



Activity Report Bordeaux - Sud-Ouest 2016

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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

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Project-Team CAGIRE

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Keywords:

Computer Science and Digital Science:

- 6.1.1. - Continuous Modeling (PDE, ODE)
- 6.2.1. - Numerical analysis of PDE and ODE
- 6.2.7. - High performance computing

Other Research Topics and Application Domains:

- 4.2.1. - Fission
- 4.3.4. - Solar Energy
- 5.2.1. - Road vehicles
- 5.2.3. - Aviation

1. Members

Research Scientists

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

Faculty Member

Jonathan Jung [Univ. Pau, Associate Professor]

Technical Staff

Benjamin Lux [Inria, Engineer, until Oct 2016]

PhD Students

Simon Delmas [Pau University, until January 2016]
Jean-François Wald [EDF, until April 2016]

Post-Doctoral Fellow

Yann Moguen [Pau University, Post-Doctoral Fellow, until May 2016]

Administrative Assistants

Sylvie Embolla [Inria, Assistant]
Nicolas Jahier [Inria, Assistant]

Others

Nicolas Hernandez Reyes [Inria internship, from Feb 2016 until Apr 2016]
Saad Jameel [Internship, from Apr 2016 until Sep 2016]

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 progressively elaborated a common vision of what should be the simulation tool of fluid dynamics of tomorrow. Our application will be focused on wall bounded turbulent flows and featuring complex phenomena such as aeroacoustics, hydrodynamic instabilities, phase change processes, wall roughness, buoyancy or localized relaminarization. Because such flows are exhibiting

a multiplicity of time and scale fluctuations resulting from complex interactions, their simulation is extremely challenging. Even if various methods of simulation (DNS⁰) and turbulence modeling (RANS⁰, LES⁰, 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 large 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. So, 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 OpenFOAM⁰ or the more recently proposed SU2⁰ 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 big 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 side, for the small companies of this sector, this may have a rather detrimental 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, AD Industrie) or indirect (European programs, WALLTURB, KIAI, IMPACT-AE, SOPRANO) 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 from 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

⁰Direct numerical simulation

⁰Reynolds averaged Navier-Stokes

⁰Large-eddy simulation

⁰<http://www.openfoam.com>

⁰<http://su2.stanford.edu/>

field of energy production and aeronautical 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 EDF and Safran group, 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 high values of the Reynolds number is governed by a spectrum of time and space scales fluctuations closely connected with the turbulent nature of the flow. The term deterministic chaos employed by Frisch in his enlightening book [42] 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) to the smallest one (Kolmogorov scale) scales as $Re^{3/4}$ per dimension. In addition, for internal flows, the viscous effects near the solid walls yield a scaling proportional to Re per dimension. 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 these scales. 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 runs themselves. If a modeling phase is on the agenda, then one has to choose again among the above mentioned variety of approaches. As it is illustrated in Fig. 1, this can be achieved either by directly solving the Navier-Stokes equations (DNS) or by first applying a statistical averaging (RANS) or a spatial filtering operator to the Navier-Stokes equations (LES). The new terms brought about by the filtering 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. 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 supposed to be more isotropic, LES proved to be quite a step through that permits to fully take advantage of the increasing power of computers to study complex flow configurations. At the same time, DNS was progressively applied to geometries of increasing complexity (channel flows with values of Re_τ multiplied by 10 during the last 15 years, jets, turbulent premixed flames, among many others), and proved to be a formidable tool that permits (i) to improve our knowledge on turbulent flows and (ii) to 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, if the steady nature of the RANS equations allows to perform iterative convergence on finer and finer meshes, 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, once chosen, a single turbulence model will (try to) do the job for modeling the whole flow. Thus, depending on its intrinsic strengths and weaknesses, the accuracy will be a rather volatile quantity strongly dependent on the flow configuration. 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 deficiencies of both approaches and to combine them for significantly improving the overall quality of the modeling, the hybrid RANS-LES approach has emerged during the last decade as a viable, intermediate way, and we are definitely inscribing our project in this innovative field of research, with an original approach though, connected with a time filtered hybrid RANS-LES and a systematic and progressive validation process against experimental data produced by the team.

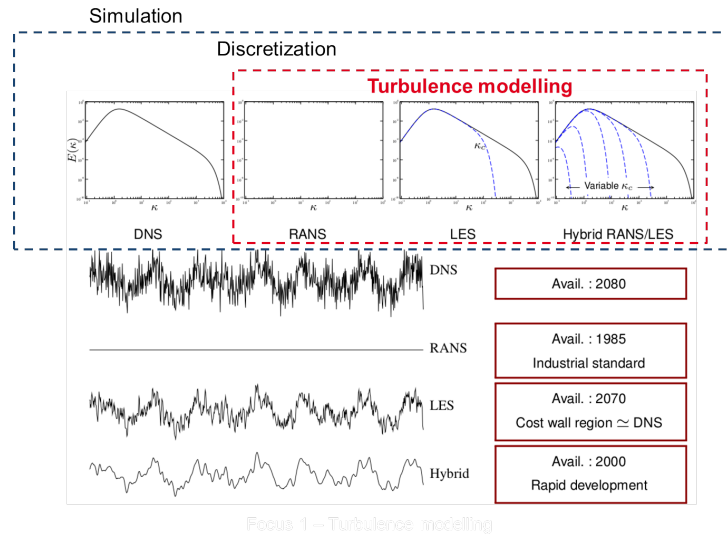


Figure 1. A schematic view of the different nested steps for turbulent flow simulation: from DNS to hybrid RANS-LES. The approximate dates at which the different approaches are or will be routinely used in the industry are indicated in the boxes on the right (extrapolations based on the present rate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

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 [53] and first studied by Lesaint and Raviart [49]. 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,

⁰http://www.transport-research.info/web/projects/project_details.cfm?id=46810

whereas specific constraints given by the finite element nature of the scheme were progressively solved, for scalar conservation laws [38], [37], one dimensional systems [36], multidimensional scalar conservation laws [35], and multidimensional systems [39]. For the same system, we can also cite the work of [41], [46], which is slightly different: the stabilization is made by adding a nonlinear term, and the time integration is implicit. Contrary 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 [28]. The first application of discontinuous Galerkin methods to Navier-Stokes equations was proposed in [33] by mean of a mixed formulation. Actually, this first attempt led to a non compact computation stencil, and was later proved to be not stable. A compactness improvement was made in [34], which was later analyzed, and proved to be stable in a more unified framework [29]. The combination with the $k - \omega$ RANS model was made in [32]. As far as Navier Stokes equations are concerned, we can also cite the work of [44], in which the stabilization is closer to the one of [29], the work of [50] on local time stepping, or the first use of discontinuous Galerkin methods for direct numerical simulation of a turbulent channel flow done in [40]. Discontinuous Galerkin methods are so 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, which require as more and more neighbors as the order increases.
- They can be developed for any kind of mesh, structured, unstructured, but also for aggregated grids [31]. This is a pro compared not only with finite differences schemes, which can be developed only on structured meshes, but also compared with continuous finite elements 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 exist 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 models. Another drawback of the discontinuous Galerkin methods is that they can be computationally costly, 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 of Flame, Physics of Fluids or Journal of Computational Physics or through websites such that of Ercoftac⁰ 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 the physical modeling and of the related 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

⁰<http://www.ercoftac.org>

DNS assessment calls for the experimental determination of time and space 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 physical modeling and the 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 level of turbulence description to a more refined one, 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 then implement it in AeroSol. On the other hand, we shall concentrate (in cooperation with EDF R&D in Chatou via a CIFRE PhD do be started next year) on the theoretical link between the local variations of the scale's 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 help in the development of missing scales of fluctuations.

