collaboration with Saint-Gobain [38]. This 2D-3stage-Guillotine cut problems are very hard to solve given the scale of the instance we have to deal with. Moreover one has to issue cutting patterns that avoid the defaults that are present in the glass sheet that are used as raw material. There are extra sequencing constraints regarding the production that make the problem even more complex.
We have also organized a European challenge on packing with society Renault. This challenge was about loading trucks under practical constraints.

4.3. Planning, Scheduling, and Logistic Problems

Inventory routing problems combine the optimization of product deliveries (or pickups) with inventory control at customer sites. We considered an industrial application where one must construct the planning of single product pickups over time; each site accumulates stock at a deterministic rate; the stock is emptied on each visit. We have developed a branch-and-price algorithm where periodic plans are generated for vehicles by solving a multiple choice knapsack subproblem, and the global planning of customer visits is coordinated by the master program [63]. We previously developed approximate solutions to a related problem combining vehicle routing and planning over a fixed time horizon (solving instances involving up to 6000 pick-ups and deliveries to plan over a twenty day time horizon with specific requirements on the frequency of visits to customers [64].

Together with our partner company GAPSO from the associate team SAMBA, we worked on the equipment routing task scheduling problem [68] arising during port operations. In this problem, a set of tasks needs to be performed using equipments of different types with the objective to maximize the weighted sum of performed tasks.

We participated to the project on an airborne radar scheduling. For this problem, we developed fast heuristics [53] and exact algorithms [35]. A substantial research has been done on machine scheduling problems. A new compact MIP formulation was proposed for a large class of these problems [34]. An exact decomposition algorithm was developed for the NP-hard maximizing the weighted number of late jobs problem on a single machine [70]. A dominant class of schedules for malleable parallel jobs was discovered in the NP-hard problem to minimize the total weighted completion time [72]. We proved that a special case of the scheduling problem at cross docking terminals to minimize the storage cost is polynomially solvable [73], [71].

Another application area in which we have successfully developed MIP approaches is in the area of tactical production and supply chain planning. In [32], we proposed a simple heuristic for challenging multi-echelon problems that makes effective use of a standard MIP solver. [31] contains a detailed investigation of what makes solving the MIP formulations of such problems challenging; it provides a survey of the known methods for strengthening formulations for these applications, and it also pinpoints the specific substructure that seems to cause the bottleneck in solving these models. Finally, the results of [39] provide demonstrably stronger formulations for some problem classes than any previously proposed. We are now working on planning phytosanitary treatments in vineries.

We have been developing robust optimization models and methods to deal with a number of applications like the above in which uncertainty is involved. In [49], [48], we analyzed fundamental MIP models that incorporate uncertainty and we have exploited the structure of the stochastic formulation of the problems in order to derive algorithms and strong formulations for these and related problems. These results appear to be the first of their kind for structured stochastic MIP models. In addition, we have engaged in successful research to apply concepts such as these to health care logistics [40]. We considered train timetabling problems and their re-optimization after a perturbation in the network [51], [50]. The question of formulation is central. Models of the literature are not satisfactory: continuous time formulations have poor quality due to the presence of discrete decision (re-sequencing or re-routing); arc flow in time-space graph blow-up in size (they can only handle a single line timetabling problem). We have developed a discrete time formulation that strikes a compromise between these two previous models. Based on various time and network aggregation strategies, we develop a 2-stage approach, solving the contiguous time model having fixed the precedence based on a solution to the discrete time model.

Currently, we are conducting investigations on a real-world planning problem in the domain of energy production, in the context of a collaboration with EDF [45], [46], [47]. The problem consists in scheduling maintenance periods of nuclear power plants as well as production levels of both nuclear and conventional power plants in order to meet a power demand, so as to minimize the total production cost. For this application, we used a Dantzig-Wolfe reformulation which allows us to solve realistic instances of the deterministic version of the problem [52]. In practice, the input data comprises a number of uncertain parameters. We deal with a scenario-based stochastic demand with help of a Benders decomposition method. We are working on Multistage Robust Optimization approaches to take into account other uncertain parameters like the duration of each maintenance period, in a dynamic optimization framework. The main challenge addressed in this work is the joint management of different reformulations and solving techniques coming from the deterministic (Dantzig-Wolfe decomposition, due to the large scale nature of the problem), stochastic (Benders decomposition, due to the number of demand scenarios) and robust (reformulations based on duality and/or column and/or row generation due to maintenance extension scenarios) components of the problem [41].

4.4. Resource Allocation for High Performance and Cloud Computing

In the context of numerical simulations on high performance machines, optimizing data locality and resource usage is very important for faster execution times and lower energy consumption. This optimization can be seen as a special case of scheduling problem on parallel resource, with several challenges. First, instances are typically large: a large matrix factorization (with 50×50 blocks) involves about $30 \cdot 10^3$ tasks. Then, HPC platforms consist of heterogeneous and unrelated resources, what is known to make scheduling problems hard to approximate. Finally, due to co-scheduling effects and shared communication resources, it is not realistic to accurately model the exact duration of tasks. All these observations make it impossible to rely on static optimal solutions, and HPC applications have gone from simple generic static allocations to runtime dynamic scheduling strategies that make their decisions based on the current state of the platform (the location of input data), the expected transfer and running times for the tasks, and some affinity and priority information that have possibly been computed offline. In this context, we are strongly involved in the design of scheduling strategies for the StarPU runtime, with two goals: proving that it is possible to design approximation algorithms whose complexity is extremely small (typically sub-linear in the number of ready tasks), and show that they can be used in practice with good performance results. We are pursuing collaborations both with teams developing the StarPU system (Storm) by designing algorithms for the generic scheduling problems [37], and with teams developing linear algebra algorithms over the runtime (Hiepacs), by proposing specialized algorithms for specific cases. For example, in the case of linear algebra applications on heterogeneous platforms, we have considered the combinatorial optimization problem associated to matrix multiplication, that is amenable to partitioning the unit square into zones of prescribed areas while minimizing the overall size of the boundaries. We have improved the best known approximation ratio to 1.15 in [36] and we have shown that the resulting distribution schemes can indeed be used to design efficient implementations using StarPU in [42].

5. Highlights of the Year

5.1. Highlights of the Year

The team has recruited Aurélien Froger as assistant professor.

Ruslan Sadykov has defended his habilitation (HDR) [2].

A paper [8] was accepted in conference IPCO, which is the most prestigious conference in the field.

6. New Software and Platforms

6.1. BaPCod

A generic Branch-And-Price-And-Cut Code

KEYWORDS: Column Generation - Branch-and-Price - Branch-and-Cut - Mixed Integer Programming - Mathematical Optimization - Benders Decomposition - Dantzig-Wolfe Decomposition - Extended Formulation

FUNCTIONAL DESCRIPTION: BaPCod is a prototype code that solves Mixed Integer Programs (MIP) by application of reformulation and decomposition techniques. The reformulated problem is solved using a branch-and-price-and-cut (column generation) algorithms, Benders approaches, network flow and dynamic programming algorithms. These methods can be combined in several hybrid algorithms to produce exact or approximate solutions (primal solutions with a bound on the deviation to the optimum).

RELEASE FUNCTIONAL DESCRIPTION: An important update to make BaPCod compatible with VRPSolver. Correction of numerous bugs.

- Participants: Artur Alves Pessoa, Boris Detienne, Eduardo Uchoa Barboza, Franck Labat, François Clautiaux, Francois Vanderbeck, Halil Sen, Issam Tahiri, Michael Poss, Pierre Pesneau, Romain Leguay and Ruslan Sadykov
- Partners: Université de Bordeaux - CNRS - IPB - Universidade Federal Fluminense
- Contact: Ruslan Sadykov
- URL: https://wiki.bordeaux.inria.fr/realopt/pmwiki.php/Project/BaPCod

6.2. ORTOJ

Operation Research Tools Under Julia

KEYWORDS: Modeling - Processing - Dashboard

FUNCTIONAL DESCRIPTION: This set of tools currently includes : 1) BlockJuMP.jl: extension of JuMP to model decomposable mathematical programs (using either Benders or Dantzig-Wolfe decomposition paradign) 2) Scanner.jl: a default data parser to ease the reading of the input data in the form that they are often encountered in operational research. 3) BenchmarkUtils.jl: Tools to ease the setup of numerical experiments to benchmark algorithmic feature performances. The test automation permits to quickly calibrate the parameters of an arbitrary algorithm control function.

- Participants: Francois Vanderbeck, Guillaume Marques, Issam Tahiri and Ruslan Sadykov
- Contact: Issam Tahiri

6.3. pmtool

KEYWORDS: Scheduling - Task scheduling - StarPU - Heterogeneity - GPGPU - Performance analysis

FUNCTIONAL DESCRIPTION: Analyse post-mortem the behavior of StarPU applications. Provide lower bounds on makespan. Study the performance of different schedulers in a simple context. Provide implementations of many scheduling algorithms from the literature

NEWS OF THE YEAR: Included many new algorithms, in particular online algorithms Better integration with StarPU by accepting .rec files as input

- Participant: Lionel Eyraud-Dubois
- Contact: Lionel Eyraud-Dubois
- Publications: Approximation Proofs of a Fast and Efficient List Scheduling Algorithm for Task-Based Runtime Systems on Multicores and GPUs - Fast Approximation Algorithms for Task-Based Runtime Systems
- URL: https://gitlab.inria.fr/eyrauddu/pmtool

7. New Results

7.1. An iterative dynamic programming approach for the temporal knapsack problem

We have developed an approach to solve the temporal knapsack problem (TKP) based on a very large size dynamic programming formulation [28]. In this generalization of the classical knapsack problem, selected items enter and leave the knapsack at fixed dates. We solve the TKP with a dynamic program of exponential size, which is solved using a method called Successive Sublimation Dynamic Programming (SSDP). This method starts by relaxing a set of constraints from the initial problem, and iteratively reintroduces them when needed. We show that a direct application of SSDP to the temporal knapsack problem does not lead to an effective method, and that several improvements are needed to compete with the best results from the literature.

7.2. A Hypergraph Model for the Rolling Stock Rotation Planning and Train Selection Problem

We investigated an integrated optimization approach for timetabling and rolling stock rotation planning in the context of passenger railway traffic [27]. Given a set of possible passenger trips, service requirement constraints, and a fleet of multiple heterogeneous self-powered railcars, our method aims at producing a timetable and solving the rolling stock problem in such a way that the use of railcars and the operational costs are minimized. To solve this hard optimization problem, we design a mixed-integer linear programming model based on network-flow in an hypergraph. We use this models to handle effectively constraints related to coupling and decoupling railcars. To reduce the size of the model, we use an aggregation and disaggregation technique combined with reduced-cost filtering. Computational experiments based on several French regional railway traffic case studies show that our method scales successfully to real-life problems.

7.3. Decomposition-based approaches for a class of two-stage robust binary optimization problems

We have studied a class of two-stage robust binary optimization problems with objective uncertainty where recourse decisions are restricted to be mixed-binary [25]. For these problems, we present a deterministic equivalent formulation through the convexification of the recourse feasible region. We then explore this formulation under the lens of a relaxation, showing that the specific relaxation we propose can be solved using the branch-and-price algorithm. We present conditions under which this relaxation is exact, and describe alternative exact solution methods when this is not the case. Despite the two-stage nature of the problem, we provide NP-completeness results based on our reformulations. Finally, we present various applications in which the methodology we propose can be applied. We compare our exact methodology to those approximate methods recently proposed in the literature under the name K-adaptability. Our computational results show that our methodology is able to produce better solutions in less computational time compared to the K-adaptability approach, as well as to solve bigger instances than those previously managed in the literature.

7.4. Primal heuristic for Branch-and-Price

Primal heuristics have become an essential component in mixed integer programming (MIP) solvers. Extending MIP based heuristics, our study outlines generic procedures to build primal solutions in the context of a branch-and-price approach and reports on their performance. Our heuristic decisions carry on variables of the Dantzig-Wolfe reformulation, the motivation being to take advantage of a tighter linear programming relaxation than that of the original compact formulation and to benefit from the combinatorial structure embedded in these variables. In [9], we focus on the so-called diving methods that use re-optimization after each LP rounding. We explore combinations with diversification-intensification paradigms such as limited discrepancy search, sub-MIPing, local branching, and strong branching. The dynamic generation of variables inherent to a column generation approach requires specific adaptation of heuristic paradigms. We manage to use simple strategies to get around these technical issues. Our numerical results on generalized assignment, cutting stock, and vertex coloring problems sets new benchmarks, highlighting the performance of diving heuristics as generic procedures in a column generation context and producing better solutions than state-of-the-art specialized heuristics in some cases.

7.5. Generic solver for vehicle routing problems

Major advances were recently obtained in the exact solution of Vehicle Routing Problems (VRPs). Sophisticated Branch-Cut-and-Price (BCP) algorithms for some of the most classical VRP variants now solve many instances with up to a few hundreds of customers. However, adapting and re-implementing those successful algorithms for other variants can be a very demanding task. In [8], [12], [11], we propose a BCP solver for a generic model that encompasses a wide class of VRPs. It incorporates the key elements found in the best existing VRP algorithms: ng-path relaxation, rank-1 cuts with limited memory, path enumeration, and rounded capacity cuts; all generalized through the new concepts of “packing set” and “elementarity set”. The concepts are also used to derive a branching rule based on accumulated resource consumption and to generalize the Ryan and Foster branching rule. Extensive experiments on several variants show that the generic solver has an excellent overall performance, in many problems being better than the best specific algorithms. Even some non-VRPs, like bin packing, vector packing and generalized assignment, can be modeled and effectively solved.

The solver is available for download and free academic use in http://vrpsolver.math.u-bordeaux.fr.

7.6. New algorithms for different vehicle routing problems

In [7], we propose a branch-cut-and-price algorithm for the two-echelon capacitated vehicle routing problem in which delivery of products from a depot to customers is performed using intermediate depots called satellites. We introduce a new route based formulation for the problem which does not use variables to determine product flows in satellites. Second, we introduce a new branching strategy which significantly decreases the size of the branch-and-bound tree. Third, we introduce a new family of satellite supply inequalities, and we empirically show that it improves the quality of the dual bound at the root node of the branch-and-bound tree. Finally, extensive numerical experiments reveal that our algorithm can solve to optimality all literature instances with up to 200 customers and 10 satellites for the first time and thus double the size of instances which could be solved to optimality.

In [22], [21], we are interested in the exact solution of the vehicle routing problem with backhauls (VRPB), a classical vehicle routing variant with two types of customers: linehaul (delivery) and backhaul (pickup) ones. We propose two branch-cut-and-price (BCP) algorithms for the VRPB. The first of them follows the traditional approach with one pricing subproblem, whereas the second one exploits the linehaul/backhaul customer partitioning and defines two pricing subproblems. The methods incorporate elements of state-of-the-art BCP algorithms, such as rounded capacity cuts, limited-memory rank-1 cuts, strong branching, route enumeration, arc elimination using reduced costs and dual stabilization. Computational experiments show that the proposed algorithms are capable of obtaining optimal solutions for all existing benchmark instances with up to 200 customers, many of them for the first time. It is observed that the approach involving two pricing subproblems is more efficient computationally than the traditional one. Moreover, new instances are also proposed for which we provide tight bounds. Also, we provide results for benchmark instances of the heterogeneous fixed fleet VRPB and the VRPB with time windows.

In [20], we consider the standard Capacitated Location-Routing Problem (LRP), which is the combination of two canonical combinatorial optimization problems : Facility Location Problem (FLP), and Vehicle Routing Problem (VRP). We have extended the Branch-and-Cut-and-Price Algorithm from [11] to solve a Mixed Integer Programming (MIP) formulation with and exponential number of varialbes. A new family of Route Load Knapsack valid inequalites is proposed to strengthen the formulation. Preliminary results showed that our algorithm could solve to optimality, for the first time, 12 open instances of the most difficult classes of LRP instances.

In the first echelon of the two-echelon stochastic multi-period capacitated location-routing problem (2E-SM-CLRP), one has to decide the number and location of warehouse platforms as well as the intermediate distribution platforms for each period; while fixing the capacity of the links between them. The system must be dimensioned to enable an efficient distribution of goods to customers under a stochastic and time-varying demand. In the second echelon of the 2E-SM-CLRP, the goal is to construct vehicle routes that visit customers from operating distribution platforms. The objective is to minimize the total expected cost. We model this hierarchical decision problem as a two-stage stochastic program with integer recourse. The first-stage includes location and capacity decisions to be fixed at each period over the planning horizon, while routing decisions of the second echelon are determined in the recourse problem. In [16], [26], we propose a Benders decomposition approach to solve this model. In the proposed approach, the location and capacity decisions are taken by solving the Benders master problem. After these first-stage decisions are fixed, the resulting subproblem is a capacitated vehicle-routing problem with capacitated multi-depot (CVRP-CMD) that is solved by a branch-cut-and-price algorithm. Computational experiments show that instances of realistic size can be solved optimally within reasonable time, and that relevant managerial insights are derived on the behavior of the design decisions under the stochastic multi-period characterization of the planning horizon.

Much of the existing research on electric vehicle routing problems (E-VRPs) assumes that the charging stations (CSs) can simultaneously charge an unlimited number of electric vehicles, but this is not the case. In [29], we investigate how to model and solve E-VRPs taking into account these capacity restrictions. In particular, we study an E-VRP with non-linear charging functions, multiple charging technologies, en route charging, and variable charging quantities, while explicitly accounting for the capacity of CSs expressed in the number of chargers. We refer to this problem as the E-VRP with non-linear charging functions and capacitated stations (E-VRP-NL-C). This problem advances the E-VRP literature by considering the scheduling of charging operations at each CS. We first introduce two mixed integer linear programming formulations showing how CS capacity constraints can be incorporated into E-VRP models. We then introduce an algorithmic framework to the E-VRP-NL-C, that iterates between two main components: a route generator and a solution assembler. The route generator uses an iterated local search algorithm to build a pool of high-quality routes. The solution assembler applies a branch-and-cut algorithm to select a subset of routes from the pool. We report on computational experiments comparing four different assembly strategies on a large and diverse set of instances. Our results show that our algorithm deals with the CS capacity constraints effectively. Furthermore, considering the well-known uncapacitated version of the E-VRP-NL-C, our solution method identifies new best-known solutions for 80 out of 120 instances.

7.7. Packing problems

In the two-dimensional guillotine cutting-stock problem, the objective is to minimize the number of large plates used to cut a list of small rectangles. We consider a variant of this problem, which arises in glass industry when different bills of order (or batches) are considered consecutively. For practical organisation reasons, leftovers are not reused, except the large one obtained in the last cutting pattern of a batch, which can be reused for the next batch. The problem can be decomposed into an independent problem for each batch. In [6] we focus on the one-batch problem, the objective of which is to minimize the total width of the cutting patterns used. We propose a diving heuristic based on column generation, in which the pricing problem is solved using dynamic programming (DP). This DP generates so-called non-proper columns, i.e. cutting patterns that cannot participate in a feasible integer solution of the problem. We show how to adapt the standard diving heuristic to this "non-proper" case while keeping its effectiveness. We also introduce the partial enumeration technique, which is designed to reduce the number of non-proper patterns in the solution space of the dynamic program. This technique strengthens the lower bounds obtained by column generation and improves the quality of the solutions found by the diving heuristic. Computational results are reported and compared on classical benchmarks from the literature as well as on new instances inspired from glass industry data. According to these results, variants of the proposed diving heuristic outperform constructive and evolutionary heuristics.instances than those previously managed in the literature.

The bin packing problem with generalized time lags (BPGL) consists of a set of items, each having a positive weight, and a set of precedence constraints with lags between pairs of items, allowing negative and non-negative lags. The items must be packed into the minimum possible number of bins with identical capacity, and the bins must be assigned to time periods satisfying the precedence constraints with lags on the items. In [18] we show a solution strategy using a generic branch-and-price algorithm (implemented in the software platform BaPCod) and applying some problem specific cuts. Our approach outperformed the compact Mixed Integer Programming (MIP) formulation solved by the MIP solver Cplex.

7.8. Covering problems

In [5], we study a covering problem where vertices of a graph have to be covered by rooted sub-trees. We present three mixed-integer linear programming models, two of which are compact while the other is based on Dantzig-Wolfe decomposition. In the latter case, we focus on the column generation sub-problem, a knapsack problem with precedence constraints on trees, for which we propose several algorithms among them a branch and bound algorithm and various dynamic programs. Numerical results are obtained using instances from the literature and instances based on a real-life districting application. Experiments show that the branch-and-price algorithm is able to solve much bigger instances than the compact model, which is limited to very small instance sizes.

7.9. Software Defined Networking

ISP networks are taking a leap forward thanks to emerging technologies such as Software Defined Networking (SDN) and Network Function Virtualization (NFV). Efficient algorithms considered too hard to be put in practice on legacy networks now have a second chance to be considered again. In this context, we rethink the ISP network dimensioning problem with protection against Shared Risk Link Group (SLRG) failures. In [30], [15], [23], we consider a path-based protection scheme with a global rerouting strategy, in which, for each failure situation, we may have a new routing of all the demands. Our optimization task is to minimize the needed amount of bandwidth. After discussing the hardness of the problem, we develop two scalable mathematical models that we handle using both Column Generation and Benders Decomposition techniques. Through extensive simulations on real-world IP network topologies and on random generated instances, we show the effectiveness of our methods. Finally, our implementation in OpenDaylight demonstrates the feasibility of the approach and its evaluation with Mininet shows that technical implementation choices may have a dramatic impact on the time needed to reestablish the flows after a failure takes place.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

We have an on-going contract with SNCF on scheduling of rolling-stock. The PhD thesis of Mohamed Benkirane is part of this contract.

Following the PhD thesis of Rodolphe Griset, our collaboration with EDF has continued through a new contract within Inria Tech. Its goal is to investigate the possibility of developing an operational prototype (called Fenix) for strategic planning of nuclear plant outages. Two scientific questions are raised. The first one concerns the new mechanisms of management of the power capacity market on the French power grid. The second one is about a new model of the stock variation during a refueling operation, which requires information of several previous production campaigns.

We also have a contract with RTE to develop strategies inspired from stochastic gradient methods to speed-up Benders' decomposition. The PhD thesis of Xavier Blanchot is part of this contract.

We have a contract with Thales Avionique to study a robust scheduling problem.

9. Partnerships and Cooperations

9.1. Regional Initiatives

- **SysNum Cluster** SysNum is a Cluster of Excellence of Bordeaux Idex that aims at bringing Bordeaux academic players in the digital sciences closer to each other around large-scale distributed digital systems. The cluster is organized around 4 methodological axes (Interconnected object systems; Reliability and safety; Modeling and numerical systems; Massive and heterogeneous data) and 3 application platforms around major societal issues (ecology, mobile systems, interconnected objects and data analysis).

  François Clautiaux is leading the methodological WP on Interconnected object systems. Understanding and controlling the complexity of systems of interconnected objects is a major challenge for both industrial and everyday life applications. We think, in particular, to fields like robotics, car industry, energy distribution or smart buildings, where it is essential to tackle autonomous heterogeneous objects and to develop robust control tools to optimize their interconnections. Our research in this direction will be developed within three interconnected tasks.

9.2. International Initiatives

9.2.1. Inria International Partners

9.2.1.1. Informal International Partners

Orlando Rivera Letelier is pursuing a co-tutelle thesis (with Universidad Adolfo Ibáñez, Peñalolén, Santiago, Chile)

We continue close collaboration with the LOGIS laboratory (Universidade Federal Fluminense, Niteroi, Brazil) after the end of the Inria Associate Team SAMBA.

9.3. International Research Visitors

9.3.1. Visits of International Scientists

Eduardo Uchoa visited the team in April 2019 for one week.

Emir Démirovic (University of Melbourne, Australia) visited the team in July for one week

Isaac Cleland (University of Auckland, New-Zealand) visited the team in July for one week

9.3.2. Visits to International Teams

9.3.2.1. Research Stays Abroad

Guillaume Marques spent 3 months in Universidade Federal Fluminense, Niteroi, Brazil (August-November 2019), financed by mobility grant of IdEx Bordeaux

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events: Organisation

10.1.1.1. General Chair, Scientific Chair

- François Clautiaux: Conférence Dataquitaine (around 300 participants) in Bordeaux, February 2019
- François Clautiaux: Workshop on Integer Programming and Algorithms in Marne-La-Vallée, November 2019

10.1.1.2. Member of the Organizing Committees

- François Clautiaux: Conférence Dataquitaine (around 300 participants) in Bordeaux, February 2019
- François Clautiaux: Workshop on Integer Programming and Algorithms in Marne-La-Vallée, November 2019

10.1.2. Scientific Events: Selection

10.1.2.1. Member of the Conference Program Committees

- François Clautiaux: Conference ROADEF 2019, Le Havre
- Pierre Pesneau: INOC 2019, in Avignon

10.1.3. Journal

10.1.3.1. Member of the Editorial Boards

- François Clautiaux : editor for Open Journal on Mathematical Optimization (OJMO)

10.1.3.2. Reviewer - Reviewing Activities

- François Clautiaux : European Journal of Operational Research, Discrete Applied Mathematics, Discrete Optimization, International Transactions on Operations Research,

- Aurélien Froger: European Journal of Operational Research, Transportation Science, Computers & Operations Research, Journal of Heuristics
- Ruslan Sadykov: Mathematical Programming, Transportation Science, International Transactions of Operations Research, ACM Transactions on Parallel Computing, Integer Programming and Combinatorial Optimization conference

10.1.4. Invited Talks

- François Clautiaux: Invited talk at the ESICUP Workshop, in Mexico (April 10th, 2019)
- Aurélien Froger: Invited talk [10] at the 2nd International Workshop on Synchronisation in Transport, SynchroTrans 2019, in Nantes (September 10th, 2019)
- Ruslan Sadykov: Invited talk [12] at the 9th International Network Optimization conference, invited talk [11] at the POC Autumn School on Advanced BCP Tools

10.1.5. Leadership within the Scientific Community

François Clautiaux has been elected president of the French O.R. association, ROADEF.

10.1.6. Scientific Expertise

François Clautiaux has been expert for HCERES

François Clautiaux has been expert for the Flander's Innovation and Entrepreneurship Agency.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

Licence : François Clautiaux, Projet d'optimisation, L3, Université de Bordeaux, France

Licence : François Clautiaux, Grands domaines de l'optimisation, L1, Université de Bordeaux, France

Master : François Clautiaux, Introduction à la programmation en variables entières, M1, Université de Bordeaux, France

Master : François Clautiaux, Integer Programming, M2, Université de Bordeaux, France

Master : François Clautiaux, Algorithmes pour l'optimisation en nombres entiers, M1, Université de Bordeaux, France

Master : François Clautiaux, Programmation linéaire, M1, Université de Bordeaux, France

Master: Boris Detienne, Combinatoire et routage, ENSEIRB INPB

Licence : Boris Detienne, Optimisation, L2, Université de Bordeaux

Licence : Boris Detienne, Groupe de travail applicatif, L3, Université de Bordeaux

Master : Boris Detienne, Optimisation continue, M1, Université de Bordeaux

Master : Boris Detienne, Integer Programming, M2, Université de Bordeaux

Master : Boris Detienne, Optimisation dans l'incertain, M2, Université de Bordeaux

Licence : Aurélien Froger, Groupe de travail applicatif, L3, Université de Bordeaux, France

Master : Aurélien Froger, Optimisation dans les graphes, M1, Université de Bordeaux, France

Master : Aurélien Froger, Gestion des opérations et planification de la production, M2, Université de Bordeaux, France

Master : Ruslan Sadykov, Introduction to Constraint Programming, M2, Université de Bordeaux, France

Licence : Pierre Pesneau, Grands domaines de l'optimisation, L1, Université de Bordeaux, France

Licence : Pierre Pesneau, Programmation pour le calcul scientifique, L2, Université de Bordeaux, France

Licence : Pierre Pesneau, Optimisation, L2, Université de Bordeaux, France

DUT : Pierre Pesneau, Recherche Opérationnelle, DUT Informatique 2ème année, Université de Bordeaux, France

Master : Pierre Pesneau, Algorithmique et Programmation 1, M1, Université de Bordeaux, France

Master : Pierre Pesneau, Algorithmique et Programmation 2, M1, Université de Bordeaux, France

Master : Pierre Pesneau, Programmation linéaire, M1, Université de Bordeaux, France

Master : Pierre Pesneau, Integer Programming, M2, Université de Bordeaux, France

10.2.2. Supervision

HdR : Ruslan Sadykov, Modern Branch-Cut-and-Price, Université de Bordeaux, 4/12/2019.

PhD : Imen Ben Mohamed, Designing Two-Echelon Distribution Networks under Uncertainty [1], Université de Bordeaux, 27/05/2019, Walid Klibi (dir), Ruslan Sadykov (dir), François Vanderbeck (co-dir).

PhD in progress : Alena Shilova, Scheduling for Deep Learning Frameworks from October 2018, Olivier Beaumont (dir) and Alexis Joly (dir)

PhD in progress: Tobias Castanet, Use of Replication in Distributed Games from September 2018, Olivier Beaumont (dir), Nicolas Hanusse (dir) and Corentin Travers (dir).

PhD in progress : Guillaume Marques, Planification de tournées de véhicules avec transbordement en logistique urbaine : approches basées sur les méthodes exactes de l'optimisation mathématique, from September 2017, Ruslan Sadykov (dir)

PhD in progress : Gaël Guillot, Aggregation and disaggregation methods for hard combinatorial problems, from November 2017, François Clautiaux (dir) and Boris Detienne (dir).

PhD in progress : Orlando Rivera Letelier, Bin Packing Problem with Generalized Time Lags, from May 2018, François Clautiaux (dir) and Ruslan Sadykov (co-dir), a co-tutelle with Universidad Adolfo Ibáñez, Peñalolén, Santiago, Chile.