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 lot of work has already been done for second order schemes for Navier Stokes equations, see [52], [55] and the huge number of papers citing it. On the one hand, we believe that strong improvements are necessary with higher order schemes: indeed, the less dissipative the scheme is, the worse impact have the spurious reflections. For this, we will first concentrate on the linearized Navier-Stokes system, and analyze the boundary condition imposition in a discontinuous Galerkin framework with a similar approach as in [43]. We will also try to extend the work of [56], which deals with Euler equations, to the Navier Stokes equations.

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 hybrid temporal RANS/LES models 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, the turbulence/wall interaction and the heat transfer at the fluid-solid interfaces 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 transfers. For our part, we will gradually use all our analysis and experimentation tools to actively participate in the improvement of the collective knowledge on such kind of transfers. The flow configurations dealt with by the beginning of the project will be those of subsonic single phase impacting jets or JICF with the possible presence of an interacting acoustic wave. The conjugate heat transfer at the wall will be also progressively tackled. The existing criteria of switching of the hybrid RANS/LES model will be tested on those 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 if it is possible to drive a change of instability regime (e.g. from absolute to convective) and so 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 one.

3.2.2.3. Improvement of turbulence models

The production and the subsequent use of DNS (AeroSol library) and experimental (bench MAVERIC) databases dedicated to the improvement of the physical models will be an important 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. It is on the improvement of the hybrid RANS/LES approach that will focus most of our initial efforts of analysis of the DNS and experimental data as soon as they will become available. This method has a decisive advantage over all other hybrid RANS/LES approaches since it relies on a well defined time filtering formalism. This greatly facilitates the proper extraction from the databases of the various terms appearing in the relevant flux balances 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 will also be to answer positively the following question: will we be 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 we wish to simulate may be 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 are 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 consists 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 use an 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 simulate in IMPACT-AE is 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 is particularly difficult, because the system is fully nonlinear, so 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 Jacobian free implementation, based on [48]. 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 [57], [58] 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 will be 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) [51]. For this, we propose to extend the scalar analysis of [59] 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 [31].

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 [54]. Already in 2003, [45] 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. In this task, we will work on the heterogeneous aspects of computation. 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 local 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 [47], 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 [30]. For this, the discontinuous Galerkin algorithm will be reformulated in term 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 task of the project will consist 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 will 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 allowing for a coarser aggregation.

The consortium will benefit from a particularly stimulating environment in the Inria Bordeaux Sud Ouest center around high performance computing, which is one of the strategic axis 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, thanks to its formalism of temporal filtering, the HTLES approach offers a 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 configuration complexity. This task is part of a the European project iHybrid, coordinated by TU Berlin, that we are currently writing in collaboration with two of our industrial partners, EDF and PSA.

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. Aeronautical combustion chambers

The combustion chamber of aeronautical engines is the system of practical interest we are interested in as far as propulsion devices are concerned. The MAVERIC test facility presented in Fig. 2 was developed by P. Bruel during the theses (CIFRE Turbomeca) of A. Most (2007) and J.-L. Florenciano (2013). The initial objective was to reproduce experimentally a simplified flow configuration (jet(s) in crossflow) representative of that encountered at the level of the effusion cooled aeronautical combustion chambers walls. The experimental data were used by Safran/Turbomeca to assess the predictive capability of LES simulations during our joint participation in the EU-FP7 KIAI program (2009-2013). Concerning DNS, the jet in crossflow configurations of our AeroSol based simulations which represent our contribution to the EU IMPACT-AE program (2011-2016) were chosen in partnership with Turbomeca who is leading the corresponding work package. On the side of turbulence modelling, in the just-started EU-SOPRANO program (2016-2020), the RANS and possibly hybrid RANS-LES models developed in CAGIRE will be compared to experimental data provided by ONERA, in order to validate their ability to represent the turbulent mixing and heat transfer in effusion cooled

walls of combustion chambers, and used to study the influence of various parameters, in order to develop approximate boundary conditions for industrial computations. Last but not least, tests aimed at demonstrating the feasibility of characterizing in situ by PIV the velocity field of flows emerging from different kinds of fuel nozzles were carried out at the Turbomeca premises in 2012 and 2013. Although our main present industrial partners are large companies, we are and will be actively targeting much smaller companies (SMEs) especially in the southwest part of France. In that respect, the partnership we just started with AD Industries which is manufacturing fuel nozzles as well as combustion chambers for business jet engines is emblematic of our involvement in such kind of partnership.

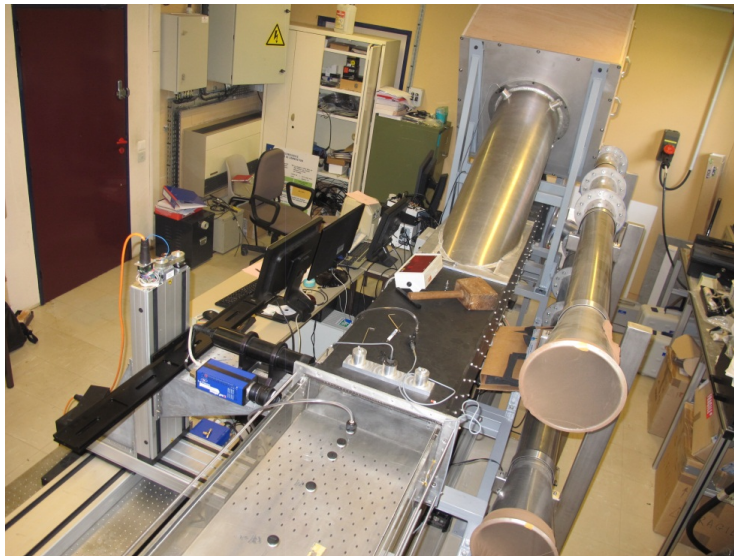


Figure 2. Overview of the Cagire test facility MAVERIC.

4.2. Power stations

The cooling of key components of power stations in case of emergency stops is a critical issue. R. Manceau has established a long term collaboration (4 PhD thesis) 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, in order to improve the physical description of the complex interaction phenomena involved in such applications. In the framework of the co-supervision of the PhD thesis (CIFRE EDF) of J.-F. Wald, defended in 2016, strategies are developed to adapt the EB-RSM turbulence model to a local modification of the scale of description of the flow in the near-wall region: refined scale (fine mesh in the near-wall region) or coarse scale (with wall functions). Indeed, the complexity of the industrial geometries is such that a fine mesh along solid boundaries in the whole system is usually not possible/desirable. This project will be pursued through the CIFRE PhD thesis of Gaetan Mangeon that will start in early 2017, dedicated to the extension of these wall functions to conjugate heat transfer and mixed/natural convection.

5. Highlights of the Year

5.1. Highlights of the Year

From Cagire to ... Cagire !

Last April 2016, after near five years of existence and a 1-year preparation/evaluation process of the new project, the common team Cagire (Computational Approximation with discontinuous Galerkin methods and comparison with Experiments) died and was reborn as the common **project** team Cagire (Computational AGility for internal flows simulations and comparisons with Experiments) with the much broader scope presented above.

A first step towards the dissemination of the AeroSol library

A deposit procedure of the AeroSol library (around 78000 lines of C++) with APP⁰ has been finalized in 2016. This will protect the library authors' rights and will open the possibility of disseminating the library in a sound way.

Launching of a long-term collaboration with a new industrial partner, PSA

In January 2016, we have been contacted by the R & D department of the PSA Group (Peugeot Citroën Automobile SA) in order to elaborate a long-term, 10-year project on the modelling and simulation of the turbulent flow in the under-hood space of road vehicles, in the framework of their *Full Digital 2025 Ambition*, i.e, their plan to switch to a design of future vehicles entirely based on simulation. In order to overcome the technological barrier of the prediction of the natural convection regime, a long-term collaboration program has been established, starting with an internship (Saad Jameel), defended in September 2016, a CIFRE PhD (same student), going to start in February 2017, and the deposit of the ANR PRCE project MONACO-2025, coordinated by R. Manceau, involving the institute PPrime of Poitiers, PSA and EDF.

6. New Software and Platforms

6.1. AeroSol

Participants: Simon Delmas [Université de Bordeaux], Sébastien de Brye [Université de Bordeaux], Benjamin Lux [Cagire], Nikolaos Pattakos [Cardamom], Vincent Perrier [Cagire, correspondent], Mario Ricchiuto [Cardamom].

Developed since 2011 by V. Perrier in partnership with the Cardamom Inria team, the AeroSol library is a high order finite element library written in C++. The code design has been carried for being able to perform efficient computations, with continuous and discontinuous finite element methods on hybrid and possibly curvilinear meshes. The work of the Cardamom team is focused on continuous finite element methods, while we focus on discontinuous Galerkin methods. However, everything is done for sharing the largest possible part of code. The distribution of the unknowns is made with the software PaMPA, first developed within the Inria teams Bacchus and Castor, and currently maintained in the Tadaam team.

The generic features of the library are Adaptive wall treatment for a second moment closure in the industrial context

- **High order.** It can be theoretically any order of accuracy, but the finite element basis, and quadrature formula are implemented for having up to a fifth order of accuracy.
- **Hybrid and curvilinear meshes.** AeroSol can deal with up to fifth order conformal meshes composed of lines, triangles, quadrangles, tetrahedra, hexahedra, prism, and pyramids.
- **Continuous and discontinuous discretization.** AeroSol deals with both continuous and discontinuous finite element methods.

⁰<http://www.app.asso.fr/en/welcome.html>

We would like to emphasize three assets of this library:

- **Its development environment** For allowing a good collaborative work and a functional library, a strong emphasis has been put on the use of modern collaborative tools for developing our software. This includes the active use of a repository, the use of CMake for the compilation, the constant development of unitary and functional tests for all the parts of the library (using CTest), and the use of the continuous integration tool Jenkins for testing the different configurations of AeroSol and its dependencies. Efficiency is regularly tested with direct interfacing with the PAPI library or with tools like scalasca.
- **Its genericity** A lot of classes are common to all the discretization, for example classes concerning I/O, finite element functions, quadrature, geometry, time integration, linear solver, models and interface with PaMPA. Adding simple features (e.g. models, numerical flux, finite element basis or quadrature formula) can be easily done by writing the class, and declaring its use in only one class of the code.
- **Its efficiency** This modularity is achieved by means of template abstraction for keeping good performances. Dedicated efficient implementation, based on the data locality of the discontinuous Galerkin method has been developed. As far as parallelism is concerned, we use point-to-point communications, the HDF5 library for parallel I/O. The behavior of the AeroSol library at medium scale (1000 to 2000 cores) was studied in [27].

The AeroSol project fits with the first axis of the Bordeaux Sud Ouest development strategy, which is to build a coherent software suite scalable and efficient on new architectures, as the AeroSol library relies on several tools developed in other Inria teams, especially for the management of the parallel aspects. At the end of 2015, AeroSol had the following features:

- **Boundary conditions** Periodic boundary conditions, time-dependent inlet and outlet boundary conditions. Adiabatic wall and isothermal wall. Steger-Warming based boundary condition. Synthetic Eddy Method for generating turbulence.
- **C++/Fortran interface** Tests for binding fortran with C++.
- **Development environment** An upgraded use of CMake for compilation (gcc, icc and xlc), CTest for automatic tests and memory checking, lcov and gcov for code coverage reports. A CDash server for collecting the unitary tests and the memory checking. An under development interface for functional tests. Optional linking with HDF5, PAPI, with dense small matrices libraries (BLAS, Eigen). An updated shared project Plafrim and joint project Aerosol/Scotch/PaMPA project on the continuous integration platform. An on-going integration of SPack for handling dependencies. A fixed ESSL interface.
- **Finite elements** up to fourth degree for Lagrange finite elements and hierarchical orthogonal finite element basis (with Dubiner transform on simplices) on lines, triangles, quadrangles, tetrahedra, prisms, hexaedra and pyramids. Finite element basis that are interpolation basis on Gauss-Legendre points for lines, quadrangles, and hexaedra, and triangle (only 1st and 2nd order).
- **Geometry** Elementary geometrical functions for first order lines, triangles, quadrangles, prisms, tetrahedra, hexaedra and pyramids. Handling of high order meshes.
- **In/Out** Link with the XML library for handling with parameter files. Parallel reader for GMSH, with an embedded geometrical pre-partitioner. Writer on the VTK-ASCII legacy format (cell and point centered). Parallel output in vtu and pvtu (Paraview) for cell-centered visualization, and XDMF/HDF5 format for both cell and point centered visualization. Ability of saving the high order solution and restarting from it. Computation of volumic and probe statistics. Ability of saving averaged layer data in quad and hexa meshes. Ability of defining user defined output visualization variables.
- **Instrumentation** Aerosol can give some traces on memory consumption/problems with an interfacing with the PAPI library. Tests have also been performed with VTUNE and TAU. Tests with Maqao and Scalasca (VIHPS workshop).

- **Linear Solvers** Link with the external linear solver UMFPack, PETSc and MUMPS. Internal solver for diagonal and block-diagonal matrices.
- **Memory handling** discontinuous and continuous, sequential and parallel discretizations based on PaMPA for generic meshes, including hybrid meshes.
- **Models** Perfect gas Euler system, real gas Euler system (template based abstraction for a generic equation of state), scalar advection, Waves equation in first order formulation, generic interface for defining space-time models from space models. Diffusive models: isotropic and anisotropic diffusion, compressible Navier-Stokes. Scalar advection-diffusion model. Linearized Euler equations, and Sutherland model for non isothermal diffusive flows. Shallow-water model.
- **Multigrid** Development of p -multigrid methods. This includes also the possibility of beginning a computation with an order and to decrease or increase the order of approximation when restarting. For the p multigrid methods, V and W cycle have been developed, and restriction and prolongation operators have also been developed. In progress implementation of h -multigrid, with the development of tests of the aggregation methods of PaMPA, and the definition of finite element basis on arbitrary cells.
- **Numerical fluxes** Centered fluxes, exact Godunov' flux for linear hyperbolic systems, and Lax-Friedrich flux. Riemann solvers for Low Mach flows. Numerical flux accurate for steady and unsteady computations.
- **Numerical schemes** Continuous Galerkin method for the Laplace problem (up to fifth order) with non consistent time iteration or with direct matrix inversion. Explicit and implicit discontinuous Galerkin methods for hyperbolic systems, diffusive and advection-diffusion problems. In progress optimization by stocking the geometry for advection problems. SUPG and Residual distribution schemes. Optimization of DG schemes for advection-diffusion problems: stocking of the geometry and use of BLAS for all the linear phases of the scheme.
- **Parallel computing** Mesh redistribution, computation of Overlap with PaMPA. Collective asynchronous communications (PaMPA based). Asynchronous point to point communications. Tests on the cluster Avakas from MCIA, and on Mésocentre de Marseille, and PlaFRIM. Tier-1 Turing (Blue-Gene). Weighted load balancing for hybrid meshes.
- **Postprocessing** High order projections over line postprocessing, possibility of stocking averaged data, such as the average flow and the Reynolds stresses.
- **Quadrature formula** up to 11th order for Lines, Quadrangles, Hexaedra, Pyramids, Prisms, up to 14th order for tetrahedron, up to 21st order for triangles. Gauss-Lobatto type quadrature formula for lines, triangles, quadrangles and hexaedra.
- **Time iteration** explicit Runge-Kutta up to fourth order, explicit Strong Stability Preserving schemes up to third order. Optimized CFL time schemes: SSP(2,3) and SSP(3,4). CFL time stepping. Implicit integration with BDF schemes from 2nd to 6th order Newton method for stationary problems. Implicit unstationary time iterator non consistent in time for stationary problems. Implementation of in house GMRES and conjugate gradient based on Jacobian free iterations.
- **Validation** Poiseuille, Taylor-Green vortex. Laplace equation on a ring and Poiseuille flow on a ring. Volumic forcing based on wall dissipation. Turbulent channel flow.