PhD in progress: Mohamed Benkirane, "Optimisation des moyens dans la recomposition commerciale de dessertes TER" from November 2016, François Clautiaux (dir), Boris Detienne (dir)

PhD in progress: Xavier Blanchot, "Accélération de la Décomposition de Benders à l'aide du Machine Learning : Application à de grands problèmes d'optimisation stochastique two-stage pour les réseaux d'électricité" from September 2019, François Clautiaux (dir), Aurélien Froger (co-dir)

PhD in progress: Johan Levêque, "Conception de réseaux de distributions urbains mutualisées en mode doux", from September 2018, François Clautiaux (dir), Gautier Stauffer (co-dir)

10.2.3. Juries

- François Clautiaux: external referee for the thesis of Arthur Kramer (Bologna), referee for the thesis of Arnaud Lazare (Université Paris Saclay) jury member for Simon Bélières (Université de Toulouse), Imen Ben Mohamed (Université de Bordeaux) jury member for the habilitation of Ruslan Sadykov (Université de Bordeaux)
- Boris Detienne: jury member for Ikram Bouras (Université de Montpellier) and Imen Ben Mohamed (Université de Bordeaux)
- Ruslan Sadykov: member of of the selection committee of the Maitre de Conference position (Université de Bordeaux)

10.3. Popularization

- Local events: Participation to "Journée emploi maths et interaction 2019". This day aims to bring together students, researchers and practitioners in mathematics in the Bordeaux area. https://uf-mi.u-bordeaux.fr/sites/jemi/

10.3.1. Interventions

- Participation to Circuit Scientifique Bordelais (Fête de la Science)
- Participation to the 80th anniversary of CNRS

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[2] R. SADYKOV.*Modern Branch-Cut-and-Price*, Université de Bordeaux, December 2019, Habilitation à diriger des recherches, https://hal.inria.fr/tel-02410101

Articles in International Peer-Reviewed Journal

[3] O. BEAUMONT, B. A. BECKER, A. DEFLUMERE, L. EYRAUD-DUBOIS, T. LAMBERT, A. LASTOVETSKY.*Recent Advances in Matrix Partitioning for Parallel Computing on Heterogeneous Platforms*, in "IEEE Transactions on Parallel and Distributed Systems", January 2019, vol. 30, n^{o} 1, 11 [*DOI :* 10.1109/TPDS.2018.2853151], https://hal.inria.fr/hal-01670672

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Project-Team SISTM

Statistics In System biology and Translational Medicine

IN PARTNERSHIP WITH:
INSERM

Université de Bordeaux

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Modeling and Control for Life Sciences

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Creation of the Team: 2013 April 02, updated into Project-Team: 2015 January 01

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1. Team, Visitors, External Collaborators

Research Scientists

Daniel Commenges [Inserm, Senior Researcher, HDR]
Melanie Prague [Inria, Researcher]

Faculty Members

Rodolphe Thiébaut [Team leader, Univ de Bordeaux, Professor, HDR]
Marta Avalos Fernandez [Univ de Bordeaux, Associate Professor, HDR]
Robin Genuer [Univ de Bordeaux, Associate Professor]
Boris Hejblum [Univ de Bordeaux, Associate Professor]
Laura Richert [Univ de Bordeaux, Associate Professor, HDR]

Technical Staff

Fabien Barbier [Inserm, Engineer, until Aug 2019]
Solenne Delahaye [Inserm, Engineer, until Dec 2019]
Melany Durand [Inserm, Engineer]

Miriam Krueger [Inserm, Engineer, from Sep 2019]
Clement Nerestan [Inria, Engineer, from Oct 2019]
Van Hung Tran [Inserm, Engineer, until Sep 2019]

PhD Students

Marie Alexandre [Inria, PhD Student]
Louis Capitaine [Univ de Bordeaux, PhD Student]
Marine Gauthier [Univ de Bordeaux, PhD Student]
Edouard Lhomme [Univ de Bordeaux, PhD Student]
Hadrien Lorenzo [Inserm, PhD Student]
Perrine Soret [Univ de Bordeaux, PhD Student]

Post-Doctoral Fellows

Quentin Clairon [Inserm, Post-Doctoral Fellow, from Mar 2019]
Irène Balelli [Inserm, Post-Doctoral Fellow, until Jul 2019]
Laura Villain [Inria, Post-Doctoral Fellow]
Binbin Xu [Univ de Bordeaux, Post-Doctoral Fellow, until Jun 2019]

Administrative Assistants

Cécile Boutros [Inria, Administrative Assistant, until Apr 2019]
Audrey Plaza [Inria, Administrative Assistant, from Jul 2019]
Sandrine Darmigny [Inserm, Administrative Assistant]
Anton Ottavi [Inserm, European Projects coordinator]
Destandau Eugénie [Inserm, Communication, until Dec 2019]

2. Overall Objectives

2.1. Overall Theoretical Objectives

The overall objective of SISTM is to develop statistical methods for the integrative analysis of health data, especially those related to clinical immunology and vaccinology to answer specific questions risen in the application field. To reach this objective we are developing statistical methods belonging to two main research areas:

- Statistical and mechanistic modeling, especially based on ordinary differential equation systems, fitted to population and sparse data
- Statistical learning methods in the context of high-dimensional data

These two approaches are used for addressing different types of questions. Statistical learning methods are developed and applied to deal with the high-dimensional characteristics of the data. The outcome of this research leads to hypotheses linked to a restricted number of markers. Mechanistic models are then developed and used for modeling the dynamics of a few markers. For example, regularized methods can be used to select relevant genes among 20000 measured with microarray/RNA-seq technologies, whereas differential equations can be used to capture the dynamics and relationship between several genes followed over time by a q-PCR assay or RNA-seq. We apply the methods developed by the team in data science approaches to vaccine trials in order to elucidate the effects and mechanisms of action of vaccines and immunotherapies and to accelerate their clinical development.

2.2. Overall Applied Objectives

Data are generated in clinical trials or biological experimentations. Our main application of interest is the immune response to vaccines or other immune interventions (such as exogenous cytokines), in the context of HIV or Ebola infection. The methods developed in this context can be applied in other circumstances but the focus of the team on immunology and vaccinology is important for the relevance of the results and their translation into practice, thanks to a longstanding collaboration with several immunologists and the implication of the team in the Labex Vaccine Research Institute (http://vaccine-research-institute.fr). Examples of objectives related to this application field are:

- To understand how immune responses are generated with immune interventions (vaccines or immunotherapies)
- To predict what would be the immune responses to a given immune intervention in order to design next studies and to adapt interventions to individual persons or to specific populations

3. Research Program

3.1. Mechanistic learning

When studying the dynamics of a given marker, say the HIV concentration in the blood (HIV viral load), one can for instance use descriptive models summarizing the dynamics over time in term of slopes of the trajectories [56]. These slopes can be compared between treatment groups or according to patients' characteristics. Another way for analyzing these data is to define a mathematical model based on the biological knowledge of what drives HIV dynamics. In this case, it is mainly the availability of target cells (the CD4+ T lymphocytes), the production and death rates of infected cells and the clearance of the viral particles that impact the dynamics. Then, a mathematical model most often based on ordinary differential equations (ODE) can be written [48]. Estimating the parameters of this model to fit observed HIV viral load gave a crucial insight in HIV pathogenesis as it revealed the very short half-life of the virions and infected cells and therefore a very high turnover of the virus, making mutations a very frequent event [47].

Having a good mechanistic model in a biomedical context such as HIV infection opens doors to various applications beyond a good understanding of the data. Global and individual predictions can be excellent because of the external validity of a model based on main biological mechanisms. Control theory may serve for defining optimal interventions or optimal designs to evaluate new interventions [40]. Finally, these models can capture explicitly the complex relationship between several processes that change over time and may therefore challenge other proposed approaches such as marginal structural models to deal with causal associations in epidemiology [39].

Therefore, we postulate that this type of model could be very useful in the context of our research that is in complex biological systems. The definition of the model needs to identify the parameter values that fit the data. In clinical research this is challenging because data are sparse, and often unbalanced, coming from populations of subjects. A substantial inter-individual variability is always present and needs to be accounted as this is the main source of information. Although many approaches have been developed to estimate the parameters of non-linear mixed models [51], [59], [43], [49], [44], [58], the difficulty associated with the complexity of ODE models and the sparsity of the data leading to identifiability issues need further research.

Furthermore, the availability of data for each individual (see below) leads to a new challenge in this area. The structural model can easily be much more complex and the observation model may need to integrate much more markers.

3.2. High-dimensional statistical learning

With the availability of omics data such as genomics (DNA), transcriptomics (RNA) or proteomics (proteins), but also other types of data, such as those arising from the combination of large observational databases (e.g. in pharmacoepidemiology or environmental epidemiology), high-dimensional data have became increasingly common. Use of molecular biological technics such as Polymerase Chain Reaction (PCR) allows for amplification of DNA or RNA sequences. Nowadays, microarray and Next Generation Sequencing (NGS) techniques give the possibility to explore very large portions of the genome. Furthermore, other assays have also evolved, and traditional measures such as cytometry or imaging have became new sources of big data. Therefore, in the context of HIV research, the dimension of the datasets has much grown in term of number of variables per individual than in term of number of included patients although this latter is also growing thanks to the multi-cohort collaborations such as CASCADE or COHERE organized in the EuroCoord network [0]. As an example, in a phase 1/2 clinical trial evaluating the safety and the immunological response to a dendritic cell-based HIV vaccine, 19 infected patients were included. Bringing together data on cell count, cytokine production, gene expression and viral genome change led to a 20 Go database [55]. This is far from big databases faced in other areas but constitutes a revolution in clinical research where clinical trials of hundred of patients sized few hundred of Ko at most. Therefore, more than the storage and calculation capacities, the challenge is the comprehensive analysis of these data-sets.

The objective is either to select the relevant information or to summarize it for understanding or prediction purposes. When dealing with high-dimensional data, the methodological challenge arises from the fact that data-sets typically contain many variables, much more than observations. Hence, multiple testing is an obvious issue that needs to be taken into account [52]. Furthermore, conventional methods, such as linear models, are inefficient and most of the time even inapplicable. Specific methods have been developed, often derived from the machine learning field, such as regularization methods [57]. The integrative analysis of large data-sets is challenging. For instance, one may want to look at the correlation between two large scale matrices composed by the transcriptome in the one hand and the proteome on the other hand [45]. The comprehensive analysis of these large data-sets concerning several levels from molecular pathways to clinical response of a population of patients needs specific approaches and a very close collaboration with the providers of data that is the immunologists, the virologists, the clinicians...

4. Application Domains

4.1. Systems Biology and Translational medicine

Biological and clinical researches have dramatically changed because of the technological advances, leading to the possibility of measuring much more biological quantities than previously. Clinical research studies can include now traditional measurements such as clinical status, but also thousands of cell populations, peptides, gene expressions for a given patient. This has facilitated the transfer of knowledge from basic to clinical science (from "bench side to bedside") and vice versa, a process often called "Translational medicine". However, the analysis of these large amounts of data needs specific methods, especially when one wants to have a global understanding of the information inherent to complex systems through an "integrative analysis". These systems like the immune system are complex because of many interactions within and between many levels (inside cells, between cells, in different tissues, in various species). This has led to a new field called "Systems biology" rapidly adapted to specific topics such as "Systems Immunology" [53], "Systems vaccinology" [50], "Systems medicine" [42]. From the data scientist point of view, two main challenges appear: i) to deal with the massive amount of data ii) to find relevant models capturing observed behaviors.

[0] see online at http://www.eurocoord.net

4.2. HIV immunotherapies

The management of HIV infected patients and the control of the epidemics have been revolutionized by the availability of highly active antiretroviral therapies. Patients treated by these combinations of antiretrovirals have most often undetectable viral loads with an immune reconstitution leading to a survival which is nearly the same to uninfected individuals [46]. Hence, it has been demonstrated that early start of antiretroviral treatments may be good for individual patients as well as for the control of the HIV epidemics (by reducing the transmission from infected people) [41]. However, the implementation of such strategy is difficult especially in developing countries. Some HIV infected individuals do not tolerate antiretroviral regimen or did not reconstitute their immune system. Therefore, vaccine and other immune interventions are required. Many vaccine candidates as well as other immune interventions (IL7, IL15) are currently evaluated. The challenges here are multiple because the effects of these interventions on the immune system are not fully understood, there are no good surrogate markers although the number of measured markers has exponentially increased. Hence, HIV clinical epidemiology has also entered in the era of Big Data because of the very deep evaluation at individual level leading to a huge amount of complex data, repeated over time, even in clinical trials that includes a small number of subjects.

4.3. Translational vaccinology

Vaccines are one of the most efficient tools to prevent and control infectious diseases, and there is a need to increase the number of safe and efficacious vaccines against various pathogens. However, clinical development of vaccines - and of any other investigational product - is a lengthy and costly process. Considering the public health benefits of vaccines, their development needs to be supported and accelerated. During early phase clinical vaccine development (phase I, II trials, translational trials), the number of possible candidate vaccine strategies against a given pathogen that needs to be down-selected in early clinical development is potentially very large. Moreover, during early clinical development there are most often no validated surrogate endpoints to predict the clinical efficacy of a vaccine strategy based on immunogenicity results that could be used as a consensus immunogenicity endpoint and down-selection criterion. This implies considerable uncertainty about the interpretation of immunogenicity results and about the potential value of a vaccine strategy as it transits through early clinical development. Given the complexity of the immune system and the many unknowns in the generation of a protective immune response, early vaccine clinical development nowadays thus takes advantage of high throughput (or “omics”) methods allowing to simultaneously assess a large number of response markers at different levels (“multi-omics”) of the immune system. This has induced a paradigm shift towards early-stage and translational vaccine clinical trials including fewer participants but with thousands of data points collected on every single individual. This is expected to contribute to acceleration of vaccine development thanks to a broader search for immunogenicity signals and a better understanding of the mechanisms induced by each vaccine strategy. However, this remains a difficult research field, both from the immunological as well as from the statistical perspective. Extracting meaningful information from these multi-omics data and transferring it towards an acceleration of vaccine development requires adequate statistical methods, state-of-the art immunological technologies and expertise, and thoughtful interpretation of the results. It thus constitutes research at the interface between disciplines: data science, immunology and vaccinology. Our main current areas of application here are early phase trials of HIV and Ebola vaccine strategies, in which we participate from the initial trial design to the final data analyses.

5. Highlights of the Year

5.1. Highlights of the Year

5.1.1. Team structure

The SISTM team was re-structured into three research axes (formerly two) in 2019:

- Axis “High Dimensional Statistical Learning” (coordinator Boris Hejblum)
- Axis “Mechanistic Learning” (coordinator Mélanie Prague)
- Axis “Translational Vaccinology” (coordinator Laura Richert)

The third research axis on "Translational vaccinology" was created in order to formalize research activities already performed previously in a less structure way. This axis is dedicated to applied research questions in early stage clinical vaccine trials, with two objectives:

– to elucidate the potential effects and mechanisms of action of vaccines and immunotherapies in integrative statistical analyses of the induced responses at various levels of the immune system

– to better inform future trial designs and statistical analysis methods by means of modelling and methodological developments.

The three axes collaborate closely with each other.

In fact, the third axis gives the motivating examples leading to the methodological work done in the two other axes. The first axis deals with the raw high-dimensional data generated in clinical epidemiology or biological studies and aims at reducing the dimension of the problem or better annotate the data available (e.g. automatic gating of cytometry data). The second axis aims at building mechanistic model to understand and predict the biological phenomenons by using the available information. The idea then is that the results of this modelling part feed the third axis to define the next strategies to be evaluated in clinical studies and the design of these studies.

5.1.2. Team composition

The SISTM team core has changed in December 2019: Daniel Commenges, DRE Inserm, HDR (emeritus from September 2014) has retired from research activities. Daniel Commenges founded the “Biostatistic” team of Bordeaux within an Inserm unit in the 1990s. The research team was officially labelled by Inserm in the early 2000s and was lead by Daniel Commenges until 2013. The team split in 2014 into two teams: the Inserm “Biostatistic” team (led by Hélène Jacqmin-Gadda), and the “SISTM” team (led by Rodolphe Thiébaut) that joined the Inria BSO center.

5.1.3. Funded projects

- Launch of the Graduate’s School Digital Public Health (PI: R Thiébaut) including the Master of Public Health Data Sciences that started with its first cohort of 9 international students in Sep 2019.
- Positive response for funding of the H2020 IP-Cure-B project (Immune profiling to guide host-directed interventions to cure hepatitis B infections, project coordinator: Pr. F. Zoulim, Inserm U1052 CRCL), in which the work package “Data Science” is led by the SISTM team. The project will be launched in January 2020.
- Kick-off of the EDTCP-2 funded project PREVAC-UP (partnership for research on Ebola vaccinations – extended follow-up and clinical research capacity build-up, project coordinator: Pr Y. Yazdanpanah, Inserm), in which the work package “Systems vaccinology” is led by the SISTM team.
- A new collaboration has started with the pharmaceutical company Ipsen on the integration of “omics” data into in-silico modelling of early-stage clinical trials in cancer. This project will be conducted with a “*CIFRE*” (*Conventions Industrielles de Formation par la REcherche*) PhD contract starting in January 2020.
- *Action de Développement technologique* VASI: Visualization and Analytics Solution for Immunologists.
- The Ebovac2 IMI project on Ebola vaccine development has been extended to 11/2020 (no cost extension).
- Associate Team DYNAMHIC: Dynamical Modeling of HIV Cure in Collaboration With Harvard Program for evolutionary dynamics.

5.1.4. Advancements in projects

- A translational phase I clinical trial of an experimental placental malaria vaccine, conducted by an interdisciplinary consortium including members of the SISTM team (Primalvac trial), has reached its publication, with a manuscript accepted for publication in the Lancet Infectious Diseases

- Two HIV clinical vaccine trials have reached their final stage with all resultats available, including integrative data analyses of the immune responses, and the corresponding manuscripts are in preparation (ANRS VRI01 trial and ANRS 149 Light trial).
- The two phase II Ebola vaccine trials conducted by the IMI-2 EBOVAC2 consortium that is coordinated by Rodolphe Thiébaut are terminated. Results have been presented at international conferences and the manuscripts with the primary results are either submitted (EBL2001 study, submitted to the Lancet) or in preparation (EBL2002 study). Systems vaccinology analyses of the data from these trials are ongoing in the SISTM team.
- Robin Genuer co-authored a book with Jean-Michel Poggi on random forests entitled *Les forêts aléatoires avec R* in *Presses Universitaires de Rennes*, Rennes, France.

5.1.5. Awards

- Award for Doctoral Supervision and Research Activity (PEDR) attributed by the University of Bordeaux to Marta Avalos and Robin Genuer

6. New Software and Platforms

6.1. marqLevAlg

KEYWORDS: Optimization - Biostatistics

FUNCTIONAL DESCRIPTION: An R package for function optimization. Available on CRAN, this package performs a minimization of function based on the Marquardt-Levenberg algorithm. This package is really useful when the surface to optimize is non-strictly convex or far from a quadratic function. A new convergence criterion, the relative distance to maximum (RDM), allows the user to have a better confidence in the stopping points, other than basic algorithm stabilization.

RELEASE FUNCTIONAL DESCRIPTION: This package has been updated so that the optimization is done in parallel and goes faster. This update has been done in collaboration Viviane Philipps and Cecile Proust-Lima from Inserm BPH

- Partner: INSERM
- Contact: Melanie Prague
- URL: https://cran.r-project.org/web/packages/marqLevAlg/index.html

6.2. VSURF

Variable Selection Using Random Forests

KEYWORDS: Classification - Statistics - Machine learning - Regression

FUNCTIONAL DESCRIPTION: An R package for Variable Selection Using Random Forests. Available on CRAN, this package performs an automatic (meaning completely data-driven) variable selection procedure. Originally designed to deal with high dimensional data, it can also be applied to standard datasets.

RELEASE FUNCTIONAL DESCRIPTION: * add RFimplem parameter which allows to choose between randomForest, ranger and Rborist to compute random forests predictors. This can be a vector of length 3 to chose a different implementation for each step of VSURF() * update of the parallel and clusterType parameters to also give the possibility to choose which step to perform in parallel with a clusterType per step * add progress bars and information of the progress of the algorithm, and also an estimated computational time for each step

- Contact: Robin Genuer
- URL: https://github.com/robingenuer/VSURF

6.3. NPflow

Bayesian Nonparametrics for Automatic Gating of Flow-Cytometry Data

KEYWORDS: Bayesian estimation - Bioinformatics - Biostatistics

FUNCTIONAL DESCRIPTION: Dirichlet process mixture of multivariate normal, skew normal or skew t-distributions modeling oriented towards flow-cytometry data pre-processing applications.

- Contact: Boris Hejblum
- URL: https://CRAN.R-project.org/package=NPflow

6.4. COVVSURF

Combination of Clustering Of Variables and Variable Selection Using Random Forests

KEYWORDS: Classification - Statistics - Cluster - Machine learning - Regression

- Contact: Robin Genuer
- URL: https://github.com/robingenuer/CoVVSURF

6.5. clogitLasso

KEYWORDS: Biostatistics - Bioinformatics - Machine learning - Regression

FUNCTIONAL DESCRIPTION: R package to fit a sequence of conditional logistic regression models with lasso, for small to large sized samples.

RELEASE FUNCTIONAL DESCRIPTION: Optimisation

- Partner: DRUGS-SAFE
- Contact: Marta Avalos Fernandez
- URL: https://cran.r-project.org/web/packages/clogitLasso/index.html

6.6. TcGSA

Time-course Gene Set Analysis

KEYWORDS: Bioinformatics - Genomics

FUNCTIONAL DESCRIPTION: An R package for the gene set analysis of longitudinal gene expression data sets. This package implements a Time-course Gene Set Analysis method and provides useful plotting functions facilitating the interpretation of the results.

- Contact: Boris Hejblum
- URL: https://CRAN.R-project.org/package=TcGSA

6.7. NIMROD

Normal approximation Inference in Models with Random effects based on Ordinary Differential equations

KEYWORDS: Ordinary differential equations - Statistical modeling

FUNCTIONAL DESCRIPTION: We have written a specific program called NIMROD for estimating parameter of ODE based population models.

- Contact: Melanie Prague
- URL: http://etudes.isped.u-bordeaux2.fr/BIOSTATISTIQUE/NIMROD/documentation/html/index.html

6.8. tcgsaseq

Time-Course Gene Set Analysis for RNA-Seq Data

KEYWORDS: Genomics - Biostatistics - Statistical modeling - RNA-seq - Gene Set Analysis

FUNCTIONAL DESCRIPTION: Gene set analysis of longitudinal RNA-seq data with variance component score test accounting for data heteroscedasticity through precision weights.

- Contact: Boris Hejblum
- URL: https://CRAN.R-project.org/package=tcgsaseq

6.9. cytometree

KEYWORDS: Clustering - Biostatistics - Bioinformatics

FUNCTIONAL DESCRIPTION: Given the hypothesis of a bimodal distribution of cells for each marker, the algorithm constructs a binary tree, the nodes of which are subpopulations of cells. At each node, observed cells and markers are modeled by both a family of normal distributions and a family of bimodal normal mixture distributions. Splitting is done according to a normalized difference of AIC between the two families.

- Contact: Boris Hejblum
- URL: https://CRAN.R-project.org/package=cytometree

6.10. CRTgeeDR

KEYWORDS: Missing data - Statistics - Regression

FUNCTIONAL DESCRIPTION: The CRTgeeDR package allows you to estimates parameters in a regression model (with possibly a link function). It allows treatment augmentation and IPW for missing outcome. It is particularly of use when the goal is to estimate the intervention effect of a prevention strategy agains epidemics in cluster randomised trials.

- Contact: Melanie Prague
- URL: https://cran.r-project.org/web/packages/CRTgeeDR/index.html

6.11. ludic

KEYWORDS: Probability - Biostatistics

FUNCTIONAL DESCRIPTION: An R package to perform probabilistic record Linkage Using only DIagnosis Codes without direct identifiers, using C++ code to speed up computations. Available on CRAN, development version on github.

- Contact: Boris Hejblum
- URL: https://CRAN.R-project.org/package=ludic

6.12. CoDaPCA

KEYWORDS: Unsupervised learning - PCA

FUNCTIONAL DESCRIPTION: R functions associated to the article Avalos et al. Representation Learning of Compositional Data. NeurIPS 2018 http://papers.nips.cc/paper/7902-representation-learning-of-compositional-data

- Contact: Marta Avalos Fernandez
- URL: https://github.com/sistm/CoDa-PCA

6.13. Left-censored Lasso

KEYWORDS: Biostatistics - Machine learning

FUNCTIONAL DESCRIPTION: R function associatied to the article Soret et al. Lasso regularization for left-censored Gaussian outcome and high-dimensional predictors. BMC Medical Research Methodology (2018) 18:159 https://doi.org/10.1186/s12874-018-0609-4

RELEASE FUNCTIONAL DESCRIPTION: https://github.com/psBiostat/left-censored-Lasso

- Contact: Marta Avalos Fernandez

6.14. dd-sPLS

Data-Driven Sparse PLS

KEYWORDS: Marker selection - Classification - Regression - Missing data - Multi-Block - High Dimensional Data - PLS - SVD

SCIENTIFIC DESCRIPTION: Allows to build Multi-Data-Driven Sparse PLS models. Multi-blocks with high-dimensional settings are particularly sensible to this. Whatsmore it deals with missing samples (entire lines missing per block) thanks to the Koh-Lanta algorithm. SVD decompositions permit to offer a fast and controlled method.

FUNCTIONAL DESCRIPTION: That software solves the missing samples problem selecting interesting variables under multi-block supervised settings.

- Contact: Hadrien Lorenzo
- URL: https://hadrienlorenzo.netlify.com/projects/ddspls/

6.15. kernscr

KEYWORDS: Genomics - Biostatistics

FUNCTIONAL DESCRIPTION: An R package to perform KERNel machine score test for pathway analysis in the presence of Semi-Competing Risks

- Contact: Boris Hejblum
- URL: https://CRAN.R-project.org/package=kernscr

6.16. phenotypr

KEYWORDS: Phenotyping - Automatic labelling - Automatic Learning

FUNCTIONAL DESCRIPTION: Machine learning prediction algorithm for predicting a clinical phenotype from structured diagnostic data and CUI occurrence data collected from medical reports, previously processed by NLP approaches.

- Contact: Boris Hejblum
- URL: https://github.com/borishejblum/phenotypr

6.17. R2GUESS

Graphical processing Unit Evolutionary Stochastic Search

FUNCTIONAL DESCRIPTION: R2GUESS package is a wrapper of the GUESS (Graphical processing Unit Evolutionary Stochastic Search) program. GUESS is a computationally optimised C++ implementation of a fully Bayesian variable selection approach that can analyse, in a genome-wide context, single and multiple responses in an integrated way. The program uses packages from the GNU Scientific Library (GSL) and offers the possibility to re-route computationally intensive linear algebra operations towards the Graphical Processing Unit (GPU) through the use of proprietary CULA-dense library.

- Contact: Rodolphe Thiebaut

7. New Results

7.1. Mechanistic learning

7.1.1. Ebola models

New models have been developed for the response to the Ebola vaccine. The first one has been fitted to Phase 1 trials and has given interesting predictions of the long term duration of the response that are confirmed with the new data coming from phase 2 trials. These results have been published in Journal of Virology. Then, a new model including the B cell memory response has been defined and its mathematical proprieties have been studied. A manuscript has been submitted to Journal of Theoretical Biology. The next step is to estimate model parameters using EBL2001 clinical trial data.

New publication: Pasin C et al. Dynamics of the Humoral Immune Response to a Prime-Boost Ebola Vaccine: Quantification and Sources of Variation. J Virol. 2019 Aug 28;93(18). pii: e00579-19. doi: 10.1128/JVI.00579-19. Print 2019 Sep 15.

7.1.2. Estimation method

A new approach is currently under development by Quentin Clairon to estimate model parameters using a regularization method based on the control theory. The estimation method used an approximation of the original ODE solution for each subject. The expected advantages of this approach are i) to mitigate the effect of model misspecification on estimation accuracy ii) to regularize the estimation problem in presence of poorly identifiable parameters, iii) to avoid estimation of initial conditions. The method is still under development but preliminary results have been presented at the Viral dynamics conference in October 2019.

7.2. High-dimensional and statistical learning

7.2.1. Automatic analysis of cell populations

New publication:

Hejblum BP, Alkhassim C, Gottardo R, Caron F, Thiébaut R, Sequential Dirichlet process mixture of skew t-distributions for model-based clustering of flow cytometry data, Annals of Applied Statistics, 13(1):638-660, 2019. DOI: 10.1214/18-AOAS1209.

7.2.2. High-dimensional compositional data analysis

Perrine Soret (PhD student in the axis "High-dimensional and statistical learning", supervised by M. Avalos) has applied our expertise in high dimensional data analysis to human microbiome field of research:

Soret P, Vandenborght LE, Francis F, Coron N, Enaud R, The Mucofong Investigation Group, Avalos M, Schaeverbeke T, Berger P, Fayon M, Thiébaut R and Delhaes L. Respiratory mycobiome and suggestion of inter-kingdom network during acute pulmonary exacerbation in cystic fibrosis. To appear in *Scientific Reports*.

7.2.3. Missing Value Treatment in Longitudinal High Dimensional Supervised Problems

Poor blood sample quality introduces a large number of missing values in the context of sequencing data production. Furthermore, strong technical biases may force the analyst to remove the considered sequenced samples. Then entire day dependent data are then missing. Hadrien Lorenzo (PhD student in the axis "High-dimensional and statistical learning", supervised by J. Saracco and R. Thiébaut) has developed a multi-block approach: the dd-sPLS method. dd-sPLS has been applied to high dimensional data analysis of different fields of research:

Lorenzo, H., Misbah, R., Odeber, J., Morange, P. E., Saracco, J., Trégouët, D. A., and Thiébaut, R. High-dimensional multi-block analysis of factors associated with thrombin generation potential. In 2019 IEEE 32nd International Symposium on Computer-Based Medical Systems (CBMS) (pp. 453-458). IEEE. https://hal.archives-ouvertes.fr/hal-02429302

Ellies-Oury, M. P., Lorenzo, H., Denoyelle, C., Saracco, J., and Picard, B. An Original Methodology for the Selection of Biomarkers of Tenderness in Five Different Muscles. Foods, 8(6), 206 (2019). https://hal.archives-ouvertes.fr/hal-02164157

7.3. Translational vaccinology

7.3.1. HIV vaccine development

We have finalized the data science analyses of two HIV vaccine clinical trials: 1) ANRS VRI01, a randomized phase I/II trial evaluating for different prime boost vaccine strategies in healthy volunteers; 2) ANRS 149 LIGHT, a randomized phase II trial comparing a prime-boost therapeutic HIV vaccine strategy to placebo in HIV-infected patients undergoing antiretroviral treatment interruption. This included integrative statistical analyses using sPLS methods (as developed by the team) to relate markers from different high-dimensional immunogenicity or gene expression assays or virological assays to each other. In the ANRS VRI01 data set this allowed to disentangle the immune responses induced by the different vaccines used in the prime-boost strategies, showing specific effects of one of the vaccines (MVA HIV-B). We further identified a gene expression signature that correlates with later functional T-cell responses across the three different prime-boost association in which the MVA HIV-B vaccine was used. The corresponding manuscripts are currently in preparation.

Other HIV vaccine trials are currently being set-up by the French VRI (Vaccine Research Institute) and the European consortium EHVA, with strong contributions of SISTM team members to the trial designs.

7.3.2. Ebola vaccine development

The main results of the two randomized phase II Ebola vaccine trials conducted by the IMI-2 EBOVAC2 consortium (coordinated by Rodophe Thiébaut from the SISTM team) were finalized in 2019. and presented at international conferences. The results showed that the tested vaccine strategy (two-dose heterologous Ad26.ZEBOV and MVA-BN®-Filo Ebola vaccine regimen, developed by Janssen) was safe and immunogenic in both European and African volunteers (EBL2001 and EBL2002 trials). Deeper analyses of the induced immune responses are currently ongoing, and systems vaccinology analyses will soon start in the SISTM team.

The SISTM team is also a partner in the related IMI-2 EBOVAC1 and EBOVAC3 consortia (assesing the same vaccine regimen in other trial populations and/or trial phases), in which the main contributions of the team are related to mechanistic modeling of the immune responses (ongoing).

7.3.3. Vaccine development against other pathogens

Two other phase I vaccine trials (one testing a placental malaria vaccine, Primalvac trial; and one testing a nasal Pertussis vaccine, BPZE-1 trial), in which members of the SISTM team were strongly involved, have shown promising results. Results of the Primalvac trial have been accepted for publication in the Lancet Infectious Disease journal, and results of the BPZE-1 trial have been submitted for publication.

7.3.4. Methodological developments for vaccine trials

At the interface between the axis on "Mechanistic learning" and the axis "Translational vaccinology", modelling done within a PhD project (M. Alexandre, supervised by R. Thiébaut and M. Prague) has informed the definition of the primary endpoint and statistical analysis method to be used in two therapeutic HIV vaccine trials with antiretroviral treatment interruption (EHVA T02 and ANRS DALIA-2). The methodological choices and their rationale have been presented to the governance bodies of the research consortia, patient associations and have been submitted for ethics and regulatory approvals. This will be subject to a specific methodology publication.

Edouard Lhomme (PhD student in the axis "Translational Vaccinology, supervised by L. Richert) has developed a statistical method for functional T-cell assay data from vaccine trials (in particular the intracellular cytokine staining assay) that takes into account non-specific immune responses. We propose using a bivariate linear model for the analysis of the cellular immune responses to obtain accurate estimations of the vaccine effect. We benchmarked the performance of the model in terms of both bias and control of type-I and -II errors, and applied it to simulated data as well as real pre- and post-vaccination data from two recent HIV vaccine trials (ANRS VRI01 and ANRS 149 LIGHT in HIV-infected participants). This method has been published in the Journal of Immunological Methods and is now used in the SISTM team as the standard method for analyses of functional cellular data with non-stimulated control conditions, for instance in the currently ongoing analysis of cellular proliferation data from the EBOVAC2 EBL2001 trial. We have also established an online interface based on R Shiny to make this analysis method available for use by immunologists without specific training in statistical modelling (https://shiny-vici.apps.math.cnrs.fr/).

7.3.5. Prediction of the survival of patients based on RNA-seq data

In collaboration with the Inria MONC team, with the Inserm Angiogenesis and Tumor micro-environment team, and with clinicians from Milan and Bergen, the project GLIOMA-PRD aims to improve the prediction of the evolution of the lower grade glioma, a primary brain tumor, based on clinical, imaging and genomic data. In the SISTM team, we first had to determine the sufficient sample size for determining a predictive signature based on RNA-seq data for the survival of the patients. We concluded that 50 patients were a good enough sample size for this aim. We then explored the potential methods to analyze these data, with a particular focus on the methods grouping the genes by pathways, as the pilot data (The Cancer Genome Atlas Research Network, NEJM, 2015) showed a high correlation structure. We particularly compared two methods, Generalized Berk-Jones (GBJ), proposed by [54], and tcgsaseq, proposed by [1]. The first method could be applied to the survival context and thus be appropriate for our data.

Once the RNA-seq data were available, we could observe a high batch effect since the data were sequenced in two different lanes. One of these two batch included only patients that exhibited a particular tumor at the PET-scan, called "COLD", while the second batch included both patient labelled as "COLD", but also the other type of tumor, called "DIFFUSE". As this experiment structure might leads to confusing the difference due to the batch effect with the one due to the biological different, we had to explore methodologies that could remove this batch effect.

Once this batch effect removed, we will then analyze the RNA-seq data in order to identify the genes, or the group of genes, that could be predictive of the survival of the patients.

8. Bilateral Contracts and Grants with Industry

8.1. Contracts and Grants with Industry

Implication in research for the development of Ebola vaccine has lead to several indirect contracts with industry:

- The EBOVAC1, EBOVAC2 and EBOVAC3 project, collaboration with Janssen from Johnson et Johnson.
- The Prevac trial vaccine trial (legal sponsors: Inserm, NIH, London School of Hygiene and Tropical Medicine) involves collaborations with Merck and Janssen. The purpose of this study is to evaluate the safety and immunogenicity of three vaccine strategies that may prevent Ebola virus disease (EVD) events in children and adults. Participants will receive either the Ad26.ZEBOV (rHAd26) vaccine with a MVA-BN-Filo (MVA) boost, or the rVSVΔG-ZEBOV-GP (rVSV) vaccine with or without boosting, or placebo. The EDCTP-2 funded Prevac-UP project is set as a continuation of Prevac trial in the same framework.

A new collaboration has started with the pharma company Ipsen on the integration of OMICS data into an in-silico trials pipeline (Cifre Phd to start in January 2020)

9. Partnerships and Cooperations

9.1. Regional Initiatives

The team have strong links with :

- Research teams of the research center Inserm U1219 : "Injury Epidemiology, Transport, Occupation" (IETO), "Biostatistics", "Pharmacoepidemiology and population impact of drugs", "Multimorbidity and public health in patients with HIV or Hepatitis" (MORPH3Eus), "Computer research applied to health" (ERIAS) emerging research team.
- Bordeaux CHU ("Centre Hospitalier Universitaire").
- Institut Bergonié, Univ Bordeaux through the Euclid F-CRIN Clinical Trials platform and CIC-EC (CIC1401)
- Inria Project-team MONC, M3DISIM and CQFD

The project team members are involved in:

- EUCLID/F-CRIN clinical trials platform (Laura Richert)
- The Clinical Epidemiology module of the Clinical Investigations Center (CIC1401) (Laura Richert)
- The research project “Self-management of injury risk and decision support systems based on predictive computer modelling. Development, implementation and evaluation in the MAVIE cohort study” funded by the Nouvelle-Aquitaine regional council (Marta Avalos).
- Phenotyping from Electronic Health Records pilot project in cooperation with with the ERIAS Inserm emerging team in Bordeaux and the Rheumatology service from the Bordeaux Hospital (Boris Hejblum)
- A cancer research project (GLIOMA-PRD) in collaboration with Inria MONC team and with the the Inserm Angiogenesis and Tumor micro-environment team on glioblastoma

9.2. National Initiatives

- Labex Vaccine Research Institute (VRI) There are strong collaborations with immunologists involved in the Labex Vaccine Research Institute (VRI) as Rodolphe Thiébaut and Laura Richert are leading the Data science division (previously Biostatistics/Bioinformatics) http://vaccine-research-institute.fr.
- Collaboration with Inserm PRC (pôle Recherche clinique).
- Collaboration with Inserm Reacting (REsearch and ACTion targeting emerging infectious diseases) network
- Collaboration with Inserm RECap (Recherche en Epidémiologie Clinique et en Santé Publique) network

9.2.1. Expert Appraisals

- Rodolphe Thiébaut is a member of the CNU 46.04 (Biostatistiques, informatique médicale et technologies de communication).
- Rodolphe Thiébaut is a member of the Scientific Council of Inserm.
- Mélanie Prague is an expert for ANRS (France Recherche Nord&Sud Sida-HIV Hépatites) in the CSS 3 (Recherches cliniques et physiopathologiques dans l’infection à VIH) and AC 47 (Dynamique et contrôle des épidémies VIH et hépatites).
- Laura Richert is an expert for the PHRC (Programme hospitalier de recherche Clinique).
- Marta Avalos is an expert for the ANSM (Agence nationale de sécurité du médicament et des produits de santé)

9.2.2. Various Partnership

The project team members are involved in:

- DRUGS-SAFE platform funded by ANSM (Marta Avalos). Initiated in 2015-2018. Renewed for 2019.
- F-CRIN (French clinical research infrastructure network), initiated in 2012 by ANR under "Programme des Investissements d'avenir". (Laura Richert)
- INCA (Institut National du Cancer) funded the project *Evaluation de l'efficacité d'un traitement sur l'évolution de la taille tumorale et autres critères de survie : développement de modèles conjoints.* (Principal PI Virginie Rondeau Inserm U1219, Mélanie Prague is responsible of Work package 4 "mechanistic modeling of cancer: 5800 euros").
- Contrat Initiation ANRS MoDeL-CI: Modeling the HIV epidemic in Ivory Coast (Principal PI Eric Ouattara Inserm U1219 in collaboration with University College London, Mélanie Prague is listed as a collaborator).

9.3. European Initiatives

9.3.1. FP7 & H2020 Projects

The member of SISTM Team are involved in EHVA (European HIV Vaccine Alliance):

EHVA: European HIV Vaccine Alliance: a EU platform for the discovery and evaluation of novel prophylactic and therapeutic vaccine candidates

Coordinator: Inserm/University of Lausanne. Other partners: EHVA consortium gathers 41 partners. Duration: 60 months. 01 /01 /2016 - 31 /12 /2020

With 37 million people living with HIV worldwide, and over 2 millions new infections diagnosed each year, an effective vaccine is regarded as the most potent public health strategy for addressing the pandemic. Despite the many advances in the under-standing, treatment and prevention of HIV made over the past 30 years, the development of broadly-effective HIV vaccine has remained unachievable. The EHVA international alliance, which includes academic and industrial research partners from all over Europe, as well as sub-Saharan Africa and North America, will work to discover and progress novel vaccine candidates through the clinic. EHVA fosters a multidisciplinary approach to the challenge of developing broadly effective HIV vaccines. EHVA's program primary goals are:

- To develop a Multidisciplinary Vaccine Platform (MVP) for prophylactic and therapeutic HIV vaccines
- To move at least two novel prophylactic vaccine candidates to clinical development
- To identify immune correlates associated with control of HIV replication following immunological intervention
- To establish a strong scientific basis for further development of EHVA vaccine candidates in larger clinical trials

  To this purpose, EHVA bring to the field 4 multidisciplinary research platforms representative of the latest advances in clinical trials and preclinical vaccine development. These four platforms cover all aspects of vaccine development from early-stage discovery to clinical trials.
- The Discovery Platform will work to disclose promising vaccine candidates based on the induction of T-cell and antibody responses (ie, neutralizing antibody and non-neutralizing antibody).
- The Immune-Profiling Platform will advance assays to predict the immunogenicity of potential vaccine candidates. The ability to generate a profile of a potential vaccine candidate, using models that emulate the immune system's response, will assist with benchmarking novel and existing vaccine candidates.

- The Data Management/Integration and Down-Selection Platform is developed around the WP10 led by Rodolphe Thiébaut. SISTM provides here state-of-the-art statistical tools for the analysis and interpretation of complex data and algorithms for the efficient selection of vaccines.
- The Clinical Trial Platform includes pharmaceutical industry expertise for late stage development, a network of top European clinical centers for conducting large cohort studies, as well as relationships with leading scientists based in Africa. Future testing of EHVA vaccine in Sub-Saharan Africa is a research priority because it is the area of the world with the greatest number of people infected with HIV.

IP-CURE-B: Immune profiling to guide host-directed interventions to cure HBV infections. Coordinated by Inserm (France), the project includes a total of 13 Beneficiaries: Centre Hospitalier Universitaire Vaudois (Switzerland), Karolinska Institutet (Sweden), Institut Pasteur (France), Universita degli studi di Parma (Italy), Fondazione IRCCS CA' Granda – Ospedale maggiore policlinico (Italy), Universitaetsklinikum Freiburg (Germany), Ethniko Kai Kapodistriako Panepistimio Athinon (Greece), Fundacio Hospital Universitari vall d'Hebron (Spain), Gilead Sciences Inc. (USA), Spring Bank Pharmaceuticals, Inc (USA), European Liver Patients Association (Belgium), Inserm Transfert SA (France). Duration: 60 months. $01/01/2020 - 31/12/2024$

HBV infections, are a major global public health threat with over 257 million people worldwide chronically infected and over 887,000 deaths per year. 4.7 million people live with HBV in the European Union (EU) and European Economic Area (EEA). W.H.O. estimates that HBV causes almost 40% of the cases of hepatocellular carcinoma (HCC), which is the 2nd leading cause of cancer-related mortality worldwide. HBV kills nearly 900,0000 people around the world each year. The current prophylactic vaccine has no impact on established chronic infection.

The objective of the IP-CURE-B project is to develop novel curative concepts for chronic hepatitis B (CHB). Specific aims will be to: 1) improve the rate of functional cure of CHB by boosting innate immunity with immune modulators and stimulating adaptive immune responses with a novel therapeutic vaccine; ii) characterize immune and viral biomarker signatures for patient stratification and treatment response monitoring; iii) integrate biological and clinical data to model the best combination treatment for future trials; iv) model the effectiveness of novel curative therapies with respect to disease spectrum, patient heterogeneity, and constraints of National Health Systems.

The project organization combines: i) a Proof of Concept clinical trial of a combination of 2 novel compounds stimulating innate immunity; ii) a preclinical immune therapy platform in humanized mice combining immune-modulatory strategies to stimulate innate immunity, rescue exhausted HBV-specific T cells and generate anti-HBV adaptive responses; iii) extensive virologic and immune profiling to identify correlates of cure in patients, iv) the integration of large biological and clinical data-sets, v) a cost-effectiveness modelling of new therapeutic interventions, vi) project management, vii) results exploitation and dissemination.

In the IP-CURE-B project, SISTM coordinates WP6 Data science platform for data integration and statistical modeling which will provide powerful data management and statistical tools for the analysis and interpretation of the complex heterogeneous and high-dimensional data generated in the other WPs. For data management and data sharing, SISTM will leverage on a data warehouse system, based on Lab-key Server, the primary structure already established within the EU funded H2020 EHVA project. SISTM will develop and apply statistical methods for integrating data from several assay platforms to better describe and understand the mechanisms of the experimental products and to define predictive signatures of viral control and functional cure. Indeed, the immune system forms a sophisticated network of tissues, cells and molecules that interact in order to achieve viral control. Understanding how this complex network responds to interventions aimed at HBV functional cure requires the use and integration of data from multiple assay technologies. Two main strategies will be used: 1) statistical approaches to relate and down-select several high-dimensional data from the various assays in humanized mice and humans; 2) a modelling approach, taking into account biological knowledge and the results from the first step, to better capture and understand the non-linear relationships between the components of the immune system, viral control and their dynamics over time. Statistical and mechanistic models will be used, based on ordinary differential equation systems or other approaches. At the end of the process, if an adequate model is identified, this can be used to down-select immunomodulatory and vaccine regimens and make in silico predictions about optimized strategies or stratified treatment approaches. These approaches have been successfully applied in HIV immunotherapy trials and in vaccine trials by SISTM.

9.3.2. Collaborations in European Programs, Except FP7 & H2020

The members of SISTM are also involved in Innovative Medicine Initiative 2 (IMI2) projects which are all under the IMI Ebola+ program that was launched in response to the Ebola virus disease outbreak of 2014. SISTM is active in 3 projects which are all in collaboration with Janssen Vaccines & Preventions B.V. The overall aim of the EBOVAC program is to assess the safety, immunogenicity and efficacy of a novel 2-dose Ad26 + MVA prophylactic vaccine regimen against Ebola Virus Disease. In this context, the 3 projects develop as follows:

EBOVAC1: Development of a Prophylactic Ebola Vaccine Using an Heterologous Prime-Boost Regimen.

Coordinated by London School of Hygiene & Tropical Medicine (United Kingdom). Other beneficiaries: Janssen a Pharmaceutical Companies of Johnson & Johnson, The Chancellor, Masters and Scholars of the University of Oxford (United Kingdom), Inserm (France), University of Sierra Leone (Sierra Leone). Duration: 84 months. 01 /12 /2014 - 30 /11 /2021.

EBOVAC1 is dedicated to the Phase I and III development of prime-boost vaccine based on Ad26.ZEBOV and MVA-BN-Filo. Phase I was conducted in the US, the UK and in Africa (Sierra Leone, Uganda, Kenya and Tanzania) for a total of 231 volunteers enrolled. Phase III was conducted in Sierra Leone in several phases leading to the successful enrolment of more than 2800 volunteers including around 500 children aged 1-17 years. In EBOVAC1, SISTM is modelling the immune response to the Ad26.ZEBOV and MVA-BN-Filo, using the data obtained in the project.

EBOVAC2: Development of a Prophylactic Ebola Vaccine Using a 2-Dose Heterologous Vaccination Regimen: Phase 2.

Coordinated by Rodolphe Thiébaut with the following partners: Inserm (France), Labex VRI (France), Janssen Pharmaceutical Companies of Johnson & Johnson, London School of Hygiene & Tropical Medicine (United Kingdom), The Chancellor, Masters and Scholars of the University of Oxford (United Kingdom), Le Centre Muraz (Burkina Faso), Inserm Transfert (France). Duration: 72 months. 01 /12 /2014 - 30 /11 /2020.

EBOVAC2 main objective is to provide extensive and robust data on the safety and immunogenicity of the Ad26.ZEBOV and MVA-BN-Filo vaccine. This was designed by: 1. Carrying out translational studies to link vaccine elicited immune responses in humans to protection from Ebola in vaccinated non-human primates 2. Carrying out Phase II trials in African and European volunteers in approximately 6 countries, four in Africa and two in the EU with an overall target enrolment of approximately 1,500 subjects. Given the compressed nature of this development program, the Phase II studies were conducted in parallel with the planned Phase III study (EBOVAC1). The rationale for inclusion of European volunteers in Phase 2, in addition to the trials in Africa, is to allow for higher sensitivity in safety signal detection in populations with low incidence of febrile illnesses, to generate negative control specimens for assay development, to allow for inclusion of health care workers or military personnel that may be deployed to Ebola-endemic regions. 3. Evaluating the vaccine response in special population groups, such as children (ages 1-17 years), the elderly (ages 50-65) and individuals infected with HIV, to confirm safety and immunogenicity. The Phase II trials started as soon as preliminary safety data were available from Phase I trials. 4. Monitoring and characterizing immune response to the proposed vaccine through different set of analysis of the humoral and cellular response with different approaches (ICS, luminex, gene expression analysis, T and B cell activation assays, Virus neutralization assays...) leading to a unique set of data. In EBOVAC2, in addition to the coordination of the whole project, SISTM is involved in the statistical analysis of the results obtained by the VRI lab responsible for an important part of the exploratory work, but also in the integrative data analysis of these high dimension and complex data. A Labkey environment was established in SISTM for EBOVAC2 to facilitate the exchange and following treatment of the project data.

EBOVAC3: Bringing a prophylactic Ebola vaccine to licensure.

Coordinated by the London School of Hygiene & Tropical Medicine (United Kingdom). Other beneficiaries: Janssen a Pharmaceutical Companies of Johnson & Johnson, Inserm (France), The University of Antwerpen (Belgium), University of Sierra Leone (Sierra Leone). Duration: 60 months. 01 /06 /2018 - 30 /05 /2023.

EBOVAC3 aims at supporting an essential part of the remaining clinical and manufacturing activities required for licensure in the European Union (EU) and the United States (US) for the candidate heterologous Ad26.ZEBOV and MVA-BN-Filo prophylactic vaccine regimen against Ebola virus disease. As a follow-up project, the IMI2 funded EBOVAC3 project, has started in June 2018. In this project, the vaccine strategy is further evaluated in specific populations in Africa (infants in Guinea and Sierra Leone; and front line workers in RDC). The project includes a work package on modelling, which is led by Rodolphe Thiébaut. Three workshop have been organized in Bordeaux (October 29th-30th, 2018), Arcachon (May 2nd-3rd, 2019) and Leiden (November 20th, 2019) to discuss and collaborate with the EBOVAC3 partners on the planned modelling work.

PREVAC-UP: The Partnership for Research on Ebola VACcinations-extended follow-UP and clinical research capacity build-UP.

SISTM is also involved in PREVAC-UP, an EDCTP2 project in direct link with the research carried out on the Ebola vaccines.

Coordinated by Inserm (France). Other beneficiaries: CNFRSR (Guinea), CERFIG (Guinea), LSHTM (UK), COMAHS (Sierra-Leone), NIAID (USA), NPHIL (Liberia), USTTB (Mali), Centre pour le Développement des Vaccins (Mali), Inserm Transfert SA (France). Duration: 60 months. 01 /01 /2019 - 31 /12 /2023.

Human-to-human transmission of Ebola virus in West Africa was interrupted in 2016 but the risk of reemergence of the disease is real. Thus, efforts to develop a safe and effective vaccine against Ebola virus disease with a durable prophylactic effect in communities must continue. The PREVAC-UP project is built around the PREVAC consortium. The Partnership for Research on Ebola Vaccinations (PREVAC) is an international consortium including the French Institute of Health and Medical Research, the London School of Hygiene & Tropical Medicine, the US National Institutes of Health, health authorities and scientists from Guinea, Liberia, Mali and Sierra Leone, a non-governmental organization (Alliance for International Medical Action), and Merck, Johnson & Johnson and Bavarian Nordic companies. The PREVAC trial is a phase IIB, randomized, placebo controlled, multicentre trial evaluating the safety and immunogenicity over 12 months of three vaccine strategies in children and adults. Participants are randomized to one of five groups: (i) vaccination with Ad26.ZEBOV prime and MVA-BN-Filo boost, (ii) vaccination with rVSVδG-ZEBOV-GP prime and a boost of the same vaccine, (iii) vaccination with rVSVδG-ZEBOV-GP vaccine without boost, (iv) placebo group 1 and (v) placebo group 2. Preliminary phases started in Liberia and Guinea in March 2017; the main phase of the trial evaluating the five regimens will begin in Liberia, Guinea Sierra Leone and Mali in April 2018 with an enrolment targets of 1,400 adults and 1,400 children.

PREVAC-UP two primary objectives are to determine (i) the long-term immunogenicity and safety and (ii) durability of humoral and cellular immune responses of Ebola vaccine regimes over 60 months. We will also evaluate the effect of co-infections, such as malaria and helminths on the immune response to vaccination. An integrative statistical analysis of the immune response will be used under the coordination of SISTM to explore the mechanism of action of the vaccines and to identify early correlates of durable antibody induction. PREVAC-UP will also build on the extensive community mobilization efforts previously generated through PREVAC to provide a trans-national platform for social and health science research and training. Finally, this research proposal will expand and sustain capacity building and training of scientists in the four participant African countries. This program is expected to significantly impact Ebola prevention and control in adults and children in Africa. PREVAC-UP will also strengthen capacity for science relevant to the development and evaluation of new vaccines in sub-Saharian Africa.

In PREVAC-UP, SISTM leads the WP4 Utilisation of a system vaccinology approach using integrative statistical analyses and mechanistic modelling of the immune response to explore the interrelationship of immune response to Ebola vaccines. System vaccinology approach helps in better understanding and predicting the response to vaccines as demonstrated in the context of yellow fever, flu and many other vaccines. The idea is to integrate the massive data generated by high-throughput technologies (transcriptomics, flow cytometry, multiplex data) and population characteristics (sociodemographics and coinfections) to isolate the main markers/signatures associated to the vaccine response. Then, a mechanistic model of the response can be built and hopefully predict the individual long-term response. The PREVAC trial is a unique opportunity for setting up such an approach and apply it to the most advanced vaccine platforms against Ebola. The Inserm-SISTM team has produced several publications highlighting how within-host mechanistic models could play an important role in predicting vaccine efficacy and in improving treatment regimens, notably in HIV. The team has started to work on modelling the response to the Ad26.ZEBOV/MVA platform. In PREVAC-UP, it is expected that signatures and the mechanistic model itself will be different according to the type of vaccine as, specifically, the rVSV is a replicative vector. Two main outcomes are expected. One is a better understanding of the individual variability of the immune response and another is the prediction of the response with two specific aspects: after a new boost and on the long-term (5 years) for a new vaccinees. Identification and validation of an early correlate of later antibody responses would allow early prediction of whether an individual, or group of individuals is likely to be a poor responder and then to recommend subsequent interventions to test in this subset (such as change in vaccination strategy or additional boosts). Heterogeneity in antibody responses is expected within each group as it has been observed in former studies. In PREVAC-UP, information will be collected to inform the reason of this variability. Specific aspects will be explored such as the impact of malaria and various infectious agents on the immune response. Integrating such information in a mechanistic model of the immune response may help understanding the pathway leading to blunted response in vaccines and also to generate new hypotheses that could be biologically validated later on. Another important aspect of the modelling approach is the quantification of the impact of each potential factor helping to order the relative importance of various factors. In conclusion, this work is definitely at the confluence of the other work packages, integrating and ordering all the available information to understand and predict the effects of the promising vaccine strategy evaluated in the PREVAC trial.

9.3.3. Collaborations with Major European Organizations

University of Oxford;

London School of Hygiene and Tropical Medicine;

University Hospital Hambourg (UKE);

Heinrich Pette Institute for Experimental Virology, Hambourg;

MRC, University College London;

MRC Biostatistics Unit, University of Cambridge;

The University of Antwerpen;

University of Milan;

University of Bergen.

9.4. International Initiatives

9.4.1. Inria International Labs

Inria@EastCoast

Associate Team involved in the International Lab:

9.4.1.1. DYNAMHIC

Title: DYNAMical modeling of HIV Cures

International Partner (Institution - Laboratory - Researcher):

Harvard University (United States) - Harvard Program for Evolutionary Dynamics - Alison HILL

Start year: 2019

See also: https://team.inria.fr/dynamhic/

The aim of the DYNAMHIC Associate Team is to bring together a mathematical biology team at Harvard and the Inria team SISTM of applied statisticians at Bordeaux Sud-ouest. This collaboration will allow the analysis of unique pre-clinical non human primates data of HIV cure interventions. In particular, we will focus on immunotherapy and therapeutic vaccine, which are very promising in term of efficacy and are at the leading edge of pre-clinical research in the area. The novelty of the approach is to propose an integrative project studying complex biological processes with novel mathematical statistical models, which has the potential to yield predictive computational tools to assist in the design of both therapeutic products and clinical trials for HIV cure

Finally, the associate team is the opportunity to provide the research group with an official administrative framework. And, to continue to develop a promising research topic connected but different from those funded up to now.

Inria@SiliconValley

Associate Team involved in the International Lab:

9.4.1.2. SWAGR

Title: Statistical Workforce for Advanced Genomics using RNAseq

International Partner (Institution - Laboratory - Researcher):

RAND Corporation (United States) - Statistics group - Denis Agniel

Start year: 2018

See also: https://team.inria.fr/swagr/

The SWAGR Associate Team aims at bringing together a statistical workforce for advanced genomics using RNAseq. SWAGR combines the biostatistics experience of the SISTM team from Inria BSO with the mathematical expertise of the statistics group at the RAND Corporation in an effort to improve RNAseq data analysis methods by developing a flexible, robust, and mathematically principled framework for detecting differential gene expression. Gene expression, measured through the RNAseq technology, has the potential of revealing deep and complex biological mechanisms underlying human health. However, there is currently a critical limitation in widely adopted approaches for the analysis of such data, as edgeR, DESeq2 and limma-voom can all be shown to fail to control the type-I error, leading to an inflation of false positives in analysis results. False positives are an important issue in all of science. In particular in biomedical research when costly studies are failing to reproduce earlier results, this is a pressing issue. SWAGR propose to develop a rigorous statistical framework modeling complex transcriptomic studies using RNAseq by leveraging the synergies between the works of B. Hejblum and D. Agniel. The new method will be implemented in open-source software as a Bioconductor R package, and a user friendly web-application will be made available to help dissemination. The new method will be applied to clinical studies to yield significant biological results, in particular in vaccine trials through existing SISTM partnerships. The developed method is anticipated to become a new standard for the analysis of RNAseq data, which are rapidly becoming common in biomedical studies, and has therefore the potential for a large impact.