In 2016, the following features have been added:

- Geometric multigrid methods: aggregation of the mesh based on PaMPA, definition of finite element basis on arbitrary shape cells. Definition of geometry, quadratures and numerical schemes on aggregated finite elements.
- Sutherland law in the Navier-Stokes equations.
- Mass matrix free implementation of discontinuous Galerkin methods.
- Improvement of installation documentation. Spack based installation.
- Implementation of Boussinesq type models and Shallow water discretizations with well balancing, positivity preserving, wet-dry handling, limiters based on entropy viscosity,
- Implementation of Barotropic Euler equations
- Implementation of Taylor-based basis on simplices.

7. New Results

7.1. Heat transfer for effusion flows

The conjugate heat-transfer problem of a flow around a multi-perforated plate under realistic conditions has been addressed by the coupling of the LES-AVBP solver for the flow and the AVTP for solving the heat equation in the solid. A description of the topology of the heat exchange has been realized for the aspiration and injection sides of the walls as well as in the inner side of the holes. This work highlights the potential of such a fluid-solid coupling strategy in the description of the heat exchange distribution for combustor liners. Different analytical expressions have been assessed for each category of exchange surface.[15]

7.2. All-Mach numerical fluxes

This study was split into three self-consistent parts. In the first one, the low Mach number problem through a linear analysis of a perturbed linear wave equation was defined and analyzed. Then, we show how to modify Godunov type schemes applied to the linear wave equation to make this scheme accurate at any Mach number. This allows to define an all Mach correction and to propose a linear all Mach Godunov scheme for the linear wave equation. In the second one, we apply the all Mach correction proposed previously to the case of the non-linear barotropic Euler system when the Godunov type scheme is a Roe scheme. A linear stability result is proposed and a formal asymptotic analysis justifies the construction in this non-linear case by showing how this construction is related with the linear analysis. At last, we apply the all Mach correction to the case of the full Euler compressible system. Numerous numerical results justify the theoretical results and show that the obtained all Mach Godunov type schemes are both accurate and stable for all Mach numbers. We also underline that the proposed approach can be applied to other schemes and allows to justify other existing all Mach schemes.

7.3. Extension and validation of the EB-RSM model

The EB-RSM RANS turbulence model, an innovative model based on second moment closure, has been developed for almost 15 years and is now gradually deployed in the industrial practise. It is already implemented in several industrial codes (Code_Saturne, StarCCM+, EZNSS), as well as the open-source code OpenFOAM. In collaboration with industrial partners, the model is now being confronted to more and more complex industrial configurations: Wall-cooling using impinging jets; Measurement/control of head losses in pipes or injectors via local restrictions of the section (diaphragms); Turbine blade cooling by pin matrices; Control of boundary layer separation by local blowing to exploit the Coanda effect; Wing-tip vortices around airfoils representative of the spoilers of Formula One racing cars; Open-water propeller. All these results confirm the interest of the model compared to well-established models, and its numerical robustness.

7.4. Creation of a database of a direct numerical simulation of a jet in cross flow with and without gyration and with non isothermal flows

This year, we performed the direct numerical simulation of a jet in cross flow without gyration and with a 90° skidding with respect to the cross flow, and with a cross flow 800 Kelvin hotter than the jet. The Sutherland law was implemented for accounting for viscous effects in the non isothermal case and was validated. Then direct numerical simulations have been performed, by using synthetic eddy methods for inlet boundary conditions. Third order discretization was used. A limiter on the density was also used for damping oscillations in strong shear layers, which in this case include both large density and velocity gradients.

The database contains the mean flow at all points, the Reynolds tensor at the degrees of freedom, and the time dependent data at some probes.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

- Collaborative research contract with EDF (UPPA): “Nouveau modèle de turbulence Haut-Bas Reynolds avec prise en compte de la thermique active ou passive. (New high-low Reynolds number turbulence model accounting for active or passive heat transfer)” associated with the PhD thesis of J.-F. Wald.
- Collaboration contract “OpenLab Fluidics” with PSA (CNRS-UPPA): “Simulation numérique d’écoulements de convection naturelle typique des situations rencontrées dans l’espace sous-capot des véhicules automobiles”.

8.2. Bilateral Grants with Industry

- PhD grant (CIFRE) of J.-F. Wald, EDF, defended in May 2016.
- Internship grant of S. Jameel, PSA, defended in September 2016.

9. Partnerships and Cooperations

9.1. Regional Initiatives

9.1.1. *Predicting pressure losses in aeronautical fuel injectors*

This is a 3-year programme, started mid-2015 and funded by Conseil Régional d’Aquitaine (2014 Call) and two small-size companies, AD Industrie (Gurmençon, France) and GDTECH (Bordes, France). The objective is to investigate the possibility of using advanced RANS or hybrid RANS-LES approaches to better predict the pressure losses in aeronautical fuel nozzles. A one-year post-doc [YM] (ending in May 2016) assessed the capability of EBRSM-based RANS simulations to predict the discharge coefficient and the pressure loss of a fluid flowing through a diaphragm [20].

9.2. National Initiatives

9.2.1. *GIS Success*

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 Yales 2. No specific technical activity has been devoted around those codes during 2016 to the noticeable exception of the post-processing and the publication of results previously obtained with AVBP [15].

9.2.2. *CEMRACS 2016*

Participants: Mohamed Essadki [PhD student, ECP], Jonathan Jung [UPPA, Cagire], Adam Larat [CNRS, ECP], Milan Peltier [PhD student, ECP], Vincent Perrier [Inria, Cagire].

The assessment of the use of a runtime (StarPU) in the context of the recourse to high order method has been at the origin of a joint project called Hodin (High Order DIScontinuous methods with ruNtime) started during CEMRACS 2016. As a first step, a low-order finite volume code has been written using a task driven implementation. This step was necessary to get acquainted with the specificities of StarPU. Then a DG based high order sequel of that FV program running only on CPU’s has been developed and will serve as a basis for the progressive adaptation of AeroSol to such a kind of runtime.

9.2.3. CDMATH

Participation in the CNRS-Needs funded action ⁰ which is aimed at applying mathematics to hydraulic problems. [JJ]

9.3. European Initiatives

9.3.1. FP7 & H2020 Projects

9.3.1.1. IMPACT-AE

Participants: Vincent Perrier [responsible of the team contribution], Pascal Bruel [substitute], Simon Delmas [PhD].

Program: Propulsion

Project acronym: IMPACT-AE

Project title: Intelligent Design Methodologies for Low Pollutant Combustors for Aero-Engines

Duration: 01/11/2011 - 31/05/2016

Coordinator: Roll Royce Deutschland

Other partners:

- France: Insa of Rouen, ONERA, Snecma, Turbomeca.
- Germany: Rolls-Royce Deutschland, MTU Aeo Engine Gmbh, DLR, Technology Institute of Karlsruhe, University of Bundeswehr (Munich)
- Italy: AVIOPROP SRL, AVIO S.P.A., University of Florence
- United Kingdom: Rolls Royce PLC, Cambridge University, Imperial College of Science, Technology and Medecine, Loughborough University.