9.5. International Research Visitors

9.5.1. Visits of International Scientists

9.5.1.1. Internships

- Eva Reiner (Germany), intern in the Translational Vaccinology axis (March-July 2019)
- Aaron Sonabend, PhD student from Harvard University, collaborator in the High-dimensional statistical learning axis (June-August 2019) funded by the Harvard Rose Fellowship.

9.5.2. Visits to International Teams

9.5.2.1. Research Stays Abroad

- Boris Hejblum did a research stay at the Biostatistics Unit of The Medical Research Council at the University of Cambridge (Cambridge, UK) for a cumulative period of 1.5 month in 2019. This stay was devoted to collaborative work with Paul DW Kirk on scalalble bayesian computational methods.
- Boris Hejblum did a research stay at the Rand Corporation (offices in both Santa Monica CA and Boston MA) and at the Harvard Medical School (Boston MA, USA) for a cumulative period of 2 weeks in 2019. This stay was devoted to collaborative work with Denis Agniel in the context of the SWAGR Associate Team and with Tianxi Cai on high-dimensional statistical inference.
- Mélanie Prague did a research stay abroad in Harvard.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Societies Involvement

- Boris Hejblum is a member of the chairing committee of the *Société Française de Biométrie*, the French Chapter of the International Biometric Society
- Boris Hejblum is a board member of the “MAchine Learning et Intelligence Artificielle” (MALIA) group of *Société Française de Statistique* (SFdS)
- Mélanie Prague is a board member of the “Jeunes Statisticien.ne.s” group of SFdS
- Marta Avalos is a board member of the “Stat&Sport” group of SFdS

10.1.2. Scientific Events: Organisation

10.1.2.1. General Chair, Scientific Chair

Mélanie Prague co-organized with Jérémy Guedj from Inserm the 4th Workshop on Virus Dynamics https://viraldynamics.sciencesconf.org, 21-23 October in Paris, France.

10.1.3. Scientific Events: Selection

10.1.3.1. Chair of Conference Program Committees

- Robin Genuer Co-organizes a reading group called "Smiling in Bordeaux" (http://www.math.u-bordeaux.fr/~mchave100p/smiling/)
- Boris Hejblum organizes the Biostatistics Seminar Series at the Bordeaux Population Health Inserm Research Center
- Boris Hejblum co-organizes the Bordeaux Statistics Seminar Series (https://indico.math.cnrs.fr/category/367/)

10.1.3.2. Member of the Conference Program Committees

- Mélanie Prague was a member of the 51th Days of Statistics (JdS), the most important annual scientific event in the French-speaking statistical community, organized by the French Statistical Society (SFdS), June 2019, Nancy, France
- Rodolphe Thiébaut was a member of the scientific committee of the national conference on clinical research (EPICLIN)
- Rodolphe Thiébaut is a member of the scientific committee of the IWHOD International Workshop on HIV Observational Databases since 2013 (http://iwhod.org/Committee) and chair in 2020.

10.1.3.3. Reviewer

- NeurIPS (Robin Genuer)
- Workshop at NeurIPS 2019 "ML4H: Machine Learning for Health" (Marta Avalos)

10.1.4. Journal

10.1.4.1. Member of the Editorial Boards

Lifetime Data Analysis (Daniel Commenges)

Statistics Surveys (Daniel Commenges)

Associate editor of International journal of Biostatistics (Melanie Prague)

IMIA Yearb Med Inform (Rodolphe Thiébaut)

10.1.4.2. Reviewer - Reviewing Activities

- AIDS (Rodolphe Thiébaut)
- Am J Public Health (Mélanie Prague)
- Biometrics (Mélanie Prague, Boris Hejblum)
- Bioinformatics (Boris Hejblum)
- IMIA Yearb Med Inform (Marta Avalos)
- International Journal of Epidemiology (Daniel Commenges)
- Journal of Computation Statistics and Data Analysis (Boris Hejblum)
- Journal of the American Statistical Association (Robin Genuer)
- Journal of the Royal Statistical Society: Interaction (Mélanie Prague)
- JRSS-B (Mélanie Prague)
- Operations research (Robin Genuer)
- PLOS Computational Biology (Boris Hejblum)
- Society of clinical trial (Mélanie Prague)
- Statistical Methods in Medical Research (Mélanie Prague)
- Statistical science (Mélanie Prague)
- Trials (Laura Richert)

10.1.5. Invited Talks

- 3rd EcoSta Conference – 25-27th June 2019. Taïchung, Taïwan. A variance component score testapplied to RNA-Seq differential analysis. [B Hejblum]
- 12th International Conference of the ERCIM Working Group on Computational and Methodological Statistics – 14-16th December 2019, London, UK. Scaling up nonparametric Bayesian clustering with MCMC for big data applications. [B Hejblum]
- The 9th International Digital Public Health Conference – 20-23 November 2019, Marseille, The Challenges of Implementing Healthcare Technology and Innovation across Europe and Beyond [R Thiebaut]

- Conférence du centre de recherche du CHU de Sainte Justine – 17 October 2019, Montreal, Canada - *Science des données en épidémiologie clinique: exemples en vaccinologie*. [R Thiebaut]
- 4th Workshop on viral dynamics – 21-23rd October 2019, Paris - Modeling to optimize vaccine development against Ebola [R Thiebaut]
- INFECTION, IMMUNITY AND INFLAMMATION PROGRAMME Mini-symposium Mathematical Immunology in memoriam Robin Callard - 3rd October 2019, Institute of Child Health, London - Modelling in Immunology from 2007 to tomorrow, an overview of the work done with and inspired by Robin Callard [R Thiebaut]
- Workshop ITUN CESI, CHU Nantes, 3rd September. Understanding and predicting the effect exogeneous IL-7 in HIV infected patients through mathematical modelling: toward personnalised medicine. [R Thiebaut]
- 14th Colloquium of ADEA *La transformation du système de santé : l'hôpital de demain*, Cambo les Bains, September. L'intelligence artificielle [R Thiebaut]
- Robin's Callard symposium – Institute of Child Health, London – 4 October [R Thiebaut]

10.1.6. Oral contributions in conferences and colloquium

- Several members contributed to the 51th Days of Statistics (JdS), the most important annual scientific event in the French-speaking statistical community, organized by the French Statistical Society (SFdS), June 2019, Nancy, France [R Genuer, M Prague, M Avalos]
- UseR! 2019, Toulouse, France – July 2019. VICI: a Shiny app for accurate esti-mation of Vaccine Induced Cellular Immunogenicity with bivariate modeling. [B Hejblum]
- Joint Statistical Meeting 2019, Denver, USA – July 2019. Can you trust differential expression methods for RNA-seq data analysis ? [B Hejblum]
- 6th *Colloque francophone international sur l'enseignement de la statistique* 2019, Nancy, France–June 2019. *Enseigner la science des données en santé publique* [B Hejblum]
- Medinfo 2019, Lyon, 25-30 August 2019 [R Thiebaut]
- Several Talks at Virus Dynamics, October, Paris [R. Thiebaut, M. Alexandre, Q. Clairon].
- 32nd IEEE International Symposium on Computer-Based Medical Systems (CBMS) [H. Lorenzo].
- GDR Statistics and Health, Paris, France, October 2019 [L. Villain].
- StatOmique day - November 2019 [M. Gauthier]

10.1.7. Poster contributions in conferences and colloquium

- The French Health Data System applied to health research Meeting - June 2019, Rennes, France [M Avalos]
- PAGE June Stocholm [M. Prague, M. Alexandre]
- StatOmique day - Novembrer 2019, Paris [L. Villain]

10.1.8. Scientific Expertise

- Rodolphe Thiébaut is an expert for INCA (Institut National du Cancer) for the PHRC (Programme hospitalier de recherche Clinique en cancérologie) and for the PRME (Programme de recherche médico-économique en cancérologie).
- Rodolphe Thiébaut is a member of the CNU 46.04 (Biostatistiques, informatique médicale et technologies de communication).
- Rodolphe Thiébaut is a member of the Scientific Council of Inserm.
- Rodolphe Thiébaut is a member of the commitee "Biologie des Systèmes et Cancer (Plan Cancer)", a member of the Scientific Advisory Board of the "Institut Pierre Louis d'Epidémiologie et de Santé Publique" (UPMC, Dir : Dominique Costagliola), a member of the independent committee of international trials ODYSSEY and SMILE, a member of the scientific council of Muraz's Center (Bobo-Dioulasso, Burkina Faso)

- Mélanie Prague is an expert for ANRS (France Recherche Nord&Sud Sida-HIV Hépatites) in the CCS13 (Recherches cliniques et physiopathologiques dans l'infection à VIH) and AC 47.
- Laura Richert is an expert for the PHRC (Programme hospitalier de recherche Clinique).
- Marta Avalos is an expert for the ANSM (Agence nationale de sécurité du médicament et des produits de santé)

10.1.9. Research Administration

Daniel Commenges is the director of the Biostat-Info axis in the Inserm BPH (Bordeaux Public Health) institute.

Rodolphe Thiébaut is the director of the department of Public Health in University of Bordeaux and a member of the Inserm Scientific Council

Laura Richert is coordinator of the Clinical epidemiology module of the Clinical Investigations Center (CIC1401 Bordeaux)

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

In class teaching

Master: Rodolphe Thiébaut is head of the Digital Public Health graduate program, University of Bordeaux.

Master : All the permanent members and several PhD students teach in the Master of Public Health (M1 Santé publique, M2 Biostatistique and/or M2 Epidemiology and/or M2 Public Health Data Science) and the Digital Public Health graduate program, University of Bordeaux.

Master : Marta Avalos, Robin Genuer, Louis Capitaine and Marine Gautier teach in the Master of Applied Mathematics and Statistics (1st and/or 2nd year), University of Bordeaux.

Master : Marta Avalos teaches in the 2nd year of the Master of “Management international : Développement pharmaceutique, Production et Qualité opérationnelle”, University of Bordeaux.

Bachelor: Laura Richert and Edouard Lhomme teach in PACES and DFASM1-3 for Medical degree at Univ. Bordeaux

Master: Hadrien Lorenzo teach in the third year engineering school ENSAI, Rennes and in the "Ecole Santé Science" Program (dual degree in Health and Science), University of Bordeaux.

Master: Laura Richert teaches in the Master of Vaccinology from basic immunology to social sciences of health (University Paris-Est Créteil, UPEC)

Teaching unit coordination: Laura Richert, Rodolphe Thiébaut, Robin Genuer, Boris Hejblum and Marta Avalos coordinate several teaching units of Master in Public Health (Biostatistics, Epidemiology, Public Health), M2 Public Health Data Science. Laura Richert coordinates the teaching unit "Experimental Designs" (M2 Epidemiology) and teaching unit "Omics Data" (M2 Public Health Data Science), University of Bordeaux

Internation summer school: Laura Richert coordinates the summer school course "Big data in immunology" University of Bordeaux. All permemanent team members teach in this course.

H Lorenzo participated to the University Course *Big data et statistique pour l'ingénieur (BDSI)*, Ecole Nationale Supérieure de Cognitique (ENSC), Bordeaux.

E-learning

Master: Marta Avalos is head of the first year of the e-learning program of the Master of Public Health, University of Bordeaux.

Master: Marta Avalos teaches in the e-learning program of the Master of Public Health (1st and 2nd year)

ODL University Course: Robin Genuer is head of the Diplôme universitaire "Méthodes statistiques en santé.

ODL University Course: Mélanie Prague teaches in the Diplôme universitaire "Méthodes statistiques de régression en épidémiologie".

ODL University Course: Laura Richert co-coordinates and teaches in the Diplôme universitaire "Recherche Clinique".

ODL University project: Robin Genuer participated to the IdEx Bordeaux University "Défi numérique" project "BeginR" (http://beginr.u-bordeaux.fr).

10.2.2. Supervision

HdR: Laura Richert, *Statistical approaches and methodological developments to optimize clinical vaccine research*, Université de Bordeaux, defence date 17th Dec 2019

PhD: Edouard Lhomme, *Analyse des déterminants de la réponse immunitaire post-vaccination dans des stratégies vaccinales expérimentales*, defence date 25th Nov, directed by Laura Richert

PhD: Hadrien Lorenzo, *Analyse supervisée multibloc en grande dimension*, defence date 27th Nov, co-directed by Rodolphe Thiébaut and Jérôme Saracco (CQFD team)

PhD: Perrine Soret, "Régression pénalisée de type Lasso pour l'analyse de données biologiques de grande dimension : application à la charge virale du VIH censurée par une limite de quantification et aux données compositionnelles du microbiote", Université de Bordeaux, defence date 28th Nov, supervisor: Marta Avalos

PhD: Soufiane Ajana "Comparison of linear and non-linear machine learning approaches to predict Age-related Macular Disease (AMD) risk in a survival framework", defense's date 4th Nov, co-supervised by Boris Hejblum and Hélène Jacqumin-Gadda (Inserm) and Cécile Delcourt (Inserm), from Sept 2016.

PhD in progress: Marie Alexandre "Mechanistic modeling and optimization of vaccine response in HIV and Ebola", co-directed by Mélanie Prague and Rodolphe Thiébaut, from Oct 2018.

PhD in progress: Marine Gauthier "Methods for bulk and single-cell RNA-seq data analysis in vaccine research", co-directed by Boris Hejblum and Rodolphe Thiébaut, from Sept 2018.

PhD in progress: Louis Capitaine, *Random forests for high-dimensional longitudinal data*, from Oct 2017, co-directed by Robin Genuer and Rodolphe Thiébaut.

PhD in progress: Madelyn Rojas *Self-management of injury risk and decision support systems based on predictive computer modelling. Development, implementation and evaluation in the MAVIE cohort study*, from Oct 2017, (Injury Epidemiology team, Inserm U1219, ED SP2) co-directed by Emmanuel Lagarde (Inserm) and Marta Avalos.

Several team's members supervised Master 2 (T. Alin, A. Devaux, G. Sotton, A. Herteau, T. Ferte) and Master 1 (V. Gasque, M.H. Ibrahim, C. Lemoigne, V. Kochegarov) internship students.

10.2.3. Juries

Boris Hejblum was involved in the PhD defence jury of Soufiane Ajana (university of Bordeaux).

Marta Avalos was involved in the PhD defence jury of Perrine Soret (University of Bordeaux).

Laura Richert was involved in the PhD defence jury of Edouard Lhomme (University of Bordeaux).

Robin Genuer was reviewer of the thesis of Antonio Sutera (University of Liège).

Rodolphe Thiébaut was involved in the PhD defence jury of Edouard Lhomme, Hadrien Lorenzo, Perrine Soret, Sophie Lefèvre-Arbogast, Corentin Segalas (University of Bordeaux), Simon Bussy, Hugo Arlegui, Jeanne Tamarelle (Paris), and Alban Caporossi (Lyon). He was also a reviewer of the HDR of Encarnita Mariotti-Ferrandiz (Sorbonne University, Paris) and took part in her defence jury.

Mélanie Prague was involved in the PhD defence jury of Chiara Nicolo (University of Bordeaux) and Steven Sanche (University of Montreal, CA)

Marta Avalos is a member of the follow-up dissertation committee of 2 PhD students: Alexandre Conanec (Statistics, IMB, ED MI) and Madelyn Rojas (Epidemiology, ED SP2).

Mélanie Prague is a member of the follow-up dissertation committee of 2 PhD students: Jonas Beal (Institut Curie) and Marie astrid Metten (University of Rennes).

Laura Richert, Rodolphe Thiébaut, Robin Genuer, Boris Hejblum, Edouard Lhomme and Marta Avalos participated to the juries of Master in Public Health (Biostatistics, Epidemiology, Public Health)

Robin Genuer and Marta Avalos participated to the juries of Master of Applied Mathematics and Statistics (2nd year), University of Bordeaux.

Edouard Lhomme participated to the juries of medical thesis defenses, Medical School of Bordeaux University

10.3. Popularization

10.3.1. Internal or external Inria responsibilities

Mélanie prague is part of two committees at Inria: "ADT - Aide au développement technologique" and "CER - Comission Emploi recherche".

10.3.2. Articles and contents

Mélanie Prague participated to the video reportage produced by the Inria's communication service

10.3.3. Interventions

Mélanie Prague participated at the "Fête de la Science" for high school students on October.

10.3.4. Internal action

R Thiébaut gave the talk "VIRUS EBOLA: Comment la modélisation permet d'aider au développement des vaccins ?" in November at "Unithé ou café", Inria BSO, Talence.

H Lorenzo presented a poster *Apprentissage supervisé pour données massives multi-blocs incomplètes* in the anual workshop (*JED*) of the Doctoral School of Societies, Politics and Public Health (ED SP2), University of Bordeaux.

11. Bibliography

Major publications by the team in recent years

[1] D. AGNIEL, B. P. HEJBLUM. *Variance component score test for time-course gene set analysis of longitudinal RNA-seq data*, in "Biostatistics", 2017, vol. 18, n^{o} 4, p. 589-604, https://hal.inria.fr/hal-01579077

[2] D. COMMENGES, C. ALKHASSIM, R. GOTTARDO, B. P. HEJBLUM, R. THIÉBAUT. *cytometree: A binary tree algorithm for automatic gating in cytometry analysis*, in "Cytometry Part A", 2018, vol. 93, n^{o} 11, p. 1132-1140, https://hal.inria.fr/hal-01887966

[3] D. COMMENGES, H. JACQMIN-GADDA.*Dynamical Biostatistical Models*, Chapman and Hall/CRC, 2015, https://hal.inria.fr/hal-01580149

[4] A. JARNE, D. COMMENGES, M. PRAGUE, Y. LEVY, R. THIÉBAUT.*Modeling CD4 + T cells dynamics in HIV-infected patients receiving repeated cycles of exogenous Interleukin 7*, in "Annals of Applied Statistics", 2017, https://hal.inria.fr/hal-01579008

[5] C. PASIN, F. DUFOUR, L. VILLAIN, H. ZHANG, R. THIÉBAUT.*Controlling IL-7 injections in HIV-infected patients*, in "Bulletin of Mathematical Biology", 2018

[6] M. PRAGUE, D. COMMENGES, J. M. GRAN, B. LEDERGERBER, J. YOUNG, H. FURRER, R. THIÉBAUT.*Dynamic models for estimating the effect of HAART on CD4 in observational studies: Application to the Aquitaine Cohort and the Swiss HIV Cohort Study*, in "Biometrics", 2017, https://hal.inria.fr/hal-01406614

[7] A. RECHTIEN, L. RICHERT, H. LORENZO, G. MARTRUS, B. P. HEJBLUM, C. DAHLKE, R. KASONTA, M. ZINSER, H. STUBBE, U. MATSCHL, A. LOHSE, V. KRÄHLING, M. EICKMANN, S. BECKER, R. THIÉBAUT, M. ALTFELD, M. ADDO.*Systems Vaccinology Identifies an Early Innate Immune Signature as a Correlate of Antibody Responses to the Ebola Vaccine rVSV-ZEBOV*, in "Cell Reports ", 2017, vol. 20, n^{o} 9, p. 2251 - 2261, https://hal.inria.fr/hal-01579246

[8] L. VILLAIN, D. COMMENGES, C. PASIN, M. PRAGUE, R. THIÉBAUT.*Adaptive protocols based on predictions from a mechanistic model of the effect of IL7 on CD4 counts*, in "Statistics in Medicine", 2018, vol. 38, n^{o} 2, p. 221-235

Publications of the year

Doctoral Dissertations and Habilitation Theses

[9] E. LHOMME.*Analysis of the determinants and modelisation of the post- vaccination immune response in experimental vaccine strategies*, Université de bordeaux, November 2019, https://hal.inria.fr/tel-02430642

[10] H. LORENZO.*Supervised analysis of high dimensional multiblock data*, Université de bordeaux, November 2019, https://hal.inria.fr/tel-02433612

[11] L. RICHERT.*Statistical approaches and methodological developments to optimize clinical vaccine research*, Université de Bordeaux, December 2019, Habilitation à diriger des recherches, https://hal.inria.fr/tel-02426909

[12] P. SORET.*Penalized Lasso regression for the analysis of high-dimensional biological data: application to HIV viral load censored by a limit of quantification and to microbiota compositional data*, Université de bordeaux, November 2019, https://hal.inria.fr/tel-02425113

Articles in International Peer-Reviewed Journal

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Project-Team STORM

STatic Optimizations, Runtime Methods

IN COLLABORATION WITH: Laboratoire Bordelais de Recherche en Informatique (LaBRI)

IN PARTNERSHIP WITH:
Institut Polytechnique de Bordeaux

Université de Bordeaux

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Distributed and High Performance Computing

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Project-Team STORM

Creation of the Team: 2015 January 01, updated into Project-Team: 2017 July 01

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A1.1.3. - Memory models
A1.1.4. - High performance computing
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2. Overall Objectives

2.1. Overall Objectives

A successful approach to deal with the complexity of modern architectures is centered around the use of runtime systems, to manage tasks dynamically, these runtime systems being either generic or specific to an application. Similarly, on the compiler side, optimizations and analyses are more aggressive in iterative compilation frameworks, suitable for library generations or DSL, in particular for linear algebra methods. To go beyond this state of the art and alleviate the difficulties for programming these machines, we believe it is necessary to provide inputs with richer semantics to runtime and compiler alike, and in particular by combining both approaches.

This general objective is declined into two sub-objectives, the first concerning the expression of parallelism itself, the second the optimization and adaptation of this parallelism by compilers and runtimes.

- Expressing parallelism: As shown in the following figure, we propose to work on parallelism expression through Domain Specific Languages, able to capture the essence of the algorithms used through usual parallel languages such as OpenCL, OpenMP and through high performance libraries. The DSLs will be driven by applications, with the idea to capture at the algorithmic level the parallelism of the problem and perform dynamic data layout adaptation, parallel and algorithmic optimizations. The principle here is to capture a higher level of semantics, enabling users to express not only parallelism but also different algorithms.

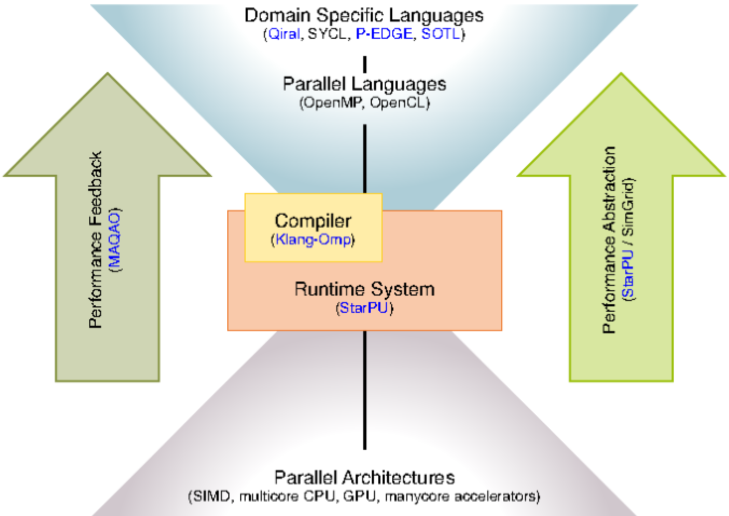

Figure 1. STORM Big Picture

- Optimizing and adapting parallelism: The goal here is to leverage the necessary adaptation to evolving hardware, by providing mechanisms allowing users to run the same code on different architectures. This implies to adapt parallelism, in particular the granularity of the work, to the architecture. This relies on the use of existing parallel libraries and their composition, and more generally the separation of concern between the description of tasks, that represent semantic units of work, and the tasks to be executed by the different processing units. Splitting or coarsening moldable tasks, generating code for these tasks and scheduling them is part of this work.

  Finally, the abstraction we advocate for requires to propose a feed back loop. This feed back has two objectives: To make users better understand their application and how to change the expression of parallelism if necessary, but also to propose an abstracted model for the machine. This allows to develop and formalize the compiling, scheduling techniques on a model, not too far from the real machine. Here, simulation techniques are a way to abstract the complexity of the architecture while preserving essential metrics.

3. Research Program

3.1. Parallel Computing and Architectures

Following the current trends of the evolution of HPC systems architectures, it is expected that future Exascale systems (i.e. Sustaining 10^{18} flops) will have millions of cores. Although the exact architectural details and trade-offs of such systems are still unclear, it is anticipated that an overall concurrency level of $O(10^9)$ threads/tasks will probably be required to feed all computing units while hiding memory latencies. It will obviously be a challenge for many applications to scale to that level, making the underlying system sound like “embarrassingly parallel hardware.”

From the programming point of view, it becomes a matter of being able to expose extreme parallelism within applications to feed the underlying computing units. However, this increase in the number of cores also comes with architectural constraints that actual hardware evolution prefigures: computing units will feature extra-wide SIMD and SIMT units that will require aggressive code vectorization or "SIMDization", systems will become hybrid by mixing traditional CPUs and accelerators units, possibly on the same chip as the AMD APU solution, the amount of memory per computing unit is constantly decreasing, new levels of memory will appear, with explicit or implicit consistency management, etc. As a result, upcoming extreme-scale system will not only require unprecedented amount of parallelism to be efficiently exploited, but they will also require that applications generate adaptive parallelism capable to map tasks over heterogeneous computing units.

The current situation is already alarming, since European HPC end-users are forced to invest in a difficult and time-consuming process of tuning and optimizing their applications to reach most of current supercomputers' performance. It will go even worse with the emergence of new parallel architectures (tightly integrated accelerators and cores, high vectorization capabilities, etc.) featuring unprecedented degree of parallelism that only too few experts will be able to exploit efficiently. As highlighted by the ETP4HPC initiative, existing programming models and tools won't be able to cope with such a level of heterogeneity, complexity and number of computing units, which may prevent many new application opportunities and new science advances to emerge.

The same conclusion arises from a non-HPC perspective, for single node embedded parallel architectures, combining heterogeneous multicores, such as the ARM big.LITTLE processor and accelerators such as GPUs or DSPs. The need and difficulty to write programs able to run on various parallel heterogeneous architectures has led to initiatives such as HSA, focusing on making it easier to program heterogeneous computing devices. The growing complexity of hardware is a limiting factor to the emergence of new usages relying on new technology.

3.2. Scientific and Societal Stakes

In the HPC context, simulation is already considered as a third pillar of science with experiments and theory. Additional computing power means more scientific results, and the possibility to open new fields of simulation requiring more performance, such as multi-scale, multi-physics simulations. Many scientific domains able to take advantage of Exascale computers, these "Grand Challenges" cover large panels of science, from seismic, climate, molecular dynamics, theoretical and astrophysics physics... Besides, embedded applications are also able to take advantage of these performance increase. There is still an on-going trend where dedicated hardware is progressively replaced by off-the-shelf components, adding more adaptability and lowering the cost of devices. For instance, Error Correcting Codes in cell phones are still hardware chips, but with the forthcoming 5G protocol, new software and adaptative solutions relying on low power multicores are also explored. New usages are also appearing, relying on the fact that large computing capacities are becoming more affordable and widespread. This is the case for instance with Deep Neural Networks where the training phase can be done on supercomputers and then used in embedded mobile systems. The same consideration applies for big data problems, of internet of things, where small sensors provide large amount of data that need to be processed in short amount of time. Even though the computing capacities required for such applications are in general a different scale from HPC infrastructures, there is still a need in the future for high performance computing applications.

However, the outcome of new scientific results and the development of new usages for mobile, embedded systems will be hindered by the complexity and high level of expertise required to tap the performance offered by future parallel heterogeneous architectures.

3.3. Towards More Abstraction

As emphasized by initiatives such as the European Exascale Software Initiative (EESI), the European Technology Platform for High Performance Computing (ETP4HPC), or the International Exascale Software Initiative (IESP), the HPC community needs new programming APIs and languages for expressing heterogeneous massive parallelism in a way that provides an abstraction of the system architecture and promotes high performance and efficiency. The same conclusion holds for mobile, embedded applications that require performance on heterogeneous systems.

This crucial challenge given by the evolution of parallel architectures therefore comes from this need to make high performance accessible to the largest number of developers, abstracting away architectural details providing some kind of performance portability, and provided a high level feed-back allowing the user to correct and tune the code. Disruptive uses of the new technology and groundbreaking new scientific results will not come from code optimization or task scheduling, but they require the design of new algorithms that require the technology to be tamed in order to reach unprecedented levels of performance.

Runtime systems and numerical libraries are part of the answer, since they may be seen as building blocks optimized by experts and used as-is by application developers. The first purpose of runtime systems is indeed to provide *abstraction*. Runtime systems offer a uniform programming interface for a specific subset of hardware (e.g., OpenGL or DirectX are well-established examples of runtime systems dedicated to hardware-accelerated graphics) or low-level software entities (e.g., POSIX-thread implementations). They are designed as thin user-level software layers that complement the basic, general purpose functions provided by the operating system calls. Applications then target these uniform programming interfaces in a portable manner. Low-level, hardware dependent details are hidden inside runtime systems. The adaptation of runtime systems is commonly handled through drivers. The abstraction provided by runtime systems thus enables portability. Abstraction alone is however not enough to provide portability of performance, as it does nothing to leverage low-level-specific features to get increased performance and does nothing to help the user tune his code. Consequently, the second role of runtime systems is to *optimize* abstract application requests by dynamically mapping them onto low-level requests and resources as efficiently as possible. This mapping process makes use of scheduling algorithms and heuristics to decide the best actions to take for a given metric and the application state at a given point in its execution time. This allows applications to readily benefit from available underlying low-level capabilities to their full extent without breaking their portability. Thus, optimization together with abstraction allows runtime systems to offer portability of performance. Numerical libraries provide sets of highly optimized kernels for a given field (dense or sparse linear algebra, FFT, etc.) either in an autonomous fashion or using an underlying runtime system.