Abstract: The environmental benefits of low emission lean burn technology in reducing NOx emissions up to 80% will only be effective when these are deployed to a large range of new aero-engine applications. While integrating methodologies for advanced engine architectures and thermodynamic cycles. It will support European engine manufacturers to pick up and keep pace with the US competitors, being already able to exploit their new low emission combustion technology to various engine applications with short turn-around times. Key element of the project will be the development and validation of design methods for low emission combustors to reduce NOx and CO emissions by an optimization of the combustor aero-design process. Preliminary combustor design tools will be coupled with advanced parametrisation and automation tools. Improved heat transfer and NOx models will increase the accuracy of the numerical prediction. The contribution of our team is to create with AeroSol a direct numerical simulations (DNS) database relevant to the configuration of film cooling for subsequent improvement of RANS based simulations of isothermal and non isothermal wall flows with discrete mass transfer.

This program ended in May 2016 and the two final deliverables due by the team and devoted to the DNS of isothermal and non isothermal single jets in crossflow with and without gyration were issued in April and May 2016.

9.3.1.2. SOPRANO

Participants: Rémi Manceau [co-responsible for the team contribution], Pascal Bruel [co-responsible for the team contribution], ? ? [Post doc starting in 2018].

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

⁰<http://cdmath.jimdo.com>

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 Medicine, Loughborough University.

Abstract: For decades, most of the aviation research activities have been focused on the reduction of noise and NO_x 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-NO_x 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 NO_x emissions.

In the SOPRANO project, our objective is to complement the experimental (ONERA) and LES (CERFACS) work by RANS computations of multiperforated plates, 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.

9.4. International Initiatives

9.4.1. Inria International Partners

9.4.1.1. Informal International Partners

- + Collaboration with E. Dick (University of Ghent, Belgium) on the development of schemes for the simulation of unsteady all-Mach flows. [PB, YM]
- + Collaboration with A. Beketaeva and A. Naïmanova (Institute of Mathematics, Almaty, Kazakhstan) related to the simulation of supersonic flows. [PB]
- + Collaboration with S. Dellacherie (Montréal Polytechnic Institute, Canada) related to all-Mach flow simulations. [JJ]
- + Collaboration with S. Lardeau (CD-Adapco, Londres, UK) on the EB-RSM model for industrial applications. [RM]

9.5. International Research Visitors

9.5.1. Visits of International Scientists

- Prof. Sergio Elaskar (Conicet and University National of Cordoba, Argentina) visited LMAP-Cagire for a 3-week stay from October 17 to November 5, 2016. Common subjects of interest were identified regarding intermittency, unsteady boundary conditions for low Mach flow and future use of AeroSol.
- Alireza Mazaheri (Nasa, Langley, USA) Hyperbolic discretization of nonlinear diffusive terms for Navier Stokes equations.

9.5.1.1. Internships

- Nicolas Hernandez from Technical University S. Maria (Chile). The objective of the stay was to compare velocity measured by LDV and PIV. When applied to MAVERIC, the results of this analysis show that to improve the coherence between LDV and PIV, an increase in the pixel size of the PIV image of particles should be sought.
- Saad Jameel from the International Master Program *Turbulence* of the Ecole Centrale de Lille/University of Poitiers. This internship, in the framework of the just-started collaboration with PSA, aimed at evaluating and overcoming the limitations of eddy-viscosity models for turbulent flows in mixed/natural convection regimes representative of the flow in under-hood space of automobiles in some particular, critical situations.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

10.1.1.1. Member of the Organizing Committees

Member [RM] of the steering committee of the Special Interest Group “Turbulence Modelling” (SIG-15) of ERCOFTAC (European Research COmmittee for Flow, Turbulence and Combustion) that organizes a series of international workshops dedicated to cross-comparisons of the results of turbulence models and experimental/DNS databases.

10.1.2. Scientific Events Selection

10.1.2.1. Member of the Conference Program Committees

- *Intl Symp. Turbulence, Heat and Mass Transfer* [RM]
- *Intl. Symp. Engineering Turbulence Modelling and Measurement* [RM]

10.1.2.2. Reviewer

This year, the team members have reviewed (6) contributions to the following conferences:

- ASME-GT Turbo Expo 2016 (Séoul, South Korea) (2) [PB]
- 6th Int. Symp. Hybrid RANS-LES models, 2016 (Strasbourg, France) (2) [RM]
- 36th IAHR World Congress, 2016 (The Hague, the Netherlands) (2) [RM]

10.1.3. Journal

10.1.3.1. Member of the Editorial Boards

- International Journal of Aerospace Engineering: co-guest editor of the special issue "The Use of Multiperforated Liners in Gas Turbine and Aeroengine Combustion Systems" ⁰ ...[PB]
- Advisory Board of *International Journal of Heat and Fluid Flow* [RM]
- Advisory Board of *Flow, Turbulence and Combustion* [RM]

⁰<https://www.hindawi.com/journals/ijae/osi/>

10.1.3.2. Reviewer - Reviewing Activities

During 2016, the team members reviewed (22) papers for the following journals:

- Aerospace Science and Technology (1) [PB]
- AIAA Journal (2) [RM]
- Comptes Rendus Mécanique (1) [PB]
- Computers and Fluids (3) [PB] [VP]
- Energy and Buildings (1) [PB]
- Experiments in Fluids (1) [RM]
- Flow, Turbulence and Combustion (3) [RM]
- International Journal of Heat and Fluid Flow (2) [RM]
- Journal of Aerospace Lab (1) [PB]
- Journal of Computational Physics (1) [VP]
- Journal of Fluid Mechanics (1) [RM]
- Journal of Petroleum Science and Engineering (1) [PB]
- Nuclear Engineering and Design (2) [RM]
- Parallel Computing (1) [VP]
- Physics of Fluids (1) [RM]

10.1.4. Invited Talks

- Manceau, R., Progress in Hybrid Temporal LES (plenary lecture), Proc. 6th Symp. Hybrid RANS-LES Methods, Strasbourg, France, 2016

10.1.5. Research Administration

- Co-responsible for the organisation of the LMAP seminar⁰ [JJ]
- Member of the LMAP council [PB]
- Member of the IPRA research federation council [RM]

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

Master : "Maths 2: Data analysis", 39h, M1 - Génie Pétrolier, Université de Pau et des Pays de l'Adour, Pau, France. [JJ]

Licence : "Stochastic simulations", 36h, L3 - MIASHS, Université de Pau et des Pays de l'Adour, Pau, France. [JJ]

Licence : "Linear regression and invariance analysis", 19h30, L3 - MIASHS, Université de Pau et des Pays de l'Adour, Pau, France. [JJ]

Master : "Finite volumes for hyperbolic systems and compressible fluid mechanics", 24h75, M2 - MMS, Université de Pau et des Pays de l'Adour, Pau, France. [VP]

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]

⁰<http://lma-umr5142.univ-pau.fr/live/seminaires>

10.2.2. Supervision

PhD Jean-François Wald, Adaptive wall treatment for a second moment closure in the industrial context , Université de Pau et des Pays de l'Adour, France, defended 10 May 2016, Supervisor: [RM].

PhD in progress : Nurtoleu Shakhan, Modelling and simulation of supersonic jet in crossflow, University of Al Faraby (Almaty, Kazakhstan), started October 2013 (the thesis subject has been modified mid-2014)), Supervisor: A. Naïmanova and Co-Supervisor :[PB].