Application domains cannot resort to libraries for all codes however, computation patterns such as stencils are a representative example of such difficulty. The compiler technology plays here a central role, in managing high level semantics, either through templates, domain specific languages or annotations. Compiler optimizations, and the same applies for runtime optimizations, are limited by the level of semantics they manage. Providing part of the algorithmic knowledge of an application, for instance knowing that it computes a 5-point stencil and then performs a dot product, would lead to more opportunities to adapt parallelism, memory structures, and is a way to leverage the evolving hardware. Besides, with the need for automatic optimization comes the need for *feed-back* to the user, corresponding to the need to debug the code and also to understand what the runtime has performed. Here the compiler plays also a central role in the analysis of the code, and the instrumentation of the program given to the runtime.

Compilers and runtime play a crucial role in the future of high performance applications, by defining the input language for users, and optimizing/transforming it into high performance code. The objective of STORM is to propose better interactions between compiler and runtime and more semantics for both approaches.

The results of the team on-going research in 2019 reflect this focus. Results presented in Sections 7.11, 7.15, 7.10 and 7.9 correspond to efforts for higher abstractions through DSL or libraries, and decouple algorithmics from parallel optimizations. Results in Section 7.8 correspond to efforts on parallelism expression and again abstraction, starting from standard parallel programming languages. Results described in Sections 7.1 and 7.16 provide feed-back information, through visualization and deadlock detection for parallel executions. The work described in Sections 7.3, 7.4, 7.5, 7.6,7.12, 7.7 and 7.13 focus in particular on StarPU and its development in order to better abstract architecture, resilience and optimizations. The work presented Section 7.2 aims to help developers with optimization.

Finally, Sections 7.14 and 7.17 present an on-going effort on improving the Chameleon library and strengthening its relation with StarPU and the NewMadeleine communication library. They represent real-life applications for the runtime methods we develop.

4. Application Domains

4.1. Application domains benefiting from HPC

The application domains of this research are the following:

- Bioinformatics (see ADT Gordon 9.2.2)
- Environment, in particular CO_2 capture (see Exa2PRO, 9.3.1)
- Health and heart disease analysis (see EXACARD, 9.2.1)
- Software infrastructures for Telecommunications (see AFF3CT, 7.9, 9.2.2)
- Aeronautics (collaboration with Airbus, J.-M. Couteyen)

4.2. Application in High performance computing/Big Data

Most of the research of the team has application in the domain of software infrastructure for HPC and BigData (ANR SOLHAR 9.2.1, Inria ADT SwLoc and Gordon 9.2.2, IPL HAC-SPECIS and BigData 9.2.3, PIA project ELCI 9.2, H2020 projects INTERTWinE and Exa2Pro 9.3.1 and PRACE project PRACE5IP 9.3.1).

5. Highlights of the Year

5.1. Highlights of the Year

- 1st year for the CoHPC team in collaboration with the Lawrence Berkeley National Lab. (9.4.1.1). A PhD student of the team obtained a joint postdoc with InriaSiliconValley at this lab to initiate the collaboration.

6. New Software and Platforms

6.1. Chameleon

KEYWORDS: Runtime system - Task-based algorithm - Dense linear algebra - HPC - Task scheduling

SCIENTIFIC DESCRIPTION: Chameleon is part of the MORSE (Matrices Over Runtime Systems @ Exascale) project. The overall objective is to develop robust linear algebra libraries relying on innovative runtime systems that can fully benefit from the potential of those future large-scale complex machines.

We expect advances in three directions based first on strong and closed interactions between the runtime and numerical linear algebra communities. This initial activity will then naturally expand to more focused but still joint research in both fields.

1. Fine interaction between linear algebra and runtime systems. On parallel machines, HPC applications need to take care of data movement and consistency, which can be either explicitly managed at the level of the application itself or delegated to a runtime system. We adopt the latter approach in order to better keep up with hardware trends whose complexity is growing exponentially. One major task in this project is to define a proper interface between HPC applications and runtime systems in order to maximize productivity and expressivity. As mentioned in the next section, a widely used approach consists in abstracting the application as a DAG that the runtime system is in charge of scheduling. Scheduling such a DAG over a set of heterogeneous processing units introduces a lot of new challenges, such as predicting accurately the execution time of each type of task over each kind of unit, minimizing data transfers between memory banks, performing data prefetching, etc. Expected advances: In a nutshell, a new runtime system API will be designed to allow applications to provide scheduling hints to the runtime system and to get real-time feedback about the consequences of scheduling decisions.

2. Runtime systems. A runtime environment is an intermediate layer between the system and the application. It provides low-level functionality not provided by the system (such as scheduling or management of the heterogeneity) and high-level features (such as performance portability). In the framework of this proposal, we will work on the scalability of runtime environment. To achieve scalability it is required to avoid all centralization. Here, the main problem is the scheduling of the tasks. In many task-based runtime environments the scheduler is centralized and becomes a bottleneck as soon as too many cores are involved. It is therefore required to distribute the scheduling decision or to compute a data distribution that impose the mapping of task using, for instance the so-called “owner-compute” rule. Expected advances: We will design runtime systems that enable an efficient and scalable use of thousands of distributed multicore nodes enhanced with accelerators.

3. Linear algebra. Because of its central position in HPC and of the well understood structure of its algorithms, dense linear algebra has often pioneered new challenges that HPC had to face. Again, dense linear algebra has been in the vanguard of the new era of petascale computing with the design of new algorithms that can efficiently run on a multicore node with GPU accelerators. These algorithms are called “communication-avoiding” since they have been redesigned to limit the amount of communication between processing units (and between the different levels of memory hierarchy). They are expressed through Direct Acyclic Graphs (DAG) of fine-grained tasks that are dynamically scheduled. Expected advances: First, we plan to investigate the impact of these principles in the case of sparse applications (whose algorithms are slightly more complicated but often rely on dense kernels). Furthermore, both in the dense and sparse cases, the scalability on thousands of nodes is still limited, new numerical approaches need to be found. We will specifically design sparse hybrid direct/iterative methods that represent a promising approach.

Overall end point. The overall goal of the MORSE associate team is to enable advanced numerical algorithms to be executed on a scalable unified runtime system for exploiting the full potential of future exascale machines.

FUNCTIONAL DESCRIPTION: Chameleon is a dense linear algebra software relying on sequential task-based algorithms where sub-tasks of the overall algorithms are submitted to a Runtime system. A Runtime system such as StarPU is able to manage automatically data transfers between not shared memory area (CPUs-GPUs, distributed nodes). This kind of implementation paradigm allows to design high performing linear algebra algorithms on very different type of architecture: laptop, many-core nodes, CPUs-GPUs, multiple nodes. For example, Chameleon is able to perform a Cholesky factorization (double-precision) at 80 TFlop/s on a dense matrix of order 400 000 (i.e. 4 min 30 s).

RELEASE FUNCTIONAL DESCRIPTION: Chameleon includes the following features:

- BLAS 3, LAPACK one-sided and LAPACK norms tile algorithms - Support QUARK and StarPU runtime systems and PaRSEC since 2018 - Exploitation of homogeneous and heterogeneous platforms through the use of BLAS/LAPACK CPU kernels and cuBLAS/MAGMA CUDA kernels - Exploitation of clusters of interconnected nodes with distributed memory (using OpenMPI)

- Participants: Cédric Castagnede, Samuel Thibault, Emmanuel Agullo, Florent Pruvost and Mathieu Faverge
- Partners: Innovative Computing Laboratory (ICL) - King Abdullha University of Science and Technology - University of Colorado Denver
- Contact: Emmanuel Agullo
- URL: https://gitlab.inria.fr/solverstack/chameleon

6.2. hwloc

Hardware Locality

KEYWORDS: NUMA - Multicore - GPU - Affinities - Open MPI - Topology - HPC - Locality

FUNCTIONAL DESCRIPTION: Hardware Locality (hwloc) is a library and set of tools aiming at discovering and exposing the topology of machines, including processors, cores, threads, shared caches, NUMA memory nodes and I/O devices. It builds a widely-portable abstraction of these resources and exposes it to applications so as to help them adapt their behavior to the hardware characteristics. They may consult the hierarchy of resources, their attributes, and bind task or memory on them.

hwloc targets many types of high-performance computing applications, from thread scheduling to placement of MPI processes. Most existing MPI implementations, several resource managers and task schedulers, and multiple other parallel libraries already use hwloc.

NEWS OF THE YEAR: hwloc 2.1 brought support for modern multi-die processors and memory-side caches. It also enhanced memory locality in heterogeneous memory architecture (e.g. with non-volatile memory DIMMs). The visualization of many-core platforms was also improved by factorizing objects when many of them are identical.

- Participants: Brice Goglin and Valentin Hoyet
- Partners: Open MPI consortium - Intel - AMD - IBM
- Contact: Brice Goglin
- Publications: hwloc: a Generic Framework for Managing Hardware Affinities in HPC Applications - Managing the Topology of Heterogeneous Cluster Nodes with Hardware Locality (hwloc) - A Topology-Aware Performance Monitoring Tool for Shared Resource Management in Multicore Systems - Exposing the Locality of Heterogeneous Memory Architectures to HPC Applications - Towards the Structural Modeling of the Topology of next-generation heterogeneous cluster Nodes with hwloc - On the Overhead of Topology Discovery for Locality-aware Scheduling in HPC - Memory Footprint of Locality Information on Many-Core Platforms - M&MMs: Navigating Complex Memory Spaces with hwloc
- URL: http://www.open-mpi.org/projects/hwloc/

6.3. KaStORS

The KaStORS OpenMP Benchmark Suite

KEYWORDS: Benchmarking - HPC - Task-based algorithm - Task scheduling - OpenMP - Data parallelism

FUNCTIONAL DESCRIPTION: The KaStORS benchmarks suite has been designed to evaluate implementations of the OpenMP dependent task paradigm, introduced as part of the OpenMP 4.0 specification.

- Participants: François Broquedis, Nathalie Furmento, Olivier Aumage, Philippe Virouleau, Pierrick Brunet, Samuel Thibault and Thierry Gautier
- Contact: Thierry Gautier
- URL: http://kastors.gforge.inria.fr/#!index.md

6.4. KStar

The KStar OpenMP Compiler

KEYWORDS: Source-to-source compiler - OpenMP - Task scheduling - Compilers - Data parallelism

FUNCTIONAL DESCRIPTION: The KStar software is a source-to-source OpenMP compiler for languages C and C++. The KStar compiler translates OpenMP directives and constructs into API calls from the StarPU runtime system or the XKaapi runtime system. The KStar compiler is virtually fully compliant with OpenMP 3.0 constructs. The KStar compiler supports OpenMP 4.0 dependent tasks and accelerated targets.

- Participants: Nathalie Furmento, Olivier Aumage, Philippe Virouleau and Samuel Thibault
- Contact: Olivier Aumage
- Publications: Bridging the gap between OpenMP and task-based runtime systems for the fast multipole method - Bridging the gap between OpenMP 4.0 and native runtime systems for the fast multipole method - Evaluation of OpenMP Dependent Tasks with the KASTORS Benchmark Suite
- URL: http://kstar.gforge.inria.fr/#!index.md

6.5. AFF3CT

A Fast Forward Error Correction Toolbox

KEYWORDS: High-Performance Computing - Signal processing - Error Correction Code

FUNCTIONAL DESCRIPTION: AFF3CT proposes high performance Error Correction algorithms for Polar, Turbo, LDPC, RSC (Recursive Systematic Convolutional), Repetition and RA (Repeat and Accumulate) codes. These signal processing codes can be parameterized in order to optimize some given metrics, such as Bit Error Rate, Bandwidth, Latency, ...using simulation. For the designers of such signal processing chain, AFF3CT proposes also high performance building blocks so to develop new algorithms. AFF3CT compiles with many compilers and runs on Windows, Mac OS X, Linux environments and has been optimized for x86 (SSE, AVX instruction sets) and ARM architectures (NEON instruction set).

- Authors: Adrien Cassagne, Bertrand Le Gal, Camille Leroux, Denis Barthou and Olivier Aumage
- Partner: IMS
- Contact: Adrien Cassagne
- Publications: AFF3CT: A Fast Forward Error Correction Toolbox! - AFF3CT : Un environnement de simulation pour le codage de canal - Toward High-Performance Implementation of 5G SCMA Algorithms - An Efficient, Portable and Generic Library for Successive Cancellation Decoding of Polar Codes - Beyond Gbps Turbo Decoder on Multi-Core CPUs - Energy Consumption Analysis of Software Polar Decoders on Low Power Processors - Fast and Flexible Software Polar List Decoders - Fast Simulation and Prototyping with AFF3CT
- URL: https://aff3ct.github.io/

6.6. MORSE

KEYWORDS: High performance computing - Matrix calculation - Fast multipole method - Runtime system

FUNCTIONAL DESCRIPTION: MORSE (Matrices Over Runtime Systems @ Exascale) is a scientific project, its objectives are to solve matrix problems on complex architectures, using runtime systems. More specifically, the goal is to write codes that reach a high level of performance for all architectures. The algorithms are written independently of the architecture, and the runtime system dispatches the different computational parts to the different computing units. This methodology has been validated on three classes of problems: dense linear algebra, sparse and dense, and fast multipole methods. The corresponding codes have been incorporated into several softwares, MAGMA, Pastix and ScalFMM.

- Contact: Emmanuel Agullo
- URL: http://icl.cs.utk.edu/morse/

6.7. SwLoc

Software Contexts for Locality

KEYWORDS: HPC - Locality - Contexts - Multicore - GPU

FUNCTIONAL DESCRIPTION: SwLoc is a library for flexible and generic partitioning of computing resources (processors, accelerators) to be able to co-excute confined parallel regions which can rely on different runtime systems (e.g. OpenMP, Intel TBB, StarPU, etc.). With all different hypervisor strategies, It is possible to adapt dynamically the computing resources of each context, in order to match each parallel region's need as closely as possible.

- Contact: Corentin Salingue
- URL: http://swloc.gforge.inria.fr/

6.8. VITE

Visual Trace Explorer

KEYWORDS: Visualization - Execution trace

FUNCTIONAL DESCRIPTION: ViTE is a trace explorer. It is a tool made to visualize execution traces of large parallel programs. It supports Pajé, a trace format created by Inria Grenoble, and OTF and OTF2 formats, developed by the University of Dresden and allows the programmer a simpler way to analyse, debug and/or profile large parallel applications.

- Participant: Mathieu Faverge
- Contact: Mathieu Faverge
- URL: http://vite.gforge.inria.fr/

6.9. PARCOACH

PARallel Control flow Anomaly CHecker

KEYWORDS: High-Performance Computing - Program verification - Debug - MPI - OpenMP - Compilation

SCIENTIFIC DESCRIPTION: PARCOACH verifies programs in two steps. First, it statically verifies applications with a data- and control-flow analysis and outlines execution paths leading to potential deadlocks. The code is then instrumented, displaying an error and synchronously interrupting all processes if the actual scheduling leads to a deadlock situation.

FUNCTIONAL DESCRIPTION: Supercomputing plays an important role in several innovative fields, speeding up prototyping or validating scientific theories. However, supercomputers are evolving rapidly with now millions of processing units, posing the questions of their programmability. Despite the emergence of more widespread and functional parallel programming models, developing correct and effective parallel applications still remains a complex task. As current scientific applications mainly rely on the Message Passing Interface (MPI) parallel programming model, new hardwares designed for Exascale with higher node-level parallelism clearly advocate for an MPI+X solutions with X a thread-based model such as OpenMP. But integrating two different programming models inside the same application can be error-prone leading to complex bugs - mostly detected unfortunately at runtime. PARallel COntrol flow Anomaly CHecker aims at helping developers in their debugging phase.

- Participants: Emmanuelle Saillard, Denis Barthou and Pierre Huchant
- Partner: CEA
- Contact: Emmanuelle Saillard
- Publications: Combining Static and Dynamic Validation of MPI Collective Communication - PARCOACH: Combining static and dynamic validation of MPI collective communications - Static Validation of Barriers and Worksharing Constructs in OpenMP Applications - Correctness Analysis of MPI-3 Non-Blocking Communications in PARCOACH - Static/Dynamic Validation of MPI Collective Communications in Multi-threaded Context - MPI Thread-Level Checking for MPI+OpenMP Applications - PARCOACH Extension for Hybrid Applications with Interprocedural Analysis - PARCOACH Extension for a Full-Interprocedural Collectives Verification - Multi-Valued Expression Analysis for Collective Checking
- URL: https://esaillar.github.io/PARCOACH/

6.10. StarPU

The StarPU Runtime System

KEYWORDS: Multicore - GPU - Scheduling - HPC - Performance

SCIENTIFIC DESCRIPTION: Traditional processors have reached architectural limits which heterogeneous multicore designs and hardware specialization (eg. coprocessors, accelerators, ...) intend to address. However, exploiting such machines introduces numerous challenging issues at all levels, ranging from programming models and compilers to the design of scalable hardware solutions. The design of efficient runtime systems for these architectures is a critical issue. StarPU typically makes it much easier for high performance libraries or compiler environments to exploit heterogeneous multicore machines possibly equipped with GPGPUs or Cell processors: rather than handling low-level issues, programmers may concentrate on algorithmic concerns.Portability is obtained by the means of a unified abstraction of the machine. StarPU offers a unified offloadable task abstraction named "codelet". Rather than rewriting the entire code, programmers can encapsulate existing functions within codelets. In case a codelet may run on heterogeneous architectures, it is possible to specify one function for each architectures (eg. one function for CUDA and one function for CPUs). StarPU takes care to schedule and execute those codelets as efficiently as possible over the entire machine. In order to relieve programmers from the burden of explicit data transfers, a high-level data management library enforces memory coherency over the machine: before a codelet starts (eg. on an accelerator), all its data are transparently made available on the compute resource.Given its expressive interface and portable scheduling policies, StarPU obtains portable performances by efficiently (and easily) using all computing resources at the same time. StarPU also takes advantage of the heterogeneous nature of a machine, for instance by using scheduling strategies based on auto-tuned performance models.

StarPU is a task programming library for hybrid architectures

The application provides algorithms and constraints: - CPU/GPU implementations of tasks - A graph of tasks, using either the StarPU's high level GCC plugin pragmas or StarPU's rich C API

StarPU handles run-time concerns - Task dependencies - Optimized heterogeneous scheduling - Optimized data transfers and replication between main memory and discrete memories - Optimized cluster communications

Rather than handling low-level scheduling and optimizing issues, programmers can concentrate on algorithmic concerns!

FUNCTIONAL DESCRIPTION: StarPU is a runtime system that offers support for heterogeneous multicore machines. While many efforts are devoted to design efficient computation kernels for those architectures (e.g. to implement BLAS kernels on GPUs), StarPU not only takes care of offloading such kernels (and implementing data coherency across the machine), but it also makes sure the kernels are executed as efficiently as possible.

- Participants: Corentin Salingue, Andra Hugo, Benoît Lize, Cédric Augonnet, Cyril Roelandt, François Tessier, Jérôme Clet-Ortega, Ludovic Courtès, Ludovic Stordeur, Marc Sergent, Mehdi Juhoor, Nathalie Furmento, Nicolas Collin, Olivier Aumage, Pierre-André Wacrenier, Raymond Namyst, Samuel Thibault, Simon Archipoff, Xavier Lacoste, Terry Cojean, Yanis Khorsi, Philippe Virouleau, LoÏc Jouans and Leo Villeveygoux
- Contact: Olivier Aumage
- Publications: Asynchronous Task-Based Execution of the Reverse Time Migration for the Oil and Gas Industry - A Compiler Algorithm to Guide Runtime Scheduling - Achieving high-performance with a sparse direct solver on Intel KNL - Modeling Irregular Kernels of Task-based codes: Illustration with the Fast Multipole Method - Scheduling of Dense Linear Algebra Kernels on Heterogeneous Resources - Critical resources management and scheduling under StarPU - Achieving High Performance on Supercomputers with a Sequential Task-based Programming Model - Programmation of heterogeneous architectures using moldable tasks - The StarPU Runtime System at Exascale ? : Scheduling and Programming over Upcoming Machines. - A Visual Performance Analysis Framework for Task-based Parallel Applications running on Hybrid Clusters - Analyzing Dynamic Task-Based Applications on Hybrid Platforms: An Agile Scripting Approach - Detecção de Anomalias de Desempenho em Aplicações de Alto Desempenho baseadas em Tarefas em Clusters Híbridos - Resource aggregation for task-based Cholesky Factorization on top of heterogeneous machines

- On Runtime Systems for Task-based Programming on Heterogeneous Platforms - Resource aggregation in task-based applications over accelerator-based multicore machines - Controlling the Memory Subscription of Distributed Applications with a Task-Based Runtime System - Exploiting Two-Level Parallelism by Aggregating Computing Resources in Task-Based Applications Over Accelerator-Based Machines - Exploiting Two-Level Parallelism by Aggregating Computing Resources in Task-Based Applications Over Accelerator-Based Machines - Achieving High Performance on Supercomputers with a Sequential Task-based Programming Model - Bridging the gap between OpenMP 4.0 and native runtime systems for the fast multipole method - Scalability of a task-based runtime system for dense linear algebra applications - Faithful Performance Prediction of a Dynamic Task-Based Runtime System for Heterogeneous Multi-Core Architectures - Towards seismic wave modeling on heterogeneous many-core architectures using task-based runtime system - Bridging the Gap between Performance and Bounds of Cholesky Factorization on Heterogeneous Platforms - Composing multiple StarPU applications over heterogeneous machines: A supervised approach - Evaluation of OpenMP Dependent Tasks with the KASTORS Benchmark Suite - A runtime approach to dynamic resource allocation for sparse direct solvers - Modeling and Simulation of a Dynamic Task-Based Runtime System for Heterogeneous Multi-Core Architectures - Toward OpenCL Automatic Multi-Device Support - Harnessing clusters of hybrid nodes with a sequential task-based programming model - Taking advantage of hybrid systems for sparse direct solvers via task-based runtimes - Modulariser les ordonnanceurs de tâches : une approche structurelle - Overview of Distributed Linear Algebra on Hybrid Nodes over the StarPU Runtime - StarPU-MPI: Task Programming over Clusters of Machines Enhanced with Accelerators - Modeling and Simulation of a Dynamic Task-Based Runtime System for Heterogeneous Multi-Core Architectures - Taking advantage of hybrid systems for sparse direct solvers via task-based runtimes - Adaptive Task Size Control on High Level Programming for GPU/CPU Work Sharing - Composing multiple StarPU applications over heterogeneous machines: a supervised approach - Implementation of FEM Application on GPU with StarPU - Le problème de la composition parallèle : une approche supervisée - Support exécutif scalable pour les architectures hybrides distribuées - SOCL: An OpenCL Implementation with Automatic Multi-Device Adaptation Support - C Language Extensions for Hybrid CPU/GPU Programming with StarPU - Programming Models and Runtime Systems for Heterogeneous Architectures - Programmation unifiée multi-accélérateur OpenCL - StarPU-MPI: Task Programming over Clusters of Machines Enhanced with Accelerators - Parallelization on Heterogeneous Multicore and Multi-GPU Systems of the Fast Multipole Method for the Helmholtz Equation Using a Runtime System - High-Level Support for Pipeline Parallelism on Many-Core Architectures - Programmability and Performance Portability Aspects of Heterogeneous Multi-/Manycore Systems - Programmation des architectures hétérogènes à l'aide de tâches divisibles - StarPU: a unified platform for task scheduling on heterogeneous multicore architectures - PEPPHER: Efficient and Productive Usage of Hybrid Computing Systems - The PEPPHER Approach to Programmability and Performance Portability for Heterogeneous many-core Architectures - Flexible runtime support for efficient skeleton programming on hybrid systems - LU Factorization for Accelerator-based Systems - QR Factorization on a Multicore Node Enhanced with Multiple GPU Accelerators - Programmation multi-accélérateurs unifiée en OpenCL - Détection optimale des coins et contours dans des bases d'images volumineuses sur architectures multicœurs hétérogènes - Association de modèles de programmation pour l'exploitation de clusters de GPUs dans le calcul intensif - Programming heterogeneous, accelerator-based multicore machines:current situation and main challenges - Scheduling Tasks over Multicore machines enhanced with acelerators: a Runtime System's Perspective - Composabilité de codes parallèles sur architectures hétérogènes - Data-Aware Task Scheduling on Multi-Accelerator based Platforms - Dynamically scheduled Cholesky factorization on multicore architectures with GPU accelerators. - StarPU: a Runtime System for Scheduling Tasks over Accelerator-Based Multicore Machines - StarPU : un support exécutif unifié pour les architectures multicoeurs hétérogènes - Automatic Calibration of Performance Models on Heterogeneous Multicore Architectures - StarPU: A Unified Platform for Task Scheduling on Heterogeneous Multicore Architectures - Exploiting the Cell/BE architecture with the StarPU unified runtime system -

Bridging the gap between OpenMP and task-based runtime systems for the fast multipole method - Composability of parallel codes on heterogeneous architectures - Are Static Schedules so Bad ? A Case Study on Cholesky Factorization - Scheduling of Linear Algebra Kernels on Multiple Heterogeneous Resources - Approximation Proofs of a Fast and Efficient List Scheduling Algorithm for Task-Based Runtime Systems on Multicores and GPUs - Resource aggregation for task-based Cholesky Factorization on top of modern architectures - Visual Performance Analysis of Memory Behavior in a Task-Based Runtime on Hybrid Platforms - Tolérance aux pannes dans l'exécution distribuée de graphes de tâches

- URL: http://starpu.gforge.inria.fr/

7. New Results

7.1. Multi-Valued Expression Analysis for Collective Checking

Determining if a parallel program behaves as expected on any execution is challenging due to non-deterministic executions. Static analysis helps to detect all execution paths that can be executed concurrently by identifying multi-valued expressions, i.e. expressions evaluated differently among processes. This can be used to find collective errors in parallel programs. The PARallel COntrol flow Anomaly CHecker (PARCOACH) framework has been extended with a multi-valued expressions detection to find such errors [9]. The new analysis corrects the previous one and analyzes parallel applications using MPI, OpenMP, UPC and CUDA.

7.2. Hiding the latency of MPI communication

As developers spend significant effort performing manual latency optimizations, the goal of Van Man Nguyen Ph.D Thesis is to automatically provide maximal communication overlap for MPI communication (collective, point-to-point and RMA Put/Get operations). A method that moves operations and their completion (e.g. Isend/Wait) as far apart as possible in the program while preserving memory consistency is under development.

7.3. Performance monitoring and Steering Framework

Two frameworks were developed within the context of the project H2020 EXA2PRO to offer performance monitoring and steering APIs into the StarPU runtime system, to be targeted by external tools.

The performance monitoring framework enables StarPU to export performance counters in a generic, safe, extensible way, to give external tools access to internal metrics and statistics, such as the peak number of tasks in the dependence waiting queue, the cumulated execution time by worker thread, and the number of ready tasks of a given kind waiting for an execution slot.

The performance steering framework defines a set of runtime-actionable knobs that can be used to steer the execution of an application on top of StarPU from an external tool, with similar properties of genericity, safety and extensibility as the performance monitoring framework.

7.4. Heterogeneous task scheduling

Taking advantage of heterogeneous systems requires to carefully choose which tasks should be accelerated. Simple heuristics allow to get fairly good performance, but do not have approximation ratio that would provide performance guarantees. The ROMA Inria team designed advanced heuristics which do have approximation ratios. We have implemented one within StarPU and indeed improved the performance over existing heuristics. The implementation required to revamp part of the StarPU toolkit dedicated to writing scheduling heuristics.

7.5. Task scheduling with memory constraints

When dealing with larger and larger datasets processed by task-based applications, the amount of system memory may become too small to fit the working set, depending on the task scheduling order. The ROMA Inria team proposed a heuristic to introduce additional dependencies to the task graph enough so that any scheduling order will meet the memory constraint, while avoiding to extend the critical path length. On the other hand, banker algorithms allow to achieve this online, within the task scheduler, but do not have an overall view of the task graph, and may thus severely increase the critical path. We have thus started to design a collaboration between visionary heuristics which take a global but coarse view of the task graph, and online heuristics which have a local but precise view of the task graph.

7.6. Leveraging compiler analysis for task scheduling

Polyhedral analysis of task graph submission loops allow to get at compilation time a representation of the task graph, and perform insightful analyses thanks to the obtained overview of the whole task graph. Task scheduling heuristics, on the other hand, usually keep only a limited view over the task graph, to avoid prohibitive algorithmic costs. We have started to collaborate with the CASH Inria team to transfer some of the insights of the compiler to the compiler. We have notably made the compiler automatically compute a cut of the task graph below which the availability parallelism is lower than the capacities of the target hardware. The scheduler can then at that point switch between a heuristic which privileges task acceleration, and a heuristic which privileges the critical path. Only preliminary results have been obtained so far.

7.7. Failure Tolerance for StarPU

Since supercomputers keep growing in terms of core numbers, the reliability decreases the same way. The project H2020 EXA2PRO aims to propose solutions for the failure tolerance problem, including StarPU. While exploring decades of research about the resilience techniques, we have identified properties in our runtime's paradigm that can be exploited in order to propose a solution with lower overhead than the generic existing ones. An implementation of a solution is currently being developed for evaluation, with an interface that can be easily plugged into StarPU.

7.8. Static and Dynamic Adaptation of Task parallelism

This work is the result of Pierre Huchant PhD thesis, and the objectives are to adapt statically and dynamically OpenCL tasks. The adaptation consists in splitting tasks automatically into multiple sub-tasks, taking into account the heterogeneity of the architecture (sub-tasks are specifically created for one processing unit), the load imbalance within a parallel OpenCL, between the different iterations in space, and if the task graph is repeatedly executed, between the iterations in time, and it takes into account the time of the communications generated by splitting the tasks [2]. The method is able to cope with sequential task graphs (tasks are parallel themselves but scheduled sequentially) and deals with tasks manipulating complex data structures as shown on an N-body particle simulation mini-app.

7.9. AFF3CT

The AFF3CT library, developed jointly between IMS and the STORM team, which aims to model error correcting codes for numerical communications has been further improved in different ways. Additional new algorithms have been designed and evaluated within the AFF3CT library [6], [7], and a new approach for generating and exploring automatically high performance error correction codes from matrix description is an on-going work. Besides, an on-going work is on the automatic parallelization of the tasks describing the simulation of a whole chain of signal transmission. In order to be able to make accessible the simulation results obtained with AFF3CT and to be able to replay easily the same simulations, a web interface allowing users to browse through the results, and the simulation setup for a large range of inputs has been designed. This graphical interface is currently in use at IMS by other researchers. Finally, a call for the creation of a consortium on AFF3CT is available on the web page of AFF3CT https://aff3ct.github.io/.

7.10. Matlab API for AFF3CT

As part of the AFF3CT development action, an API compatible with the Matlab mathematical software was designed on top of the AFF3CT fast forward error correction toolbox to allow the library to be used in a high-level manner, directly from the Matlab environment. Due to the relatively large number of classes exported by AFF3CT, an automatized process was designed to let AFF3CT classes be wrapped adequately for Matlab's MEX interface to external libraries.

7.11. InKS framework

The InKS framework was developed by Ksander Ejjaaouani as part of his Ph.D Thesis co-supervised by the university of Strasbourg, the Maison de la Simulation and the STORM team. It enables separating algorithms of time loop based scientific simulations into platform independent algorithms and platform specific optimisation files, thus enforcing separation of concerns between the algorithmic design process on one side, and the optimization process of specifying platform-dependent aspects such as operation ordering and memory placement on the other side.

7.12. HPC Big Data Convergence

A Java interface for StarPU has been implemented and allows to execute Map Reduce applications on top of StarPU. We have made some preliminary experiments on Cornac, a big data application for visualising huge graphs.

7.13. Hierarchical Tasks

We are continuing our work, on the partitioning of the data and the prioritization of task graphs to optimize the use of resources of a machine. Hierarchical tasks allow a better control over the submission of an application's task graph by allowing to dynamically adapt the granularity of the calculations. In the ANR project Solharis, hierarchical tasks are proposed as a solution for a better management of dynamic task graphs. We have continued to explore new solutions for maximizing the performance of hierarchical tasks.

7.14. ADT Gordon

In collaboration with the HIEPACS and TADAAM Inria teams, we are strengthening the relations between the Chameleon linear algebra library from HIEPACS, our StarPU runtime scheduler, and the NewMadeleine high-performance communication library from TADAAM. More precisely, we have improved the interoperation between StarPU and NewMadeleine, to more carefully decide when NewMadeleine should proceed with communications. We have then introduced the notion of dynamic collective operations, which opportunistically introduce communication trees to balance the communication load.

7.15. StarPU in Julia

Julia is a modern language for parallelism and simulation that aims to ease the effort for developing high performance codes. In this context, we carry on the development of a StarPU binding inside Julia. It is possible to launch StarPU tasks inside Julia, either given as libraries, or described in Julia directly. The tasks described in Julia are compiled into either source OpenMP code or CUDA code. We improved further the support of StarPU in Julia, but this is still a work in progress.

7.16. Simulation of OpenMP task based programs

A simulator for OpenMP task based programs is being designed as part of Inria's IPL HAC-Specis project, and the Ph.D Thesis of Idriss Daoudi. The goal is to extend the SimGrid HPC simulation framework with the ability to simulate OpenMP applications.

7.17. OpenMP enabled version of Chameleon

An OpenMP enabled version of the Chameleon linear algebra library was designed within the context of European Project PRACE-5IP. This enables the Chameleon library to be available on any platform for which an OpenMP compiler is installed, without any requirement for third party task-based runtime systems. A preliminary support of the OpenMP port for heterogeneous, accelerated platform was also designed as part of this work.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

- Contract with ATOS/Bull for the PhD CIFRE of Tassadit Célia Ait Kaci (2019-2021),
- Contract with Airbus for 1 year, renewable, on StarPU in Flusepa code (2019-), for the engineer contract of Alexis Juven,
- Contract with CEA for the PhD of Arthur Loussert (2017-2019), for the PhD of Van Man Nguyen (2019-2021) and other short contracts.

9. Partnerships and Cooperations

9.1. Regional Initiatives

HPC/Big-Data Convergence

- Team participants : Olivier Aumage, Nathalie Furmento, Samuel Thibault.
- Other participants : David Auber, Olivier Beaumont, Lionel Eyraud-Dubois, Gérald Point
- Abstract: The goal of this project is to gather teams from the HPC and Big Data communities to work at the intersection between these domains. We will focus on how StarPU can be adapted to achieve good performances on Big Data platforms.

9.2. National Initiatives

ELCI The ELCI PIA project (Software Environment for HPC) aims to develop a new generation of software stack for supercomputers, numerical solvers, runtime and programming development environments for HPC simulation. The ELCI project also aims to validate this software stack by showing its capacity to offer improved scalability, resilience, security, modularity and abstraction on real applications. The coordinator is Bull, and the different partners are CEA, Inria, SAFRAN, CERFACS, CNRS CORIA, CENAERO, ONERA, UVSQ, Kitware and AlgoTech.

9.2.1. ANR

ANR SOLHAR (http://solhar.gforge.inria.fr/doku.php?id=start).

ANR MONU 2013 Program, 2013 - 2018 (36 months extended)

Identification: ANR-13-MONU-0007

Coordinator: Inria Bordeaux/LaBRI

Other partners: CNRS-IRIT, Inria-LIP Lyon, CEA/CESTA, EADS-IW

Abstract: This project aims at studying and designing algorithms and parallel programming models for implementing direct methods for the solution of sparse linear systems on emerging computers equipped with accelerators. The ultimate aim of this project is to achieve the implementation of a software package providing a solver based on direct methods for sparse linear systems of equations. Several attempts have been made to accomplish the porting of these methods on such architectures; the proposed approaches are mostly based on a simple offloading of some computational tasks (the coarsest grained ones) to the accelerators and rely on fine hand-tuning of the code and accurate performance modeling to achieve efficiency. This project proposes an innovative approach which relies on the efficiency and portability of runtime systems, such as the StarPU tool developed in the runtime team (Bordeaux). Although the SOLHAR project will focus on heterogeneous computers equipped with GPUs due to their wide availability and affordable cost, the research accomplished on algorithms, methods and programming models will be readily applicable to other accelerator devices such as ClearSpeed boards or Cell processors.

ANR EXACARD

AAPG ANR 2018 (42 months)

Coordinator: Yves Coudière (Carmen) Inria Bordeaux

Abstract: Cardiac arrhythmia affect millions of patients and cause 300,000 deaths each year in Europe. Most of these arrhythmia are due to interaction between structural and electrophysiological changes in the heart muscle. A true understanding of these phenomena requires numerical simulations at a much finer resolution, and larger scale, than currently possible. Next-generation, heterogeneous, high-performance computing (HPC) systems provide the power for this. But the large scale of the computations pushes the limits of current runtime optimization systems, and together with task-based parallelism, prompts for the development of dedicated numerical methods and HPC runtime optimizations. With a consortium including specialists of these domains and cardiac modeling, we will investigate new task-based optimization techniques and numerical methods to utilize these systems for cardiac simulations at an unprecedented scale, and pave the way for future use cases.

9.2.2. ADT - Inria Technological Development Actions

ADT SwLoc (http://swloc.gforge.inria.fr/web/)

Participants: Raymond Namyst, Pierre-André Wacrenier, Andra Hugo, Brice Goglin, Corentin Salingue.

Inria ADT Campaign 2017, 10/2017 - 9/2019 (24 months)

Coordinator: Raymond Namyst

Abstract: The Inria action ADT SwLoc is aiming at developing a library allowing dynamic flexible partitioning of computing resources in order to execute parallel regions concurrently inside the same processes.

ADT Gordon

Participants: Denis Barthou, Nathalie Furmento, Samuel Thibault, Pierre-André Wacrenier.

Inria ADT Campaign 2018, 11/2018 - 11/2020 (24 months)

Coordinator: Emmanuel Jeannot (Tadaam)

Other partners: HiePACS, PLEIADE, Tadaam (Inria Bordeaux)

Abstract: Teams HiePACS, Storm and Tadaam develop each a brick of an HPC software stack, namely solver, runtime, and communication library. The goal of the Gordon project is to consolidate the HPC stack, to improve interfaces between each brick, and to target a better scalability. The bioinformatics application involved in the project has been selected so as to stress the underlying systems.

ADT AFF3CT Matlab

Participants: Denis Barthou, Olivier Aumage, Adrien Cassagne, Kun He.

Inria ADT Campaign 2018, 12/2018 - 12/2019 (12 months)

Coordinator: Denis Barthou

Other partners: C.Jégo and C.Leroux (IMS lab, U.Bordeaux)

Abstract: AFF3CT is a toolchain for designing, validation and experimentation of new Error Correcting codes. This toolchain is written in C++, and this constitutes a difficulty for many industrial users, who are mostly electronics engineers. The goal of this ADT is to widen the number of possible users by designing a Matlab and Python interface for AFF3CT, in collaboration with existing users, and proposing a parallel framework in OpenMP.

9.2.3. IPL - Inria Project Lab

HAC-SPECIS (High-performance Application and Computers, Studying PErformance and Correctness In Simulation)

Participants: Samuel Thibault, Emmanuelle Saillard, Olivier Aumage, Idriss Daoudi.

Inria IPL 2016 - 2020 (48 months)

Coordinator: Arnaud Legrand (team Polaris, Inria Rhône Alpes)

Since June 2016, the team is participating to the HAC-SPECIS http://hacspecis.gforge.inria.fr/ Inria Project Lab (IPL). This national initiative aims at answering methodological needs of HPC application and runtime developers and allowing to study real HPC systems both from the correctness and performance point of view. To this end, it gathers experts from the HPC, formal verification and performance evaluation community.

HPC-BigData (High Performance Computing and Big Data)

Participant: Samuel Thibault.

Inria IPL 2018 - 2022 (48 months)

Coordinator: Bruno Raffin (team DataMove, Inria Rhône Alpes)

Since June 2018, the team is participating to the HPC-BigData https://project.inria.fr/hpcbigdata/ Inria Project Lab (IPL). The goal of this HPC-BigData IPL is to gather teams from the HPC, Big Data and Machine Learning (ML) areas to work at the intersection between these domains. Research is organized along three main axes: high performance analytics for scientific computing applications, high performance analytics for big data applications, infrastructure and resource management.

9.3. European Initiatives

9.3.1. FP7 & H2020 Projects

Exa2PRO

- Title: Enhancing Programmability and boosting Performance Portability for Exascale Computing systems
- Program: H2020-FETHPC
- Duration: May 2018 - April 2021
- Coordinator: ICCS
- Inria contact: Samuel Thibault
- Partners:
  - Institute of Communications and Computer Systems (ICCS) (Greece)
  - Linköpiung University (LIU) (Sweden)
  - Centre for Research and Technology Hellas (CERTH) (Greece)

  * Institut National de Recherche en Informatique et en Automatique (Inria) (France)
  * Maxeler Technologies Limited (MAX) (UK)
  * Forschungszentrum Jülich (JUELICH) (Germany)
  * Centre National de la Recherche Scientifique (CNRS) (France)

The vision of EXA2PRO is to develop a programming environment that will enable the productive deployment of highly parallel applications in exascale computing systems. EXA2PRO programming environment will integrate tools that will address significant exascale challenges. It will support a wide range of scientific applications, provide tools for improving source code quality, enable efficient exploitation of exascale systems' heterogeneity and integrate tools for data and memory management optimization. Additionally, it will provide various fault-tolerance mechanisms, both user-exposed and at runtime system level and performance monitoring features. EXA2PRO will be evaluated using 4 use cases from 4 different domains, which will be deployed in JUELICH supercomputing center. The use cases will leverage the EXA2PRO tool-chain and we expect:

  * Increased applications performance based on EXA2PRO optimization tools (data and memory management)
  * Efficient exploitation of heterogeneity by the applications that will allow the evaluation of more complex problems.
  * Identification of trade-offs between design qualities (source code maintainability/reusability) and run-time constraints (performance/energy consumption).
  * Evaluation of various fault-tolerance mechanisms for applications with different characteristics.

EXA2PRO outcome is expected to have major impact in a) the scientific and industrial community that focuses on application deployment in supercomputing centers: EXA2PRO environment will allow efficient application deployment with reduced effort. b) on application developers of exascale application: EXA2PRO will provide tools for improving source code maintainability/ reusability, which will allow application evaluation with reduced developers' effort. c) on the scientific community and the industry relevant to the EXA2PRO use cases. At least two of the EXA2PRO use cases will have significant impact to the CO2 capture and to the Supercapacitors industry.

9.3.2. Collaborations in European Programs, Except FP7 & H2020

PRACE-5IP

- Title: PRACE 5th Implementation Phase
- Program: PRACE
- Duration: 2017 - 2019
- Coordinator: PRACE
- Inria contact for team STORM: Olivier Aumage
- Abstract: The objectives of PRACE-5IP are to build on and seamlessly continue the successes of PRACE and start new innovative and collaborative activities proposed by the consortium. These include:
  * assisting the transition to PRACE2 including analysis of TransNational Access;
  * strengthening the internationally recognised PRACE brand;
  * continuing and extend advanced training which so far provided more than 18 800 person-training days;
  * preparing strategies and best practices towards Exascale computing;

* coordinating and enhancing the operation of the multi-tier HPC systems and services;
* supporting users to exploit massively parallel systems and novel architectures.

A high level Service Catalogue is provided. The proven project structure will be used to achieve each of the objectives in 6 dedicated work packages. The activities are designed to increase Europe's research and innovation potential especially through:

* seamless and efficient Tier-0 services and a pan-European HPC ecosystem including national capabilities;
* promoting take-up by industry and new communities and special offers to SMEs;
* implementing a new flexible business model for PRACE 2;
* proposing strategies for deployment of leadership systems;
* collaborating with the ETP4HPC, CoEs and other European and international organisations on future architectures, training, application support and policies.

9.4. International Initiatives

9.4.1. Inria International Labs

Inria@SiliconValley

Associate Team involved in the International Lab:

9.4.1.1. COHPC

Title: Correctness and Performance of HPC Applications

International Partner (Institution - Laboratory - Researcher):

Lawrence Berkeley National Laboratory (United States) - Costin Iancu

Start year: 2019

See also: https://team.inria.fr/cohpc/

High Performance Computing (HPC) plays an important role in many fields like health, materials science, security or environment. The current supercomputer hardware trends lead to more complex HPC applications (heterogeneity in hardware and combinations of parallel programming models) that pose programmability challenges. As indicated by a recent US DOE report, progress to Exascale stresses the requirement for convenient and scalable debugging and optimization methods to help developers fully exploit the future machines; despite all recent advances these still remain manual complex tasks.

This collaboration aims to develop tools to aid developers with problems of correctness and performance in HPC applications for Exascale systems. There are several requirements for such tools: precision, scalability, heterogeneity and soundness. In order to improve developer productivity, we aim to build tools for guided code transformations (semi-automatic) using a combination of static and dynamic analysis. Static analysis techniques will enable soundness and scalability in execution time. Dynamic analysis techniques will enable precision, scalability in LoCs and heterogeneity for hybrid parallelism. A key aspect of the collaboration is to give precise feedback to developers in order to help them understand what happens in their applications and facilitate the debugging and optimization processes.

9.5. International Research Visitors

9.5.1. Visits of International Scientists

- Scott Baden, LBNL (USA), from April 29 to May 3, 2019

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Selection

10.1.1.1. Member of the Conference Program Committees

- Emmanuelle Saillard: Correctness workshop, Compas 2019, PPAM 2019, OMASE'19, 4PAD'19
- Olivier Aumage: SC Asia 2019, Euro-Par 2019, ICPADS 2019, PAW-ATM
- Samuel Thibault: HCW 19
- Raymond Namyst: SC 19, HiPC 19, CCGRID 19, ISC 19, ICCS 19, PPAM 19, RADR 19

10.1.1.2. Reviewer

STORM members have conducted reviewing activities for the following conferences and workshops: Correctness workshop, Compas, PPAM, OMASE, 4PAD, HCW 19

10.1.2. Journal

10.1.2.1. Reviewer - Reviewing Activities

STORM members have conducted reviewing activities for the following journals: JPDC, IEEE TII

10.1.3. Invited Talks

- Olivier Aumage: Cluster SysNum (Bordeaux, Jan. 24, 2019 and Mar. 8, 2019), 10-Year PlaFRIM (Bordeaux, May. 23, 2019), SPPEXA (Dresden, Germany, Oct. 21, 2019)
- Samuel Thibault: ENS Lyon seminar (Lyon, Jan 2019), ENS Lyon seminar (Lyon, May 2019), Workshop SIAM CSE (Spokane, Feb 2019), Workshop PADAL (Bordeaux, Sep 2019)
- Raymond Namyst: Aristote Seminar about "Toward ExaScale Computing" (Ecole Polytechnique, May 2019)

10.1.4. Scientific Expertise

- Olivier Aumage: Review of one project proposal for the French national research agency (ANR)
- Raymond Namyst: Scientific Advisor for CEA/DAM (French Department of Energy) HPC research groups

10.1.5. Research Administration

- Olivier Aumage: Permanent Contact for Team STORM.
- Emmanuelle Saillard: Member of the Commission de délégation at Inria Bordeaux Sud-Ouest

10.1.6. Standardization Activities

- Olivier Aumage represents Inria at the OpenMP ARB Standardization Committee.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

- Engineering School: Emmanuelle Saillard, Introduction to Algorithms, 16HeCI, L3, ENSEIRB-MATMECA.
- Engineering School: Emmanuelle Saillard, Tree Structure, 16HeCI, L3, ENSEIRB-MATMECA.
- Engineering School: Emmanuelle Saillard, Harmonisation, 10HeTD, L3, ENSEIRB-MATMECA.
- Engineering School: Emmanuelle Saillard, Languages of parallelism, 12HeC, M2, ENSEIRB-MATMECA.

- Engineering School: Adrien Cassagne, Microprocessors architecture, 20HeTD, L3, ENSEIRB-MATMECA.
- Engineering School: Romain Lion, System Programming, 18HeTD, M1, ENSEIRB-MATMECA.
- Licence: Marie-Christine Counilh, Introduction to Computer Science (64HeTD), Introduction to C programming (52HeTD), L1, University of Bordeaux.
- Master MIAGE: Marie-Christine Counilh, Object oriented programming in Java (30HeTD), M1, University of Bordeaux.
- Licence: Samuel Thibault is responsible for the computer science topic of the first university year.
- Licence: Samuel Thibault is responsible for the new Licence Pro ADSILLH (Administration et Développeur de Systèmes Informatiques à base de Logiciels Libres et Hybrides).
- Licence: Samuel Thibault is responsible for the 1st year of the computer science Licence.
- Licence: Samuel Thibault, Introduction to Computer Science, 32HeTD, L1, University of Bordeaux.
- Licence: Samuel Thibault, Networking, 51HeTD, Licence Pro, University of Bordeaux.
- Master: Samuel Thibault, Operating Systems, 24HeTD, L1, University of Bordeaux.
- Engineering School: Denis Barthou is the head of the computer science teaching department of ENSEIRB-MATMECA (300 students, 20 faculties, 120 external teachers)
- Engineering School: Denis Barthou, Architectures (L3), Parallel Architectures (M2), Procedural Generation for 3D Games (M2), C/Algorithm projects (L3)
- Licence, Pierre-André Wacrenier, is responsible for the 3rd year of the computer science Licence.
- Licence, Pierre-André Wacrenier, Introduction to Computer Science (64HeTD, L1), Systems Programming (64HeTD, L3), University of Bordeaux.
- Master, Pierre-André Wacrenier, Parallel Programming (64HeTD), University of Bordeaux.
- Raymond Namyst was involved in the introduction of Computer Science courses in the French High School (Lycée) scholar program. In particular, he was in charge of organizing a one-week condensed training session to 96 High School teachers on the following topics: Computer Architecture, Operating Systems, Networks and Robotics. The goal was to prepare then to teach computer science basics to students starting from September 2019, and to help them to prepare material for practice sessions.
- Denis Barthou was teacher for the previous courses, in Computer Architecture.

10.2.2. Supervision

- PhD in progress: Tassadit Célia Ait Kaci, March 2019, Emmanuelle Saillard, Marc Sergent, Denis Barthou
- PhD in progress: Paul Beziau, October 2018, Raymond Namyst
- PhD in progress: Adrien Cassagne, October 2017, Olivier Aumage, Denis Barthou, Christophe Jégo, Camille Leroux.
- PhD in progress: Idriss Daoudi, October 2018, Olivier Aumage, Thierry Gautier.
- PhD in progress: Romain Lion, October 2018, Samuel Thibault
- PhD in progress: Gwenolé Lucas, November 2019, Raymond Namyst, Abdou Guermouche
- PhD in progress: Van Man Nguyen, November 2019, Emmanuelle Saillard, Julien Jaeger, Denis Barthou, Patrick Carribault
- Internship: Firmin Martin, June 2019 - August 2019, Emmanuelle Saillard
- Internship: Radjasouria Vinayagame, November 2019 - January 2020, Emmanuelle Saillard
- Internship: Pierre-Antoine Rouby, May - July 2019 , Samuel Thibault
- Internship: Mehdi Naciri, January - August 2019, Adrien Cassagne, Denis Barthou

- Internship: Mael Keryell, January - April 2019, Denis Barthou
- Master's Thesis: Van Man Nguyen, January - September 2019 , Emmanuelle Saillard, Julien Jaeger, Denis Barthou, Patrick Carribault
- Master's Thesis: Gwenolé Lucas, March - Septembre 2019, Pierre-André Wacrenier, Abdou Guermouche, Mathieu Faverge
- PhD completed: Hugo Brunie, March 2019, Denis Barthou
- PhD completed: Pierre Huchant, March 2019, Denis Barthou
- PhD completed: Arthur Loussert, December 2019
- PhD completed: Raphaël Prat, October 2019

10.2.3. Juries

- Marie-Christine Counilh : Ph.D defense of Pierre Huchant at the University of Bordeaux, Mar. 2019 (member)
- Olivier Aumage : Ph.D defense of Ksander Ejjaaouani at the Maison de la simulation in Saclay, Oct. 25, 2019 (invited member)
- Denis Barthou was member of the following PhD/HdR committees:
  - PhD of Fabian Gruber (reviewer): "Debogage de performance pour code binaire: Analyse de sensitivité et profilage de dépendence", Grenoble Alpes University, December 2019
  - HdR of Guillaume Mercier (president): "Évolutions du passage de messages face aux défis de la gestion des topologies matérielles hiérarchiques", University of Bordeaux, December 2019
  - PhD of Maxime Schmitt (reviewer): "Génération automatique de codes adaptatifs", University of Strasbourg, September 2019
  - PhD of Gauthier Sornet (reviewer): "Parallélisme des calculs numériques appliqué aux géosciences", University of Orléans, September 2019
  - PhD of Youenn Lebras (president): "Code optimization based on source to source transformations using profile guided metrics", University of Paris Saclay, July 2019
  - PhD of Filip Arvid Jakobson (reviewer): "Static Analysis for BSPlib programs", University of Orléans, June 2019
  - PhD of Fotis Nicolaidis (president): "TROMOS: a SDK for virtual storage systems", University of Paris Saclay, May 2019
- Raymond Namyst was member of the following committees:
  - PhD of Benjamin Lorendeau (president): "Improving performance of a CFD code with unstructured meshes through multi level parallelism", University of Bordeaux, December 2019
  - PhD of Georgious Christodoulis (president): "Adapting a HPC runtime system to FPGAs", University of Grenoble, December 2019

10.3. Popularization

10.3.1. Internal or external Inria responsibilities

- Samuel Thibault : Organization of a meet-a-researcher day for ENS Lyon, December 2019

10.3.2. Interventions

- Emmanuelle Saillard, Raymond Namyst: Fête de la Science, Inria, October 2019.
- Emmanuelle Saillard: Printemps de la mixité, Inria, April 2019.
- Emmanuelle Saillard, Sabrina Duthil: Forum des métiers, Lycée des graves, April 2019.

- Emmanuelle Saillard: Moi Informaticienne - Moi Mathématicienne, University of Bordeaux, April 2019.
- Olivier Aumage, Nathalie Furmento, Emmanuelle Saillard, Adrien Cassagne: Welcoming ENS-Lyon undergraduate students, Inria, December 2019.
- Olivier Aumage, Marie-Christine Counilh, Emmanuelle Saillard, Kun He: Welcoming Schoolchildren, Inria, December 2019.

10.3.3. Creation of media or tools for science outreach

- Pierre-André Wacrenier and Raymond Namyst have developed a software platform named EasyPAP to provide students with an easy-to-use programming environment to quickly learn parallel programming (using Pthreads, OpenMP, OpenCL and MPI). The platform has a nice graphical interface which makes it suitable for showing the benefits of High Performance Computing to a broad audience. More information on the web site: https://gforgeron.gitlab.io/easypap/

11. Bibliography

Publications of the year

Doctoral Dissertations and Habilitation Theses

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[2] P. HUCHANT.*Static Analysis and Dynamic Adaptation of Parallelism*, Université de Bordeaux, March 2019, https://hal.inria.fr/tel-02429785

[3] A. LOUSSERT.*Understanding and Guiding the Computing Resource Management in a Runtime Stacking Context*, Université de Bordeaux, October 2019, https://hal.inria.fr/tel-02438652

[4] R. PRAT.*Dynamic load balancing on exaflop supercomputer applied to molecular dynamics*, Université de Bordeaux, October 2019, https://tel.archives-ouvertes.fr/tel-02413331

Articles in International Peer-Reviewed Journal

[5] A. CASSAGNE, O. HARTMANN, M. LEONARDON, K. HE, C. LEROUX, R. TAJAN, O. AUMAGE, D. BARTHOU, T. TONNELLIER, V. PIGNOLY, B. LE GAL, C. JEGO.*AFF3CT: A Fast Forward Error Correction Toolbox!*, in "SoftwareX", July 2019, vol. 10, 7, 100345 [*DOI :* 10.1016/J.SOFTX.2019.100345], https://hal.inria.fr/hal-02358306

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[9] P. HUCHANT, E. SAILLARD, D. BARTHOU, P. CARRIBAULT.*Multi-Valued Expression Analysis for Collective Checking*, in "EuroPar", Göttingen, Germany, August 2019, https://hal.archives-ouvertes.fr/hal-02390025

[10] L. LEANDRO NESI, S. THIBAULT, L. STANISIC, L. MELLO SCHNORR.*Visual Performance Analysis of Memory Behavior in a Task-Based Runtime on Hybrid Platforms*, in "CCGrid 2019 - 19th Annual IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing", Larnaca, Cyprus, IEEE, May 2019, p. 142-151 [*DOI :* 10.1109/CCGRID.2019.00025], https://hal.inria.fr/hal-02275363

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[11] R. LION.*Tolérance aux pannes dans l'exécution distribuée de graphes de tâches*, in "COMPAS'2019 - Conférence d'informatique en Parallélisme, Architecture et Système", Anglet, France, June 2019, https://hal.inria.fr/hal-02296118

Conferences without Proceedings

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[SWH-ID : swh:1:dir:b6e19d99449a78805e7a55a341fbaba2bc431973], Software, https://hal.inria.fr/hal-02443512

Project-Team TADAAM

Topology-aware system-scale data management for high-performance computing

IN COLLABORATION WITH: Laboratoire Bordelais de Recherche en Informatique (LaBRI)

IN PARTNERSHIP WITH:
Institut Polytechnique de Bordeaux

Université de Bordeaux

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Distributed and High Performance Computing

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Project-Team TADAAM

Creation of the Team: 2015 January 01, updated into Project-Team: 2017 December 01

Keywords:

Computer Science and Digital Science:

A1.1.1. - Multicore, Manycore
A1.1.2. - Hardware accelerators (GPGPU, FPGA, etc.)
A1.1.3. - Memory models
A1.1.4. - High performance computing
A1.1.5. - Exascale
A1.1.9. - Fault tolerant systems
A1.2. - Networks
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A2.2.5. - Run-time systems
A2.6.1. - Operating systems
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A3.1.2. - Data management, quering and storage
A3.1.3. - Distributed data
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A6.3.3. - Data processing
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Other Research Topics and Application Domains:

B6.3.2. - Network protocols
B6.3.3. - Network Management
B6.5. - Information systems
B9.5.1. - Computer science
B9.8. - Reproducibility

1. Team, Visitors, External Collaborators

Research Scientists

Emmanuel Jeannot [Team leader, Inria, Senior Researcher, HDR]

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Julien Herrmann [Inria, until Sep 2019]

2. Overall Objectives

2.1. Overall Objectives

In TADAAM, we propose a new approach where we allow the application to explicitly express its resource needs about its execution. The application needs to express its behavior, but in a different way from the compute-centric approach, as the additional information is not necessarily focused on computation and on instructions execution, but follows a high-level semantics (needs of large memory for some processes, start of a communication phase, need to refine the granularity, beginning of a storage access phase, description of data affinity, etc.). These needs will be expressed to a service layer though an API. The service layer will be system-wide (able to gather a global knowledge) and stateful (able to take decision based on the current request but also on previous ones). The API shall enable the application to access this service layer through a well-defined set of functions, based on carefully designed abstractions.

Hence, **the goal of** TADAAM **is to design a stateful system-wide service layer for HPC systems, in order to optimize applications execution according to their needs**.

This layer will abstract low-level details of the architecture and the software stack, and will allow applications to register their needs. Then, according to these requests and to the environment characteristics, this layer will feature an engine to optimize the execution of the applications at system-scale, taking into account the gathered global knowledge and previous requests.