Young Engineer: Benjamin Lux, Implementation of h-p multigrid in Aerosol, Supervisor: [VP]

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):

- PhD: F. Laurendeau, "Analyse expérimentale et modélisation numérique d'un actionneur plasma de type jet synthétique", University of Toulouse, France, 18 October 2016. Supervisors: G. Casalis and F. Chedeveigne. [RM, referee]
- PhD: G. Arroyo-Callejo « Modélisation thermique avancée d'une paroi multi-perforée de chambre de combustion aéronautique avec dilution giratoire » University of Toulouse, France, 3 May 2016. Supervisor: P. Millan. [PB, referee]
- PhD: M. Nini, "Analysis of a novel hybrid RANS/LES technique based on Reynolds stress tensor reconstruction", Politecnico di Milano, Italy, 3 March 2016. Supervisors: Antonella Abba and Massimo Germano. [RM, referee]
- PhD: L. Labarrère "Étude théorique et numérique de la combustion à volume constant appliquée à la propulsion », University of Toulouse, France, 21 March 2016. Supervisor and co-supervisor: T. Poinsot et A. Dauplain. [PB]
- PhD: V. Popie « Modélisation asymptotique de la réponse acoustique de plaques perforées dans un cadre linéaire avec étude des effets visqueux », University of Toulouse, France, 14 January 2016. Supervisor and co-supervisor: S. Tordeux et E. Piot. [PB]

10.3. Popularization

- Unithé ou café, "Modelling and approximation in fluid mechanics", 21 June 2016, Inria BSO Center. [JJ]

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Major publications by the team in recent years

- [1] S. DELLACHERIE, J. JUNG, P. OMNES, P.-A. RAVIART. *Construction of modified Godunov type schemes accurate at any Mach number for the compressible Euler system*, in "Mathematical Models and Methods in Applied Sciences", November 2016 [DOI : 10.1142/S0218202516500603], <https://hal.archives-ouvertes.fr/hal-00776629>.
- [2] J.-L. FLORENCIANO, P. BRUEL. *LES fluid-solid coupled calculations for the assessment of heat transfer coefficient correlations over multi-perforated walls*, in "Aerospace Science and Technology", 2016, vol. 53, 13 [DOI : 10.1016/J.AST.2016.03.004], <https://hal.inria.fr/hal-01353952>.
- [3] E. FRANQUET, V. PERRIER. *Runge-Kutta discontinuous Galerkin method for interface flows with a maximum preserving limiter*, in "Computers and Fluids", March 2012, vol. 65, p. 2-7 [DOI : 10.1016/J.COMPFLUID.2012.02.021], <https://hal.inria.fr/hal-00739446>.

- [4] E. FRANQUET, V. PERRIER. *Runge-Kutta discontinuous Galerkin method for the approximation of Baer and Nunziato type multiphase models*, in "Journal of Computational Physics", February 2012, vol. 231, n^o 11, p. 4096-4141 [DOI : 10.1016/J.JCP.2012.02.002], <https://hal.inria.fr/hal-00684427>.
- [5] J.-M. HÉRARD, J. JUNG. *An interface condition to compute compressible flows in variable cross section ducts*, in "Comptes Rendus Mathématique", February 2016 [DOI : 10.1016/J.CRMA.2015.10.026], <https://hal.inria.fr/hal-01233251>.
- [6] R. MANCEAU. *Recent progress in the development of the Elliptic Blending Reynolds-stress model*, in "Int. J. Heat Fluid Fl.", 2015, vol. 51, p. 195-220, <http://dx.doi.org/10.1016/j.ijheatfluidflow.2014.09.002>.
- [7] Y. MOGUEN, P. BRUEL, E. DICK. *Semi-implicit characteristic-based boundary treatment for acoustics in low Mach number flows*, in "Journal of Computational Physics", 2013, vol. 255, p. 339-361 [DOI : 10.1016/J.JCP.2013.08.019], <http://hal.inria.fr/hal-00929713>.
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- [9] B. DE LAAGE DE MEUX, B. AUDEBERT, R. MANCEAU, R. PERRIN. *Anisotropic Linear Forcing for synthetic turbulence generation in LES and hybrid RANS/LES modeling*, in "Phys. Fluids", 2015, vol. 27, n^o 035115, <http://dx.doi.org/10.1063/1.4916019>.

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Doctoral Dissertations and Habilitation Theses

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Articles in International Peer-Reviewed Journal

- [11] F. DEHOUX, S. BENHAMADOUCHE, R. MANCEAU. *An elliptic blending differential flux model for natural, mixed and forced convection*, in "International Journal of Heat and Fluid Flow", 2016 [DOI : 10.1016/J.IJHEATFLUIDFLOW.2016.09.003], <https://hal.inria.fr/hal-01391900>.
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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

Keywords:

Computer Science and Digital Science:

- 6.1.1. - Continuous Modeling (PDE, ODE)
- 6.1.4. - Multiscale modeling
- 6.1.5. - Multiphysics modeling
- 6.2.1. - Numerical analysis of PDE and ODE
- 6.2.6. - Optimization
- 6.2.8. - Computational geometry and meshes
- 6.3.1. - Inverse problems
- 6.3.4. - Model reduction
- 6.3.5. - Uncertainty Quantification

Other Research Topics and Application Domains:

- 3.3.2. - Water: sea & ocean, lake & river
- 3.3.3. - Littoral
- 3.4.1. - Natural risks
- 4.3.2. - Hydro-energy
- 5.2.1. - Road vehicles
- 5.2.3. - Aviation
- 5.2.4. - Aerospace
- 5.5. - Materials

1. Members

Research Scientists

- Pietro Marco Congedo [Inria, Researcher, HDR]
- Maria Kazolea [Inria, Researcher]
- Mario Ricchiuto [Team leader, Inria, Senior Researcher, HDR]

Faculty Members

- H eloise Beaugendre [Bordeaux INP, Associate Professor, HDR]
- Mathieu Colin [Bordeaux INP, Associate Professor, HDR]
- Cecile Dobrzynski [Bordeaux INP, Associate Professor]
- Luc Mieussens [Bordeaux INP, Professor]

Technical Staff

- Algiane Froehly [Univ. Bordeaux]
- Nikolaos Pattakos [Inria (SED)]
- Jean Mercat [Inria]

PhD Students

- Luca Arpaia [Inria]
- Stevan Bellec [Univ. Bordeaux]
- Umberto Bosi [Inria]
- Andrea Cortesi [Inria]

Aurore Fallourd [Univ. Bordeaux, from Oct 2016]
Andrea Filippini [Inria]
Xi Lin [Univ. Bordeaux]
Leo Nouveau [Inria]
Simon Peluchon [CEA]
Nassim Auguste Razaaly Jamal [Inria]
Barbara Re [Politecnico di Milano, until Sep 2016]
Mickael Rivier [Inria]
François Sanson [Inria]
Quentin Viville [Univ. Bordeaux]

Post-Doctoral Fellows

Sebastien de Brye [Univ. Bordeaux]
Ghina El Jannoun [Inria, until Feb 2016]
Marco Lorini [Inria, from Nov 2016]
Giorgio Martalo [Univ. Bordeaux]

Administrative Assistants

Anne-Laure Gautier [Inria]
Nicolas Jahier [Inria]

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 [131], [67]. 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 [73], [98]. 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 propagate [75]. 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 [81], [93], [111], [67] or for wave energy conversion [91]), or parametric studies of complex environments (e.g. harbour dynamics [100], or estuarine hydrodynamics [62]), or hazard assessment and prevention [95]. 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 [135]. 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 [57], [124]. 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 [83]). 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 standard way a certification study may be conducted 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 [103] 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,

evaluation 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, and 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 form 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 analogs 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 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 anisotropic finite element 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 [106], [110] 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 [60] 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 initial results of [64], [66] by developing more robust nonlinear variants allowing to embed rapidly moving objects. For this the use of non-linear mesh PDEs (cf e.g. [120], [127], [76]), combined with Bezier type approximations for the mesh displacements to accommodate high order curved meshes [60], 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 [107], [113], [112] 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. [86], [133], [132] 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. [61], [96], [134], [84] 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 [66], [64]. 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, and 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 [65]. 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. [105]). The use of penalization will also provide a natural setting to compute immediate approximations of the forces on the immersed body [111], [114]. 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 [97], or on some iterative Defect Correction method (see e.g. [78]) ;
- 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 [92] 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 methods 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 [122], [63], [123] 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 [77], allowing to have a more flexible approach similar to the so-called P^pP^m method [89], [126]. 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 [94] ;

- 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 [74], as well as spatial partitioning techniques [102]. 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 remeshing 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 [59]. 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 [59], 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 [59] 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 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 reasons, 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 Simplex² method [82];
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 Simplex² 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 immersed boundary capturing of moving ice debris, whose movements are computed using basic mechanical laws.

In [68] 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 [58], [114]. In these methods we compensate for the error at solid walls introduced by the penalization by using anisotropic mesh adaptation [87], [104], [105]. 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 [70]. 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 [72], [67] 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 [118], 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. Space re-entry

As already mentioned, atmospheric re-entry involves multi-scale fluid flow physics including highly rarefied effects, aerothermochemistry, radiation. All this must be coupled to the response of thermal protection materials to extreme conditions. This response is most often the actual objective of the study, to allow the certification of Thermal Protection Systems (TPS).

One of the applications we will consider is the so-called post-flight analysis of a space mission. This involves reconstructing the history of the re-entry module (trajectory and flow) from data measured on the spacecraft by means of a Flush Air Data System (FADS), a set of sensors flush mounted in the thermal protection system to measure the static pressure (pressure taps) and heat flux (calorimeters). This study involves the accurate determination of the freestream conditions during the trajectory. In practice this means determining temperature, pressure, and Mach number in front of the bow shock forming during re-entry. As shown by zur Nieden and Olivier [136], state of the art techniques for freestream characterization rely on several approximations, such as e.g. using an equivalent calorically perfect gas formulas instead of taking into account the complex aero-thermo-chemical behaviour of the fluid. These techniques do not integrate measurement errors nor the heat flux contribution, for which a correct knowledge drives more complex models such as gas surface interaction. In this context, CFD supplied with UQ tools permits to take into account chemical effects and to include both measurement errors and epistemic uncertainties, e.g. those due to the fluid approximation, on the chemical model parameters in the bulk and at the wall (surface catalysis).

Rebuilding the freestream conditions from the stagnation point data therefore amounts to solving a stochastic inverse problem, as in robust optimization. Our objective is to build a robust and global framework for rebuilding freestream conditions from stagnation-point measurements for the trajectory of a re-entry vehicle. To achieve this goal, methods should be developed for

- an accurate simulation of the flow in all the regimes, from rarefied, to transitional, to continuous ;
- providing a complete analysis about the reliability and the prediction of the numerical simulation in hypersonic flows, determining the most important source of error in the simulation (PDE model, discretization, mesh, etc)
- reducing the overall computational cost of the analysis .

Our work on the improvement of the simulation capabilities for re-entry flows will focus both on the models and on the methods. We will in particular provide an approach to extend the use of standard CFD models in the transitional regime, with CPU gains of several orders of magnitude w.r.t. Boltzmann solvers. To do this we will use the results of a boundary layer analysis allowing to correct the Navier-Stokes equations. This theory gives modified (or extended) boundary conditions that are called "slip velocity" and "temperature jump" conditions. This theory seems to be completely ignored by the aerospace engineering community. Instead, people rather use a simpler theory due to Maxwell that also gives slip and jump boundary conditions: however, the coefficients given by this theory are not correct. This is why several teams have tried to modify these coefficients by some empirical methods, but it seems that this does not give any satisfactory boundary conditions.

Our project is twofold. First, we want to revisit the asymptotic theory, and to make it known in the aerospace community. Second, we want to make an intensive sensitivity analysis of the model to the various coefficients of the boundary conditions. Indeed, there are two kinds of coefficients in these boundary conditions. The first one is the accommodation coefficient: in the kinetic model, it gives the proportion of molecules that are specularly reflected, while the others are reflected according to a normal distribution (the so-called diffuse reflexion). This coefficient is a data of the kinetic model that can be measured by experiments: it depends on the material and the structure of the solid boundary, and of the gas. Its influence on the results of a Navier-Stokes simulation is certainly quite important. The other coefficients are those of the slip and jump boundary conditions: they are issued from the boundary layer analysis, and we have absolutely no idea of the order of magnitude of their influence on the results of a Navier-Stokes solution. In particular, it is not clear if these results are more sensitive to the accommodation coefficient or to these slip and jump coefficients.

In this project, we shall make use of the expertise of the team on uncertainty quantification to investigate the sensitivity of the Navier-Stokes model with slip and jump coefficients to these various coefficients. This would be rather new in the field of aerospace community. It could also have some impacts in other sciences in which slip and jump boundary conditions with incorrect coefficients are still used, like for instance in spray simulations: for very small particles immersed in a gas, the drag coefficient is modified to account for rarefied effects (when the radius of the particle is of the same order of magnitude as the mean free path in the gas), and slip and jump boundary conditions are used.

Another application which has very close similarities to the physics of de-anti icing systems is the modelling of the solid and liquid ablation of the thermal protective system of the aircraft. This involves the degradation and recession of the solid boundary of the protection layer due to the heating generated by the friction. As in the case of de-anti icing systems, the simulation of these phenomena need to take into account the heat conduction in the solid, its phase change, and the coupling between a weakly compressible and a compressible phase. Fluid/Solid coupling methods are generally based on a weak approach. Here we will both study, by theoretical and numerical techniques, a strong coupling method for the interaction between the fluid and the solid, and, as for de-anti icing systems, attempt at developing appropriate asymptotic models. These would constitute some sort of thin layer/wall models to couple to the external flow solver.

These modelling capabilities will be coupled to high order adaptive discretizations to provide high fidelity flow models. One of the most challenging problems is the minimization of the influence of mesh and scheme on the wall conditions on the re-entry module. To reduce this influence, we will investigate both high order adaptation across the bow shock, and possibly adaptation based on uncertainty quantification high order moments related to the heat flux estimation, or shock fitting techniques [71], [109]. These tools will be coupled to our robust inverse techniques. One of our objectives is to development of a low-cost strategy for improving the numerical prediction by taking into account experimental data. Some methods have been recently introduced [117] for providing an estimation of the numerical errors/uncertainties. We will use some metamodels for solving the inverse problem, by considering all sources of uncertainty, including those on physical models. We will validate the framework using the experimental data available in strong collaboration with the von Karman Institute for Fluid dynamics (VKI). In particular, data coming from the VKI Longshot facility will be used. We will show application of the developed numerical tool for the prediction in flight conditions.

These activities will benefit from our strong collaborations with the CEA and with the von Karman Institute for Fluid Dynamics and ESA.

4.3. 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

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

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 than 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 $\Gamma \ll 1$, 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 [80]). 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 [135], 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 [91], 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 anisotropic 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 [91], asymptotic models for 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 OCEANerant 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).

4.4. 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 [121].

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 with 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 for the transport equations (Fick's laws) with chemical reactions sources, plus a potential model for the flow of oxide [83], [88], [119]. 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 (see e.g. [79]) 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.