This approach exhibits several key characteristics:

- It is independent from the application parallelization, the programming model, the numerical scheme and, largely, from the data layout. Indeed, high-level semantic requests can easily be added to the application code after the problem has been modeled, parallelized, and most of the time after the data layout has been designed and optimized. Therefore, this approach is – to a large extent – orthogonal to other optimization mechanisms and does not require application developers to rewrite their code.
- Application developers are the persons who know best their code and therefore the needs of their application. They can easily (if the interface is well designed and the abstractions are correctly exposed), express the application needs in terms of resource usage and interaction with the whole environment.

- Being stateful and shared by all the applications in the parallel environment, the proposed layer will therefore enable optimizations that:
  - cannot be performed statically but require information only known at launch- or run-time,
  - are incremental and require minimal changes to the application execution scheme,
  - deal with several parts of the environment at the same time (e.g., batch scheduler, I/O, process manager and storage),
  - take into account the needs of several applications at the same time and deal with their interaction. This will be useful, for instance, to handle network contention, storage access or any other shared resources.

3. Research Program

3.1. Need for System-Scale Optimization

Firstly, in order for applications to make the best possible use of the available resources, it is impossible to expose all the low-level details of the hardware to the program, as it would make impossible to achieve portability. Hence, the standard approach is to add intermediate layers (programming models, libraries, compilers, runtime systems, etc.) to the software stack so as to bridge the gap between the application and the hardware. With this approach, optimizing the application requires to express its parallelism (within the imposed programming model), organize the code, schedule and load-balance the computations, etc. In other words, in this approach, the way the code is written and the way it is executed and interpreted by the lower layers drives the optimization. In any case, this approach is centered on how computations are performed. Such an approach is therefore no longer sufficient, as the way an application is executing does depend less and less on the organization of computation and more and more on the way its data is managed.

Secondly, modern large-scale parallel platforms comprise tens to hundreds of thousand nodes [0]. However, very few applications use the whole machine. In general, an application runs only on a subset of the nodes [0]. Therefore, most of the time, an application shares the network, the storage and other resources with other applications running concurrently during its execution. Depending on the allocated resources, it is not uncommon that the execution of one application interferes with the execution of a neighboring one.

Lastly, even if an application is running alone, each element of the software stack often performs its own optimization independently. For instance, when considering an hybrid MPI/OpenMP application, one may realize that threads are concurrently used within the OpenMP runtime system, within the MPI library for communication progression, and possibly within the computation library (BLAS) and even within the application itself (pthreads). However, none of these different classes of threads are aware of the existence of the others. Consequently, the way they are executed, scheduled, prioritized does not depend on their relative roles, their locations in the software stack nor on the state of the application.

The above remarks show that in order to go beyond the state-of-the-art, it is necessary to design a new set of mechanisms allowing cross-layer and system-wide optimizations so as to optimize the way data is allocated, accessed and transferred by the application.

[0] More than 22,500 XE6 compute node for the BlueWaters system; 5040 B510 Bullx Nodes for the Curie machine; more than 49,000 BGQ nodes for the MIRA machine.

[0] In 2014, the median case was 2048 nodes for the BlueWaters system and, for the first year of the Curie machine, the median case was 256 nodes

3.2. Scientific Challenges and Research Issues

In TADAAM, we will tackle the problem of efficiently executing an application, at system-scale, on an HPC machine. We assume that the application is already optimized (efficient data layout, use of effective libraries, usage of state-of-the-art compilation techniques, etc.). Nevertheless, even a statically optimized application will not be able to be executed at scale without considering the following dynamic constraints: machine topology, allocated resources, data movement and contention, other running applications, access to storage, etc. Thanks to the proposed layer, we will provide a simple and efficient way for already existing applications, as well as new ones, to express their needs in terms of resource usage, locality and topology, using a high-level semantic.

It is important to note that we target the optimization of each application independently but also several applications at the same time and at system-scale, taking into account their resource requirement, their network usage or their storage access. Furthermore, dealing with code-coupling application is an intermediate use-case that will also be considered.

Several issues have to be considered. The first one consists in providing relevant **abstractions and models to describe the topology** of the available resources **and the application behavior**.

Therefore, the first question we want to answer is: **"How to build scalable models and efficient abstractions enabling to understand the impact of data movement, topology and locality on performance?"** These models must be sufficiently precise to grasp the reality, tractable enough to enable efficient solutions and algorithms, and simple enough to remain usable by non-hardware experts. We will work on (1) better describing the memory hierarchy, considering new memory technologies; (2) providing an integrated view of the nodes, the network and the storage; (3) exhibiting qualitative knowledge; (4) providing ways to express the multi-scale properties of the machine. Concerning abstractions, we will work on providing general concepts to be integrated at the application or programming model layers. The goal is to offer means, for the application, to express its high-level requirements in terms of data access, locality and communication, by providing abstractions on the notion of hierarchy, mesh, affinity, traffic metrics, etc.

In addition to the abstractions and the aforementioned models we need to **define a clean and expressive API in a scalable way**, in order for applications to express their needs (memory usage, affinity, network, storage access, model refinement, etc.).

Therefore, the second question we need to answer is: "**how to build a system-scale, stateful, shared layer that can gather applications needs expressed with a high-level semantic?**". This work will require not only to define a clean API where applications will express their needs, but also to define how such a layer will be shared across applications and will scale on future systems. The API will provide a simple yet effective way to express different needs such as: memory usage of a given portion of the code; start of a compute intensive part; phase where the network is accessed intensively; topology-aware affinity management; usage of storage (in read and/or write mode); change of the data layout after mesh refinement, etc. From an engineering point of view, the layer will have a hierarchical design matching the hardware hierarchy, so as to achieve scalability.

Once this has been done, the service layer, will have all the information about the environment characteristics and application requirements. We therefore need to design a set of **mechanisms to optimize applications execution**: communication, mapping, thread scheduling, data partitioning/mapping/movement, etc.

Hence, the last scientific question we will address is: "**How to design fast and efficient algorithms, mechanisms and tools to enable execution of applications at system-scale, in full a HPC ecosystem, taking into account topology and locality?**" A first set of research is related to thread and process placement according to the topology and the affinity. Another large field of study is related to data placement, allocation and partitioning: optimizing the way data is accessed and processed especially for mesh-based applications. The issues of transferring data across the network will also be tackled, thanks to the global knowledge we have on the application behavior and the data layout. Concerning the interaction with other applications, several directions will be tackled. Among these directions we will deal with matching process placement with resource allocation given by the batch scheduler or with the storage management: switching from a best-effort application centric strategy to global optimization scheme.

4. Application Domains

4.1. Mesh-based applications

TADAAM targets scientific simulation applications on large-scale systems, as these applications present huge challenges in terms of performance, locality, scalability, parallelism and data management. Many of these HPC applications use meshes as the basic model for their computation. For instance, PDE-based simulations using finite differences, finite volumes, or finite elements methods operate on meshes that describe the geometry and the physical properties of the simulated objects. This is the case for at least two thirds of the applications selected in the 9th PRACE. call [0], which concern quantum mechanics, fluid mechanics, climate, material physic, electromagnetism, etc.

Mesh-based applications not only represent the majority of HPC applications running on existing supercomputing systems, yet also feature properties that should be taken into account to achieve scalability and performance on future large-scale systems. These properties are the following:

Size Datasets are large: some meshes comprise hundreds of millions of elements, or even billions.

Dynamicity In many simulations, meshes are refined or coarsened at each time step, so as to account for the evolution of the physical simulation (moving parts, shockwaves, structural changes in the model resulting from collisions between mesh parts, etc.).

Structure Many meshes are unstructured, and require advanced data structures so as to manage irregularity in data storage.

Topology Due to their rooting in the physical world, meshes exhibit interesting topological properties (low dimensionality embedding, small maximum degree, large diameter, etc.). It is very important to take advantage of these properties when laying out mesh data on systems where communication locality matters.

All these features make mesh-based applications a very interesting and challenging use-case for the research we want to carry out in this project. Moreover, we believe that our proposed approach and solutions will contribute to enhance these applications and allow them to achieve the best possible usage of the available resources of future high-end systems.

5. Highlights of the Year

5.1. Highlights of the Year

- Guillaume PALLEZ was an invited speaker at the Royal Society https://royalsociety.org/science-events-and-lectures/2019/04/high-performance-computing/
- Brice GOGLIN is co-chair of the Architecture & Networks area of the SuperComputing 2020 conference.
- François PELLEGRINI has been re-appointed a member of the French *Commission Nationale de l'Informatique et des Libertés* (French data protection authority) by the President of the French Senate.

5.1.1. Awards

- Guillaume PALLEZ was one of the recipient of the IEEE Computer Society TCHPC Early Career Researchers Award for Excellence in High Performance Computing
- François PELLEGRINI was bestowed *Chevalier dans l'Ordre des Palmes Académiques* (Order of Academic Palms), promotion of July 2019.

6. New Software and Platforms

6.1. Hsplit

Hardware communicators split

[0] http://www.prace-ri.eu/prace-9th-regular-call/

KEYWORDS: MPI communication - Topology - Hardware platform

SCIENTIFIC DESCRIPTION: Hsplit is a library that implements an abstraction allowing the programmer using MPI in their parallel applications to access the underlying hardware structure through a hierarchy of communicators. Hsplit is based on the MPI_Comm_split_type routine and provides a new value for the split_type argument that specifically creates a hierarchy a subcommunicators where each new subcommunicator corresponds to a meaningful hardware level. The important point is that only the structure o the hardware is exploited and the number of levels or the levels names are not fixed so as to propose a solution independent from future hardware evolutions (such as new levels for instance). Another flavor of this MPI_Comm_split_type function is provided that creates a roots communicators at the same time a subcommunicator is produced, in order to ease the collective communication and/or synchronization among subcommunicators.

FUNCTIONAL DESCRIPTION: Hsplit implements an abstraction that allows the programmer using MPI in their parallel applications to access the underlying hardware structure through a hierarchy of communicators. Hsplit is based on the MPI_Comm_split_type routine and provides a new value for the split_type argument that specifically creates a hierarchy a subcommunicators where each new subcommunicator corresponds to a meaningful hardware level. The important point is that only the structure o the hardware is exploited and the number of levels or the levels names are not fixed so as to propose a solution independent from future hardware evolutions (such as new levels for instance). Another flavor of this MPI_Comm_split_type function is provided that creates a roots communicators at the same time a subcommunicator is produced, in order to ease the collective communication and/or synchronization among subcommunicators.

NEWS OF THE YEAR: Most of our proposal had been officially read in front of the MPI Forum at the last physical meeting in December at Albuquerque. This concerns hte guided and the unguided mode of the split function. This now has to pass two votes in the next physical meetings in 2020 to be part of the new version of the standard: MPI 4.0 that shall be ratified and released at the end of 2020. Since no other MPI library currently implements the unguided mode, Hsplit will be the only sofware that is currently able to provide it.

- Participants: Guillaume Mercier, Brice Goglin and Emmanuel Jeannot
- Contact: Guillaume Mercier
- Publications: A hierarchical model to manage hardware topology in MPI applications - A Hierarchical Model to Manage Hardware Topology in MPI Applications
- URL: http://mpi-topology.gforge.inria.fr/

6.2. hwloc

Hardware Locality

KEYWORDS: NUMA - Multicore - GPU - Affinities - Open MPI - Topology - HPC - Locality

FUNCTIONAL DESCRIPTION: Hardware Locality (hwloc) is a library and set of tools aiming at discovering and exposing the topology of machines, including processors, cores, threads, shared caches, NUMA memory nodes and I/O devices. It builds a widely-portable abstraction of these resources and exposes it to applications so as to help them adapt their behavior to the hardware characteristics. They may consult the hierarchy of resources, their attributes, and bind task or memory on them.

hwloc targets many types of high-performance computing applications, from thread scheduling to placement of MPI processes. Most existing MPI implementations, several resource managers and task schedulers, and multiple other parallel libraries already use hwloc.

NEWS OF THE YEAR: hwloc 2.1 brought support for modern multi-die processors and memory-side caches. It also enhanced memory locality in heterogeneous memory architecture (e.g. with non-volatile memory DIMMs). The visualization of many-core platforms was also improved by factorizing objects when many of them are identical.

- Participants: Brice Goglin and Valentin Hoyet
- Partners: Open MPI consortium - Intel - AMD - IBM

- Contact: Brice Goglin
- Publications: hwloc: a Generic Framework for Managing Hardware Affinities in HPC Applications - Managing the Topology of Heterogeneous Cluster Nodes with Hardware Locality (hwloc) - A Topology-Aware Performance Monitoring Tool for Shared Resource Management in Multicore Systems - Exposing the Locality of Heterogeneous Memory Architectures to HPC Applications - Towards the Structural Modeling of the Topology of next-generation heterogeneous cluster Nodes with hwloc - On the Overhead of Topology Discovery for Locality-aware Scheduling in HPC - Memory Footprint of Locality Information on Many-Core Platforms - M&MMs: Navigating Complex Memory Spaces with hwloc
- URL: http://www.open-mpi.org/projects/hwloc/

6.3. NetLoc

Network Locality

KEYWORDS: Topology - Locality - Distributed networks - HPC - Parallel computing - MPI communication

FUNCTIONAL DESCRIPTION: netloc (Network Locality) is a library that extends hwloc to network topology information by assembling hwloc knowledge of server internals within graphs of inter-node fabrics such as Infiniband, Intel OmniPath or Cray networks.

Netloc builds a software representation of the entire cluster so as to help applications properly place their tasks on the nodes. It may also help communication libraries optimize their strategies according to the wires and switches.

Netloc targets the same challenges as hwloc but focuses on a wider spectrum by enabling cluster-wide solutions such as process placement. It interoperates with the Scotch graph partitioner to do so.

Netloc is distributed within hwloc releases starting with hwloc 2.0.

- Participants: Brice Goglin, Clément Foyer and Cyril Bordage
- Contact: Brice Goglin
- Publications: netloc: Towards a Comprehensive View of the HPC System Topology - Netloc: a Tool for Topology-Aware Process Mapping
- URL: http://www.open-mpi.org/projects/netloc/

6.4. NewMadeleine

NewMadeleine: An Optimizing Communication Library for High-Performance Networks

KEYWORDS: High-performance calculation - MPI communication

FUNCTIONAL DESCRIPTION: NewMadeleine is the fourth incarnation of the Madeleine communication library. The new architecture aims at enabling the use of a much wider range of communication flow optimization techniques. Its design is entirely modular: drivers and optimization strategies are dynamically loadable software components, allowing experimentations with multiple approaches or on multiple issues with regard to processing communication flows.

The optimizing scheduler SchedOpt targets applications with irregular, multi-flow communication schemes such as found in the increasingly common application conglomerates made of multiple programming environments and coupled pieces of code, for instance. SchedOpt itself is easily extensible through the concepts of optimization strategies (what to optimize for, what the optimization goal is) expressed in terms of tactics (how to optimize to reach the optimization goal). Tactics themselves are made of basic communication flows operations such as packet merging or reordering.

The communication library is fully multi-threaded through its close integration with PIOMan. It manages concurrent communication operations from multiple libraries and from multiple threads. Its MPI implementation MadMPI fully supports the MPI_THREAD_MULTIPLE multi-threading level.

- Participants: Alexandre Denis, Clément Foyer, Nathalie Furmento, Raymond Namyst, Adrien Guilbaud, Florian Reynier and Philippe Swartvagher
- Contact: Alexandre Denis
- Publications: NewMadeleine: a Fast Communication Scheduling Engine for High Performance Networks - Ordonnancement et qualité de service pour réseaux rapides - Improving Reactivity and Communication Overlap in MPI using a Generic I/O Manager - PIOMan : un gestionnaire d'entrées-sorties générique - A multithreaded communication engine for multicore architectures - A multicore-enabled multirail communication engine - About the interactions between communication and thread scheduling in clusters of multicore machines - Scalability of the NewMadeleine Communication Library for Large Numbers of MPI Point-to-Point Requests - An analysis of the impact of multi-threading on communication performance - A scalable and generic task scheduling system for communication libraries - A Generic and High Performance Approach for Fault Tolerance in Communication Library - A High-Performance Superpipeline Protocol for InfiniBand - A sampling-based approach for communication libraries auto-tuning - High performance checksum computation for fault-tolerant MPI over InfiniBand - pioman: a Generic Framework for Asynchronous Progression and Multithreaded Communications - pioman: a pthread-based Multithreaded Communication Engine - Updating MadMPI to MPI-3: Remote Memory Access - Portage de StarPU sur la bibliothèque de communication NewMadeleine
- URL: http://pm2.gforge.inria.fr/newmadeleine/

6.5. PaMPA

Parallel Mesh Partitioning and Adaptation

KEYWORDS: Dynamic load balancing - Unstructured heterogeneous meshes - Parallel remeshing - Subdomain decomposition - Parallel numerical solvers

SCIENTIFIC DESCRIPTION: PaMPA is a parallel library for handling, redistributing and remeshing unstructured meshes on distributed-memory architectures. PaMPA dramatically eases and speeds-up the development of parallel numerical solvers for compact schemes. It provides solver writers with a distributed mesh abstraction and an API to: - describe unstructured and possibly heterogeneous meshes, on the form of a graph of interconnected entities of different kinds (e.g. elements, faces, edges, nodes), - attach values to the mesh entities, - distribute such meshes across processing elements, with an overlap of variable width, - perform synchronous or asynchronous data exchanges of values across processing elements, - describe numerical schemes by means of iterators over mesh entities and their connected neighbors of a given kind, - redistribute meshes so as to balance computational load, - perform parallel dynamic remeshing, by applying adequately a user-provided sequential remesher to relevant areas of the distributed mesh.

PaMPA runs concurrently multiple sequential remeshing tasks to perform dynamic parallel remeshing and redistribution of very large unstructured meshes. E.g., it can remesh a tetrahedral mesh from 43Melements to more than 1Belements on 280 Broadwell processors in 20 minutes.

FUNCTIONAL DESCRIPTION: Parallel library for handling, redistributing and remeshing unstructured, heterogeneous meshes on distributed-memory architectures. PaMPA dramatically eases and speeds-up the development of parallel numerical solvers for compact schemes.

NEWS OF THE YEAR: PaMPA has been used to remesh an industrial mesh of a helicopter turbine combustion chamber, up to more than 1 billion elements.

- Participants: Cécile Dobrzynski, Cedric Lachat and François Pellegrini
- Partners: Université de Bordeaux - CNRS - IPB
- Contact: François Pellegrini
- URL: http://project.inria.fr/pampa/

6.6. TopoMatch

KEYWORDS: Intensive parallel computing - High-Performance Computing - Hierarchical architecture - Placement

SCIENTIFIC DESCRIPTION: TreeMatch embeds a set of algorithms to map processors/cores in order to minimize the communication cost of the application.

Important features are : the number of processors can be greater than the number of applications processes , it assumes that the topology is a tree and does not require valuation of the topology (e.g. communication speeds) , it implements different placement algorithms that are switched according to the input size.

Some core algorithms are parallel to speed-up the execution. Optionally embeds scotch for fix-vertex mapping. enable exhaustive search if required. Several metric mapping are computed. Allow for oversubscribing of ressources. multithreaded.

TreeMatch is integrated into various software such as the Charm++ programming environment as well as in both major open-source MPI implementations: Open MPI and MPICH2.

FUNCTIONAL DESCRIPTION: TreeMatch is a library for performing process placement based on the topology of the machine and the communication pattern of the application.

- Participants: Adele Villiermet, Emmanuel Jeannot, François Tessier, Guillaume Mercier and Pierre Celor
- Partners: Université de Bordeaux - CNRS - IPB
- Contact: Emmanuel Jeannot
- URL: http://treematch.gforge.inria.fr/

6.7. SCOTCH

KEYWORDS: Mesh partitioning - Domain decomposition - Graph algorithmics - High-performance calculation - Sparse matrix ordering - Static mapping

FUNCTIONAL DESCRIPTION: Scotch is a graph partitioner. It helps optimise the division of a problem, by means of a graph, into a set of independent sub-problems of equivalent sizes. These sub-problems can also be solved in parallel.

RELEASE FUNCTIONAL DESCRIPTION: Version 6.0 offers many new features:

sequential graph repartitioning

sequential graph partitioning with fixed vertices

sequential graph repartitioning with fixed vertices

new, fast, direct k-way partitioning and mapping algorithms

multi-threaded, shared memory algorithms in the (formerly) sequential part of the library

exposure in the API of many centralized and distributed graph handling routines

embedded pseudo-random generator for improved reproducibility

and even more...

NEWS OF THE YEAR: In 2019, several versions of Scotch have been released, from v6.0.7 up to v6.0.9. While they are mostly bugfix updates, several new features and API routines have been added, to increase its use by third-party software, notably routines handling target topologies. Also, code quality has been improved by the addition of many tests in the continuous integration process. A new graphical system has been developed by Amaury Jacques (Inria intern, Feb.-May 2019) to display differences in result quality across versions and builds. This system has been adopted by other Inria projects.

- Participants: François Pellegrini, Sébastien Fourestier, Jun-Ho Her, Cédric Chevalier and Amaury Jacques

- Partners: Université de Bordeaux - IPB - CNRS - Region Aquitaine
- Contact: François Pellegrini
- Publications: Process Mapping onto Complex Architectures and Partitions Thereof - Multi-criteria Graph Partitioning with Scotch - Adaptation au repartitionnement de graphes d'une méthode d'optimisation globale par diffusion - Contributions au partitionnement de graphes parallèle multi-niveaux - A parallelisable multi-level banded diffusion scheme for computing balanced partitions with smooth boundaries - PT-Scotch: A tool for efficient parallel graph ordering - Design and implementation of efficient tools for parallel partitioning and distribution of very large numerical problems - Improvement of the Efficiency of Genetic Algorithms for Scalable Parallel Graph Partitioning in a Multi-Level Framework - PT-Scotch : Un outil pour la renumérotation parallèle efficace de grands graphes dans un contexte multi-niveaux - PT-Scotch: A tool for efficient parallel graph ordering
- URL: http://www.labri.fr/~pelegrin/scotch/

6.8. disk-revolve

KEYWORDS: Automatic differentiation - Gradients - Machine learning

FUNCTIONAL DESCRIPTION: This software provides several algorithms (Disk-Revolve, 1D-Revolve, Periodic-Disk-Revolve,...) computing the optimal checkpointing strategy when executing a adjoin chain with limited memory. The considered architecture has a level of limited memory that is free to access (writing and reading costs are negligible) and a level of unlimited memory with non-negligible access costs. The algorithms describe which data should be saved in the memory to minimize the number of re-computation during the execution.

- Authors: Guillaume Aupy and Julien Herrmann
- Contact: Julien Herrmann
- Publications: H-Revolve: A Framework for Adjoint Computation on Synchrone Hierarchical Platforms - Periodicity in optimal hierarchical checkpointing schemes for adjoint computations - Optimal Multistage Algorithm for Adjoint Computation
- URL: https://gitlab.inria.fr/adjoint-computation/disk-revolve-public

7. New Results

7.1. Management of heterogeneous and non-volatile memories in HPC

The emergence of non-volatile memory that may be used either as fast storage or slow high-capacity memory brings many opportunities for application developers.

We studied the impact of those new technologies on the allocation of resources in HPC platforms. We showed that co-scheduling HPC applications will possibly different needs in term of storage and memories brings constraints of the way non-volatile memory should be exposed by the hardware and operating system to bring both flexibility and performance. [21]

We also worked with Lawrence Livermore National Lab to propose an API to help application choose between the different kinds of available memory (high-bandwidth (HBM), normal (DDR), slow (non-volatile)). We exposed several useful criteria for selecting target memories as well as ways to rank them. [22]

7.2. Modeling and Visualizing Many-core HPC Platforms

As the number of cores keeps increasing inside processors, new kinds of hierarchy are added to organize and interconnect them. We worked with Intel to leverage new groups of cores such as *Dies* in newest Xeon Advanced Performance models. We also designed ways to clarify the modeling and visualisation of those many cores by factorizing identical parts of the platforms.

7.3. Co-scheduling HPC workloads on cache-partitioned CMP platforms

Co-scheduling techniques are used to improve the throughput of applications on chip multiprocessors (CMP), but sharing resources often generates critical interferences.

In collaboration with ENS Lyon and Georgia Tech, we looked at the interferences in the last level of cache (LLC) and use the *Cache Allocation Technology* (CAT) recently provided by Intel to partition the LLC and give each co-scheduled application their own cache area.

We considered m iterative HPC applications running concurrently and answer the following questions: (i) how to precisely model the behavior of these applications on the cache partitioned platform? and (ii) how many cores and cache fractions should be assigned to each application to maximize the platform efficiency? Here, platform efficiency is defined as maximizing the performance either globally, or as guaranteeing a fixed ratio of iterations per second for each application. Through extensive experiments using CAT, we demonstrated the impact of cache partitioning when multiple HPC application are co-scheduled onto CMP platforms. [2]

7.4. Modeling High-throughput Applications for in situ Analytics

In this work [3], we proposed to model HPC applications in the framework of in situ analytics. Typically, an HPC application is composed of a simulation tasks (data and compute intensive), and a set of analysis tasks that post-process the data. Currently, the performance of the I/O system in HPC platform prohibits the storage of all simulation data to process analysis post-mortem. Hence, in situ framework proposes to treat the data "on the fly", directly where it is produced. Hence, it leverages the amount of data to store as we only keep the result of analytics phase. However, simulation and analysis have to be scheduled in parallel and compete for shared resources. It generates resource conflicts and can lead to severe performance degradation for the simulation.

Hence, we proposed to model both platform (number of nodes and cores, memory, etc) and application (profile of each tasks) in order to optimize the execution of such applications. We propose a resource partitioning model that affects computational resources to the different tasks, as so as a scheduling of those tasks in order to maximize resource usage and minimize total application makespan. Tasks are assumed to be fully parallel to solve the partitioning problem.

We evaluated different scheduling heuristics combined to the resource partitioning model and show important features that influence in situ analytics performance.

This work is done in collaboration with Bruno RAFFIN from Inria team DATAMOVE of Inria Grenoble.

7.5. Modeling Non-Uniform Memory Access and Heterogeneous Memories on Large Compute Nodes with the Cache-Aware Roofline Model

The trend of increasing the number of cores on-chip is enlarging the gap between compute power and memory performance. This issue leads to design systems with heterogeneous memories, creating new challenges for data locality. Before the release of those memory architectures, the Cache-Aware Roofline Model [43] (CARM) offered an insightful model and methodology to improve application performance with knowledge of the cache memory subsystem.

With the help of the HWLOC library, we are able to leverage the machine topology to extend the CARM for modeling NUMA and heterogeneous memory systems, by evaluating the memory bandwidths between all combinations of cores and NUMA nodes. The new Locality Aware Roofline Model [6] (LARM) scopes most contemporary types of large compute nodes and characterizes three bottlenecks typical of those systems, namely contention, congestion and remote access. We also designed a hybrid memory bandwidth model to better estimate the roof when heterogeneous memories are involved or when read and write bandwidths differ.

We also developed an hybrid bandwidth model that combines the performance of different memories and their respective read/write bandwidth with the application memory access pattern to predict the performance of these accesses on heterogeneous memory platforms.

This work has been achieved in collaboration with the authors of the CARM from University of Lisbon.

7.6. Statistical Learning for Task and Data Placement in NUMA Architecture

Achieving high performance for multi-threaded application requires both a careful placement of threads on computing units and a thorough allocation of data in memory. Finding such a placement is a hard problem to solve, because performance depends on complex interactions in several layers of the memory hierarchy.

We proposed a black-box approach to decide if an application execution time can be impacted by the placement of its threads and data, and in such a case, to choose the best placement strategy to adopt [18]. We show that it is possible to reach near-optimal placement policy selection by looking at hardware performance counters, and at counters obtained from application instrumentation. Furthermore, solutions work across several recent processor architectures (from Haswell to Skylake), across several applications, and decisions can be taken with a single run of low overhead profiling.

This work has been achieved in collaboration with Thomas ROPARS from University of Grenoble.

7.7. On-the-fly scheduling vs. reservation-based scheduling for unpredictable workflows

Scientific insights in the coming decade will clearly depend on the effective processing of large datasets generated by dynamic heterogeneous applications typical of workflows in large data centers or of emerging fields like neuroscience. In this work [8], we show how these big data workflows have a unique set of characteristics that pose challenges for leveraging HPC methodologies, particularly in scheduling. Our findings indicate that execution times for these workflows are highly unpredictable and are not correlated with the size of the dataset involved or the precise functions used in the analysis. We characterize this inherent variability and sketch the need for new scheduling approaches by quantifying significant gaps in achievable performance. Through simulations, we show how on-the-fly scheduling approaches can deliver benefits in both system-level and user-level performance measures. On average, we find improvements of up to 35% in system utilization and up to 45% in average stretch of the applications, illustrating the potential of increasing performance through new scheduling approaches.

7.8. Scheduling strategies for stochastic jobs

Following the observations of made in 7.7, we studied stochastic jobs (coming from neuroscience applications) which we want to schedule on a reservation-based platform (e.g. cloud, HPC).

The execution time of jobs is modeled using a (known) probability distribution. The platform to run the job is reservation-based, meaning that the user has to request fixed-length time slots for its job to be executed. The aim of this project is to study efficient strategies of reservation for an user given the cost associated to the machine. These reservations are all paid until a job is finally executed.

As a first step we derived efficient strategies without any additional asumptions [15]. This allowed us to set up properly the problem. These strategies were general enough that they could take as input any probability distributions, and performed better than any more natural strategies. Then we extended our strategies by including checkpoint/restart to well-chosen reservations in order to avoid wasting the benefits of work during underestimated reservations [35]. We were able to develop a fully polynomial-time approximation for continuous distribution of job execution time whose performance we then experimentally studied.

The final works of this project focused on the case without checkpointing: we studied experimentally how the strategies developed in [15] would perform in a parallel setup and showed that they improve both system utilization and job response time. Finally we started to study the robustness of such solutions when the job distributions were not perfectly known [19] and observed that the performance were still correct even with a very low quantity of information.

7.9. Online Prediction of Network Utilization

Stealing network bandwidth helps a variety of HPC runtimes and services to run additional operations in the background without negatively affecting the applications. A key ingredient to make this possible is an accurate prediction of the future network utilization, enabling the runtime to plan the background op- erations in advance, such as to avoid competing with the application for network bandwidth. In this work [23], we have proposed a portable deep learning predictor that only uses the information available through MPI introspection to construct a recurrent sequence-to-sequence neural network capable of forecasting network utilization. We leverage the fact that most HPC applications exhibit periodic behaviors to enable predictions far into the future (at least the length of a period). Our online approach does not have an initial training phase, it continuously improves itself during application execution without incurring significant computational overhead. Experimental results show better accuracy and lower computational overhead compared with the state-of-the-art on two representative applications.

7.10. An Introspection Monitoring Library

In this work [36] we have described how to improve communication time of MPI parallel applications with the use of a library that enables to monitor MPI applications and allows for introspection (the program itself can query the state of the monitoring system). Based on previous work, this library is able to see how collective communications are decomposed into point-to-point messages. It also features monitoring sessions that allow suspending and restarting the monitoring, limiting it to specific portions of the code. Experiments show that the monitoring overhead is very small and that the proposed features allow for dynamic and efficient rank reordering enabling up to 2-time reduction of communication parts of some program.

7.11. Tag matching in constant time

Tag matching is the operation, inside an MPI library, of pairing a packet arriving from the network, with its corresponding receive request posted by the user. This operation is not straightforward given that matching criterions are the communicator, the source of the message, a user-supplied tag, and since there are wildcards for tag and source. State of the art algorithms are linear with the number of pending packets and requests, or don't support wildcards.

We proposed [17] an algorithm that is able perform the matching operation in constant time, in all cases, even with wildcard requests. We implemented the algorithm in our NEWMADELEINE communication library, and demonstrated it actually improves performance of Cholesky factorization with CHAMELEON running on top of STARPU.

7.12. Dynamic broadcasts in StarPU/NewMadeleine

We worked on the improvement of broadcast performance in STARPU runtime with NEWMADELEINE. Although STARPU supports MPI, its distributed and asynchronous model to schedule tasks makes it impossible to use MPI optimized routines, such as `MPI_Bcast`. Indeed these functions need that all nodes participating in the collective are synchronized and know each others, which makes it unusable in practice for STARPU.

We proposed [42], a dynamic broadcast algorithm that runs without synchronization among participants, and where only the root node needs to know the others. Recipient don't even have to know whether the message will arrive as a plain send/receive or through a dynamic broadcast, which allows for a seamless integration in STARPU. We implemented the algorithm in our NEWMADELEINE communication library, leveraging its event-based paradigm and background progression of communications. Preliminary experiments using Cholesky factorization from the CHAMELEON library show a sensible performance improvement.

7.13. Task based asynchronous MPI collectives optimisation

Asynchronous collectives are more complex than plain non-blocking point-to-point communications. They need specific mechanisms for progression. Task based progression is a good way to improve the performance of applications with overlap.

We worked on a benchmarking tool [41] measuring specific collective overlapping, taking into account time shift between different nodes. Using this tool, we were able to experiment with different task execution policies in the NEWMADELEINE communication library.

We propose a progression policy consisting of a dedicated a core for progression tasks; modern processors have more and more cores, so it is profitable on that kind of processors. The only function of this core is to progress communications, so we use a particularly aggressive algorithm for this progression.

7.14. Dynamic placement of progress thread for overlapping MPI non-blocking collectives on manycore processor

To amortize the cost of MPI collective operations, non-blocking collectives have been proposed so as to allow communications to be overlapped with computation. Unfortunately, collective communications are more CPU-hungry than point-to-point communications and running them in a communication thread on a single dedicated CPU core makes them slow. On the other hand, running collective communications on the application cores leads to no overlap. To address these issues, we proposed [5] an algorithm for tree-based collective operations that splits the tree between communication cores and application cores. To get the best of both worlds, the algorithm runs the short but heavy part of the tree on application cores, and the long but narrow part of the tree on one or several communication cores, so as to get a trade-off between overlap and absolute performance. We provided a model to study and predict its behavior and to tune its parameters. We implemented it in the MPC framework, which is a thread-based MPI implementation. We have run benchmarks on manycore processors such as the KNL and Skylake and got good results both in terms of performance and overlap.

7.15. Dynamic placement of Hybrid MPI +X coupled applications

We continued our collaboration with CERFACS in order to propose the HIPPO software that addresses the issue of dynamic placement of computing kernels that feature each their own placement/mapping/binding policy of MPI processes and OpenMP threads. In such a case, enforcing a global placement policy for the whole application composed of several such kernels may be detrimental to the overall performance. HIPPO (based on our HSPLIT library and the HWLOC software) is able to make the selection of the relevent resource on which some master MPI processes are going to execute and spawn OpenMP parallel sections while the remaining MPI processes are put in a "quiescence" state. HIPPO is currently at the prototype stage and the interface and the set of provided functionnalities need some refinement, however, preliminary results are very encouraging, especially on climate modelling applications from Météo France.

7.16. Scheduling on Two Unbounded Resources with Communication Costs

Heterogeneous computing systems are popular and powerful platforms, containing several heterogeneous computing elements (e.g. CPU+GPU). In [13], we consider a platform with two types of machines , each containing an unbounded number of elements. We want to execute an application represented as a Directed Acyclic Graph (DAG) on this platform. Each task of the application has two possible execution times, depending on the type of machine it is executed on. In addition we consider a cost to transfer data from one platform to the other between successive tasks. We aim at minimizing the execution time of the DAG (also called makespan). We show that the problem is NP-complete for graphs of depth at least three but polynomial for graphs of depth at most two. In addition, we provide polynomial-time algorithms for some usual classes of graphs (trees, series-parallel graphs).

7.17. H-Revolve: A Framework for Adjoint Computation on Synchrone Hierarchical Platforms

In this work [38], we study the problem of checkpointing strategies for adjoint computation on synchrone hierarchical platforms. Specifically we consider computational platforms with several levels of storage with different writing and reading costs. When reversing a large adjoint chain, choosing which data to checkpoint and where is a critical decision for the overall performance of the computation. We introduce H-Revolve, an optimal algorithm for this problem. We make it available in a public Python library along with the implementation of several state-of-the-art algorithms for the variant of the problem with two levels of storage. We provide a detailed description of how one can use this library in an adjoint computation software in the field of automatic differentiation or backpropagation. Finally, we evaluate the performance of H-Revolve and other checkpointing heuristics though an extensive campaign of simulation.

7.18. Sizing and Partitioning Strategies for Burst-Buffers to Reduce IO Contention

Burst-Buffers are high throughput and small size storage which are being used as an intermediate storage between the PFS (Parallel File System) and the computational nodes of modern HPC systems. They can allow to hinder to contention to the PFS, a shared resource whose read and write performance increase slower than processing power in HPC systems. A second usage is to accelerate data transfers and to hide the latency to the PFS. In this work [14], we concentrate on the first usage. We propose a model for Burst-Buffers and application transfers. We consider the problem of dimensioning and sharing the Burst-Buffers between several applications. This dimensioning can be done either dynamically or statically. The dynamic allocation considers that any application can use any available portion of the Burst-Buffers. The static allocation considers that when a new application enters the system, it is assigned some portion of the Burst-Buffers, which cannot be used by the other applications until that application leaves the system and its data is purged from it. We show that the general sharing problem to guarantee fair performance for all applications is an NP-Complete problem. We propose a polynomial time algorithms for the special case of finding the optimal buffer size such that no application is slowed down due to PFS contention, both in the static and dynamic cases. Finally, we provide evaluations of our algorithms in realistic settings. We use those to discuss how to minimize the overhead of the static allocation of buffers compared to the dynamic allocation.

7.19. Optimal Memory-aware Backpropagation of Deep Join Networks

Deep Learning training memory needs can prevent the user to consider large models and large batch sizes. In our work [4] (extended version [34]), we propose to use techniques from memory-aware scheduling and Automatic Differentiation (AD) to execute a backpropagation graph with a bounded memory requirement at the cost of extra recomputations. The case of a single homogeneous chain, i.e. the case of a network whose all stages are identical and form a chain, is well understood and optimal solutions have been proposed in the AD literature. The networks encountered in practice in the context of Deep Learning are much more diverse, both in terms of shape and heterogeneity. In this work, we define the class of backpropagation graphs, and extend those on which one can compute in polynomial time a solution that minimizes the total number of recomputations. In particular we consider join graphs which correspond to models such as Siamese or Cross Modal Networks.

7.20. Optimal checkpointing for heterogeneous chains: how to train deep neural networks with limited memory

This work [33] introduces a new activation checkpointing method which allows to significantly decrease memory usage when training Deep Neural Networks with the back-propagation algorithm. Similarly to checkpoint-ing techniques coming from the literature on Automatic Differentiation, it consists in dynamically selecting the forward activations that are saved during the training phase, and then automatically recomputing missing activations from those previously recorded. We propose an original computation model that combines two types of activation savings: either only storing the layer inputs, or recording the complete history of operations that produced the outputs (this uses more memory, but requires fewer recomputations in the backward phase), and we provide an algorithm to compute the optimal computation sequence for this model. This paper also describes a PyTorch implementation that processes the entire chain, dealing with any sequential DNN whose internal layers may be arbitrarily complex and automatically executing it according to the optimal checkpointing strategy computed given a memory limit. Through extensive experiments, we show that our implementation consistently outperforms existing checkpoint-ing approaches for a large class of networks, image sizes and batch sizes.

7.21. I/O scheduling strategy for HPC applications

With the ever-growing need of data in HPC applications, the congestion at the I/O level becomes critical in supercomputers. Architectural enhancement such as burst buffers and pre-fetching are added to machines, but are not sufficient to prevent congestion. Recent online I/O scheduling strategies have been put in place, but they add an additional congestion point and overheads in the computation of applications.

In this project, we studied application pattern (such as periodicity), in order to develop efficient scheduling strategies [7], [32] for their I/O transfers.

7.22. A New Framework for Evaluating Straggler Detection Mechanisms in MapReduce

In this work [10] we present a new framework for evaluating straggler detection mechanisms in MapReduce. We then show how to use it efficiently.

7.23. Clarification of the MPI semantics

In the framework of the MPI Forum, we have been involved in several active working groups, in particular the “Terms and Conventions” Working Group. The work carried out in this group has lead to a timely study and proposed clarifications, revisions, and enhancements to the Message Passing Interface’s (MPI’s) Semantic Terms and Conventions. To enhance MPI, a clearer understanding of the meaning of the key terminology has proven essential, and, surprisingly, important concepts remain underspecified, ambiguous and, in some cases, inconsistent and/or conflicting despite 26 years of standardization. This work [16] addresses these concerns comprehensively and usefully informs MPI developers, implementors, those teaching and learning MPI, and power users alike about key aspects of existing conventions, syntax, and semantics. This work will also be a useful driver for great clarity in current and future standardization and implementation efforts for MPI.

7.24. Adaptive Request Scheduling for the I/O Forwarding Layer using Reinforcement Learning

I/O optimization techniques such as request scheduling can improve performance mainly for the access patterns they target, or they depend on the precise tune of parameters. In this work [40], we propose an approach to adapt the I/O forwarding layer of HPC systems to the application access patterns by tuning a request scheduler. Our case study is the TWINS scheduling algorithm, where performance improvements depend on the time window parameter, which depends on the current workload. Our approach uses a reinforcement learning technique — contextual bandits — to make the system capable of learning the best parameter value to each access pattern during its execution, without a previous training phase. We evaluate our proposal and demonstrate it can achieve a precision of 88% on the parameter selection in the first hundreds of observations of an access pattern. After having observed an access pattern for a few minutes (not necessarily contiguously), we demonstrate that the system will be able to optimize its performance for the rest of the life of the system (years).

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Grants with Industry

8.1.1. Intel

INTEL granted $30k and provided information about future many-core platforms and memory architectures to ease the design and development of the HWLOC software with early support for next generation hardware.

8.1.2. EDF

With Yvan Fournier from EDF R&D, we co-advise the PhD thesis of Benjamin Lorendeau under a CIFRE funding.

8.1.3. CEA

CEA/DAM granted the CIFRE PhD thesis of Florian Reynier on non-blocking MPI collectives.

9. Partnerships and Cooperations

9.1. Regional Initiatives

9.1.1. CRA HPC Scalable Ecosystem, 2018-2021

2018 - 2021 (36 months)

Coordinator: Emmanuel AGULLO

Other partners: INRA, Institut Pprime, UPPA, Airbus, CEA, CATIE

Abstract: The goal is to design a unified runtime-system for numerical simulation at large-scale and with a large amount of data. We aim at contributing significantly to the convergence between HPC and BigData. TADAAM is involved in scheduling data access and managing communication efficiently on large-scale system.

9.2. National Initiatives

9.2.1. ANR

ANR SATAS SAT as a Service (http://www.agence-nationale-recherche.fr/Project-ANR-15-CE40-0017).

AP générique 2015, 01/2016 - 12/2019 (48 months)

Coordinator: Laurent Simon (LaBRI)

Other partners: CRIL (Univ. Artois), Inria Lille (Spirals)

Abstract: The SATAS project aims to advance the state of the art in massively parallel SAT solving. The final goal of the project is to provide a "pay as you go" interface to SAT solving services and will extend the reach of SAT solving technologies, daily used in many critical and industrial applications, to new application areas, which were previously considered too hard, and lower the cost of deploying massively parallel SAT solvers on the cloud.

ANR DASH Data-Aware Scheduling at Higher scale (https://project.inria.fr/dash/).

AP générique JCJC 2017, 03/2018 - 02/2022 (48 months)

Coordinator: Guillaume PALLEZ (Tadaam)

Abstract: This project focuses on the effecient execution of I/O for High-Performance applications. The idea is to take into account some knowledge on the behavior of the different I/O steps to compute efficient schedules, and to update them dynamically with the online information.

ANR Solharis SOLvers for Heterogeneous Architectures over Runtime systems, Investigating Scalability .

AAPG ANR 2019, 2019 - 2023 (48 months)

Coordinator: Alfredo BUTTARI (IRIT-INPT)

Abstract: The Solharis project aims at producing scalable methods for the solution of large sparse linear systems on large heterogeneous supercomputers, using the STARPU runtime system, and to address the scalability issues both in runtime systems and in solvers.

9.2.2. ADT - Inria Technological Development Actions

ADT Gordon

10/2018 - 09/2020 (24 months)

Coordinator: Emmanuel JEANNOT

Other partners: Storm, HiePACS, PLEIADE (Inria Bordeaux)

Abstract: Teams HiePACS, Storm and Tadaam develop each a brick of an HPC software stack, namely solver, runtime, and communication library. The goal of the Gordon project is to consolidate the HPC stack, to improve interfaces between each brick, and to target a better scalability. The bioinformatics application involved in the project has been selected so as to stress the underlying systems.

9.2.3. IPL - Inria Project Lab

High-Performance computing and BigData

Participants: Guillaume Pallez, Emmanuel Jeannot, Nicolas Vidal, Francieli Zanon-Boito

HPC and Big Data evolved with their own infrastructures (supercomputers versus clouds), applications (scientific simulations versus data analytics) and software tools (MPI and OpenMP versus Map/Reduce or Deep Learning frameworks). But Big Data analytics is becoming more compute-intensive (thanks to deep learning), while data handling is becoming a major concern for scientific computing. The goal of this HPC-BigData IPL is to gather teams from the HPC, Big Data and Machine Learning (ML) areas to work at the intersection between these domains. Research is organized along three main axes: high performance analytics for scientific computing applications, high performance analytics for big data applications, infrastructure and resource management

9.2.4. Collaboration with CERFACS

Developments on the HIPPO software

Participants: Brice Goglin, Guillaume Mercier

A Memorandum of Understanding is currently being negociated between Inria and CERFACS to organize the collaboration between both entities pertaining to the developements on the HIPPO software. The goal is to provide a portable solution to address the issue of dynamic placement of hybrid coupled MPI + OpenMP applications, especially for climate modelling. Météo France is one of the targer of this work but other teams/institutes around the globe have expressed an interest in HIPPO. Therefore we want to create a solution that would match the needs of the community on the whole.

9.3. European Initiatives

9.3.1. Collaborations with Major European Organizations

Partner 1: INESC-ID, Lisbon, (Portugal)

Subject 1: Application modeling for hierarchical memory system

Partner 2: University Carlos III de Madrid, (Spain)

Subject 2: I/O Scheduling

9.4. International Initiatives

9.4.1. Inria International Labs

Joint-Lab on Extreme Scale Computing (JLESC):

Coordinators: Franck Cappello (general) and Yves Robert (Inria coordinator).

Other partners: Argonne National Lab, University of Urbanna Champaign (NCSA), Tokyo Riken, Jülich Supercomputing Center, Barcelona Supercomputing Center (BSC).

Abstract: The purpose of the Joint Laboratory for Extreme Scale Computing (JLESC) is to be an international, virtual organization whose goal is to enhance the ability of member organizations and investigators to make the bridge between Petascale and Extreme computing. The founding partners of the JLESC are Inria and UIUC. Further members are ANL, BSC, JSC and RIKEN-AICS.

9.4.2. Inria International Partners

9.4.2.1. Informal International Partners

Partner 1: Argonne National Lab

Subject 1: Binomial Checkpointing Strategies for Machine Learning (recipient of a FACCTS grant, 2018-2020) as well as network performance prediction.

Partner 2: Vanderbilt University

Subject 2: Scheduling for Neurosciences 7.8

Partner 3: ICL at University of Tennessee

Subject 3: on instrumenting MPI applications and modeling platforms (works on HWLOC take place in the context of the Open MPI consortium) and MPI and process placement

Partner 4: Lawrence Livermore National Laboratory

Subject 4: Exposing Heterogeneous Memory Characteristics to HPC Applications 7.1

9.5. International Research Visitors

9.5.1. Visits of International Scientists

- Ana Gainaru, Reseach Assistant Professor at U. Vanderbilt, visited the team for one week in December 2019.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events: Organisation

10.1.1.1. General Chair, Scientific Chair

- Brice GOGLIN and Emmanuel JEANNOT organized (with Didem UNAT from Ko c University, Turkey), PADAL 2019 (Fifth Workshop on Programming Abstractions for Data Locality) in Bordeaux (workshop by invitation): 25 participants from 10 different countries.
- François PELLEGRINI was, along with Nataliia BIELOVA (from Inria team PRIVATICS), the co-chair of this year's jury of the CNIL-Inria European prize awarded to research scientific papers on the subject of data protection and privacy.

10.1.1.2. Member of the steering committee

- Emmanuel JEANNOT is member of the steering committee of Euro-Par and the Cluster international conference.

10.1.2. Scientific Events: Selection

10.1.2.1. Chair of Conference Program Committees

- Brice GOGLIN is the *Architecture & Networks* area co-chair of SuperComputing 2020.
- Emmanuel JEANNOT is the track program chair of Cluster 2020 (area: application, algorithms, and libraries)
- Emmanuel JEANNOT was the program chair of the COLOC workshop (collocated with Euro-Par).
- Emmanuel JEANNOT was the program chair of the RADR workshop (collocated with IPDPS).
- François PELLEGRINI was a co-chair (along with Roberto DI COSMO) of the workshop on *Software and Open Science: issues and opportunities*, National days on Open science (JNSO 2019), Paris (https://jnso2019.sciencesconf.org/resource/page/id/2).

10.1.2.2. Member of Conference Program Committees

- Alexandre DENIS was a member of the program committee of CCGrid 2019.
- Brice GOGLIN was a member of the program committee of ICPP 2019, EuroMPI 2019, HotInterconnects 26, ROME 2019, ROSS 2019, RADR 2019.
- Emmanuel JEANNOT was member of the program committee of SuperComputing 2019, Euro-MPI 2019, ROSS 2019, Heteropar 2019.
- Guillaume MERCIER was a member of the programm committee of CCGrid 2019 and EuroMPI 2019.
- Guillaume PALLEZ was a member of the program committee of SC 2019 (Tutorials), ICPP 2019, IPDPS 2020, ICA3PP 2019, PMBS 2019.
- François PELLEGRINI was a member of the program committee of ENISA's "EU Privacy Forum".

10.1.3. Journal

10.1.3.1. Member of the Editorial Boards

- Emmanuel JEANNOT is associate editor of the International Journal of Parallel, Emergent & Distributed Systems (IJPEDS).

10.1.3.2. Reviewer - Reviewing Activities

- Emmanuel JEANNOT was a reviewer for JPDC, Parallel Computing, Transaction on Computers.
- Guillaume MERCIER was a reviewer for IEEE Transactions on Computers and for Cluster Computing.
- François PELLEGRINI was a reviewer for journal Terminal.

10.1.4. Invited Talks

- Emmanuel JEANNOT was invited to the panel *Heterogeneous Computing for Energy Efficiency* of 10th International Green and Sustainable Computing Conference (Alexandia VA, USA, octobre 2019, https://www.igscc.org/copy-of-schedule).
- Emmanuel JEANNOT was invited to the panel *Resilience in High Performance Computing* to the HiPEAC event (at Bilbao Spain, October 2019, https://www.hipeac.net/csw/2019/bilbao/#/schedule/).
- Guillaume MERCIER was invited to make a presentation at the PADAL workshop 2019.
- Guillaume PALLEZ was invited to give a talk at the Royal Society of London, UK, as a part of the event *Numerical algorithms for high-performance computational science* [11] (https://royalsociety.org/science-events-and-lectures/2019/04/high-performance-computing/).
- François PELLEGRINI was invited to deliver a common talk with Emmanuel NETTER, "*Is code law?*", at the Symposium of the Agorantic research federation, University of Avignon (https://agorantic.univ-avignon.fr/symposium/symposium-agorantic-28-janvier-2019/).

10.1.5. Scientific Expertise

- Emmanuel JEANNOT was a member of the hiring committee of an Inria junior researcher position at Nancy and at the National Level.
- Guillaume PALLEZ is an elected member of the Inria evaluation committee.
- François PELLEGRINI is co-chair (along with Roberto DI COSMO) of the workgroup on Free software of the Permanent Secretariat for Open Science (SPSO) of the French Ministry of Higher Education (MENESR).
- François PELLEGRINI was heard in an expert panel commissioned by the *Information mission on digital identity* of the French *Assemblée nationale*, chaired by Mrs Marietta KARAMANLI, assisted by Mrs Paula FORTEZA and Christine HENNION.

10.1.6. Research Administration

- Alexandre DENIS is head of the Inria Bordeaux CUMI-R (IT users committee).
- Brice GOGLIN and Guillaume MERCIER are elected members of the Inria Bordeaux center committee.
- Emmanuel JEANNOT is deputy head of science of the Inria Bordeaux research center.
- Emmanuel JEANNOT is member of the Inria evaluation committee
- Emmanuel JEANNOT is member of LaBRI scientific council and head of the Satanas team.
- Guillaume PALLEZ is a worker representative at the Prevention, Health, Security committee (CHSCT) for the Inria center of Bordeaux.

10.1.7. Standardization Activities

TADAAM attended the MPI Forum meetings on behalf of Inria (where the MPI standard for communication in parallel applications is developed and maintained). Guillaume MERCIER leads the *Hardware Topologies* working group. Part of the HSPLIT proposal was discussed and read at the last physical meeting in December 2019 in Albuquerque and has been approved to enter the voting process for an eventual inclusion in the next revision (4.0) of the MPI standard. This voting process will take place in the first semester of 2020 and the release of the 4.0 revision is expected for the end of 2020. Guillaume MERCIER is also the chair of the standard chapter committee *Groups, Contexts, Communicators, Caching* and member of several other chapter committees.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

Members of the TADAAM project gave hundreds of hours of teaching at Université de Bordeaux and the Bordeaux INP engineering school, covering a wide range of topics from basic use of computers, introduction to algorithmics and C programming to advanced topics such as probabilities and statistics, scheduling, computer architecture, operating systems, parallel programming and high-performance runtime systems, as well as software law and personal data.

- Brice GOGLIN gave courses about Operating Systems to teachers as part of the *Diplôme Inter Universitaire* to prepare them for teaching the new Computer Science track in high-school.
- François PELLEGRINI did a training session on "*Information science, digital technologies and law*" for the continuous education of magistrates, École nationale de la magistrature (National School for Magistrates), Paris.
- François PELLEGRINI did two training sessions on "*Strategic issues of information technologies*" and "*Personal data law*" to a group of administration heads and civil society activists of several French-speaking west-African countries, in the context of FFGI 2019 at Ouagadougou, Burkina Faso.

10.2.2. Supervision

PhD: Benjamin LORENDEAU, Amélioration des performances via un parallélisme multi-niveaux sur un code CFD en maillages non structurés. Defense at Université de Bordeaux on December 16th. Advisors : Yvan FOURNIER and Emmanuel JEANNOT.

PhD in progress: Valentin Honoré, Partitioning Strategies for high throughput Applications, started in November 2017. Advisors: Guillaume PALLEZ and Brice GOGLIN.

PhD in progress: Andrès RUBIO, Management on heterogeneous and non-volatile memories, started in October 2018. Advisor: Brice GOGLIN.

PhD in progress: Nicolas VIDAL, IO scheduling strategies, started in October 2018. Advisors: Guillaume PALLEZ and Emmanuel JEANNOT.

PhD started: Philippe SWARTVAGHER, Interactions at large scale between high performance communication libraries and task-based runtime, started in October 2019. Advisors: Alexandre DENIS and Emmanuel JEANNOT.

PhD started: Florian REYNIER, Task-based communication progression, started in January 2019. Advisors: Alexandre DENIS and Emmanuel JEANNOT.

PhD started: Pierre FERENBACH, The legal regime of video games, started in January 2019. Advisors: Xavier DAVERAT and François PELLEGRINI.

Master: Léa CHEVALIER, M2 student at Université Paris Nanterre supervised by François PELLEGRINI, won the Disney–Microsoft–Orange–TF1 prize on Media Law for her master thesis on "*Artistic creations generated by automated processing: are they works like others?*".

10.2.3. Juries

Emmanuel JEANNOT was member of the Ph.D defense jury of:

- Hugo BRUNIE, U. Bordeaux (Member);
- Jean-Baptiste KECK, U. Grenoble Alpes (Reviewer);
- Hamza DEROUI, Insa Rennes and U. Rennes (Reviewer);
- Arthur LOUSSERT, U. Bordeaux (Member).

FrançoisPELLEGRINI was member of the Ph.D defense jury of:

- Maximilien LANNA, U. Paris II Panthéon Assas (Member).

10.3. Popularization

10.3.1. Internal or external Inria responsibilities

Brice GOGLIN is in charge of the diffusion of the scientific culture for the Inria Research Centre of Bordeaux. He organized several popularization activities involving colleagues.

10.3.2. Articles and contents

- Guillaume PALLEZ wrote a blog article for *Binaire* on autonomous vehicles [37].
- François PELLEGRINI was interviewed on the subject of "*Resisting algorithmic governance*" (cover page), Expertises droit/technologies/prospectives, nr 443, Feb. 2019 (https://www.expertises.info/#anciens-numeros).

10.3.3. Interventions

- Brice GOGLIN is the sponsor (*parrain*) of the *Edouard Vaillant* middle school (Bordeaux) for their scientific projects with the fondation *La main à la pâte*.
- Guillaume PALLEZ, Brice GOGLIN, Valentin HONORÉ, Philippe SWARTVAGHER and Nicolas VIDAL gave seminars and hands-on session about computer science to schools attending *Fete de la Science*, Oct. 2019.
- François PELLEGRINI participated in the round table "*GDPR and cyber-security*" during the OpenS'IAE event, Pau.
- François PELLEGRINI participated in the rountable on "*Legal aspects, GDPR and anonymization technologies*" during the annual congress of *Société informatique de France* (SIF), Bordeaux.
- François PELLEGRINI gave a conference on the security of personal data during the *Mars@Hack* event, in Mont-de-Marsan.
- François PELLEGRINI participated in the round table "*Is our legal framework IA-compatible?*" during the NAIA (*Nouvelle-Aquitaine Intelligence Artificielle*) event, Bordeaux.

- François PELLEGRINI participated in the round table "*What alternatives and what regulations in the GAFAM era?*" during the second edition of the *Rencontres Culture:Tech*, Assemblée nationale, Paris.
- François PELLEGRINI gave a conference on "*Freedom in the digital age*" to students of first and second year of all departments at ENS Cachan (250 people).
- François PELLEGRINI participated in a round table on "*The future of choice*" in the context of the "de-inauguration" of the exhibition textitUnder influence, the science of choice at Espace Pierre-Gilles de Gennes (ESPGG), Paris.
- François PELLEGRINI answered the public at the movie theater Utopia Bordeaux after the display of the movie *Meeting Snowden*.
- François PELLEGRINI gave a public conference on "*How does personal data processing interfere with our privacy?*" during the *IA Pau* conference, Pau.

10.3.4. Internal action

- François PELLEGRINI participated in a round table on "*Digital security: technical, ethical and legal aspects*", Inria scientific days 2019, Lyon (https://project.inria.fr/journeesscientifiques2019/).

10.3.5. Creation of media or tools for science outreach

- Brice GOGLIN was involved in the building of the MOOC *Sciences Numériques et Technologie* which focus at bringing basics about computer science to high-school teachers and general audience. More than 18 000 people registered to the course.
- François PELLEGRINI is one of the 14 people appearing in the documentary "*LOL: Logiciel libre, une affaire sérieuse*" ("LOL: Free software, a serious matter").

11. Bibliography

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