4.5. 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 [101], [125], [116], [85], to hybrid methods coupling dispersive PDEs with hyperbolic ones, and trying to mimic wave breaking with travelling bores [129], [130], [128], [99], [92]. 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 investigated, 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 [69].

5. New Software and Platforms

5.1. AeroSol

Participants: Simon Delmas [Universit de Bordeaux], Sbastien de Brye [Universit de Bordeaux], Benjamin Lux [Cagire], Nikolaos Pattakos [Cardamom], Vincent Perrier [Cagire, correspondent], Mario Ricchiuto [Cardamom].

Developed since 2011 by V. Perrier in partnership with the Cardamom Inria team, the AeroSol library is a high order finite element library written in C++. The code design has been carried for being able to perform efficient computations, with continuous and discontinuous finite element methods on hybrid and possibly curvilinear meshes.

The work of the Cardamom team is focused on continuous finite element methods, while we focus on discontinuous Galerkin methods. However, everything is done for sharing the largest possible part of code. The distribution of the unknowns is made with the software PaMPA, first developed within the Inria teams Bacchus and Castor, and currently maintained in the Tadaam team.

The generic features of the library are Adaptive wall treatment for a second moment closure in the industrial context

- **High order.** It can be theoretically any order of accuracy, but the finite element basis, and quadrature formula are implemented for having up to a fifth order of accuracy.
- **Hybrid and curvilinear meshes.** AeroSol can deal with up to fifth order conformal meshes composed of lines, triangles, quadrangles, tetrahedra, hexahedra, prism, and pyramids.
- **Continuous and discontinuous discretization.** AeroSol deals with both continuous and discontinuous finite element methods.

We would like to emphasize three assets of this library:

- **Its development environment** For allowing a good collaborative work and a functional library, a strong emphasis has been put on the use of modern collaborative tools for developing our software. This includes the active use of a repository, the use of CMake for the compilation, the constant development of unitary and functional tests for all the parts of the library (using CTest), and the use of the continuous integration tool Jenkins for testing the different configurations of AeroSol and its dependencies. Efficiency is regularly tested with direct interfacing with the PAPI library or with tools like scalasca.
- **Its genericity** A lot of classes are common to all the discretization, for example classes concerning I/O, finite element functions, quadrature, geometry, time integration, linear solver, models and interface with PaMPA. Adding simple features (e.g. models, numerical flux, finite element basis or quadrature formula) can be easily done by writing the class, and declaring its use in only one class of the code.
- **Its efficiency** This modularity is achieved by means of template abstraction for keeping good performances. Dedicated efficient implementation, based on the data locality of the discontinuous Galerkin method has been developed. As far as parallelism is concerned, we use point-to-point communications, the HDF5 library for parallel I/O. The behavior of the AeroSol library at medium scale (1000 to 2000 cores) was studied in [108].

The AeroSol project fits with the first axis of the Bordeaux Sud Ouest development strategy, which is to build a coherent software suite scalable and efficient on new architectures, as the AeroSol library relies on several tools developed in other Inria teams, especially for the management of the parallel aspects. At the end of 2015, AeroSol had the following features:

- **Boundary conditions** Periodic boundary conditions, time-dependent inlet and outlet boundary conditions. Adiabatic wall and isothermal wall. Steger-Warming based boundary condition. Synthetic Eddy Method for generating turbulence.
- **C++/Fortran interface** Tests for binding fortran with C++.
- **Development environment** An upgraded use of CMake for compilation (gcc, icc and xlc), CTest for automatic tests and memory checking, lcov and gcov for code coverage reports. A CDash server for collecting the unitary tests and the memory checking. An under development interface for functional tests. Optional linking with HDF5, PAPI, with dense small matrices libraries (BLAS, Eigen). An updated shared project Plafrim and joint project Aerosol/Scotch/PaMPA project on the continuous integration platform. An on-going integration of SPack for handling dependencies. A fixed ESSL interface.
- **Finite elements** up to fourth degree for Lagrange finite elements and hierarchical orthogonal finite element basis (with Dubiner transform on simplices) on lines, triangles, quadrangles, tetrahedra, prisms, hexaedra and pyramids. Finite element basis that are interpolation basis on Gauss-Legendre points for lines, quadrangles, and hexaedra, and triangle (only 1st and 2nd order).
- **Geometry** Elementary geometrical functions for first order lines, triangles, quadrangles, prisms, tetrahedra, hexaedra and pyramids. Handling of high order meshes.
- **In/Out** Link with the XML library for handling with parameter files. Parallel reader for GMSH, with an embedded geometrical pre-partitioner. Writer on the VTK-ASCII legacy format (cell and point centered). Parallel output in vtu and pvtu (Paraview) for cell-centered visualization, and XDMF/HDF5 format for both cell and point centered visualization. Ability of saving the high order solution and restarting from it. Computation of volumic and probe statistics. Ability of saving averaged layer data in quad and hexa meshes. Ability of defining user defined output visualization variables.
- **Instrumentation** Aerosol can give some traces on memory consumption/problems with an interfacing with the PAPI library. Tests have also been performed with VTUNE and TAU. Tests with Maqao and Scalasca (VIHPS workshop).

- **Linear Solvers** Link with the external linear solver UMFPack, PETSc and MUMPS. Internal solver for diagonal and block-diagonal matrices.
- **Memory handling** discontinuous and continuous, sequential and parallel discretizations based on PaMPA for generic meshes, including hybrid meshes.
- **Models** Perfect gas Euler system, real gas Euler system (template based abstraction for a generic equation of state), scalar advection, Waves equation in first order formulation, generic interface for defining space-time models from space models. Diffusive models: isotropic and anisotropic diffusion, compressible Navier-Stokes. Scalar advection-diffusion model. Linearized Euler equations, and Sutherland model for non isothermal diffusive flows. Shallow-water model.
- **Multigrid** Development of p -multigrid methods. This includes also the possibility of beginning a computation with an order and to decrease or increase the order of approximation when restarting. For the p multigrid methods, V and W cycle have been developed, and restriction and prolongation operators have also been developed. In progress implementation of h -multigrid, with the development of tests of the aggregation methods of PaMPA, and the definition of finite element basis on arbitrary cells.
- **Numerical fluxes** Centered fluxes, exact Godunov' flux for linear hyperbolic systems, and Lax-Friedrich flux. Riemann solvers for Low Mach flows. Numerical flux accurate for steady and unsteady computations.
- **Numerical schemes** Continuous Galerkin method for the Laplace problem (up to fifth order) with non consistent time iteration or with direct matrix inversion. Explicit and implicit discontinuous Galerkin methods for hyperbolic systems, diffusive and advection-diffusion problems. In progress optimization by stocking the geometry for advection problems. SUPG and Residual distribution schemes. Optimization of DG schemes for advection-diffusion problems: stocking of the geometry and use of BLAS for all the linear phases of the scheme.
- **Parallel computing** Mesh redistribution, computation of Overlap with PaMPA. Collective asynchronous communications (PaMPA based). Asynchronous point to point communications. Tests on the cluster Avakas from MCIA, and on Mésocentre de Marseille, and PlaFRIM. Tier-1 Turing (Blue-Gene). Weighted load balancing for hybrid meshes.
- **Postprocessing** High order projections over line postprocessing, possibility of stocking averaged data, such as the average flow and the Reynolds stresses.
- **Quadrature formula** up to 11th order for Lines, Quadrangles, Hexaedra, Pyramids, Prisms, up to 14th order for tetrahedron, up to 21st order for triangles. Gauss-Lobatto type quadrature formula for lines, triangles, quadrangles and hexaedra.
- **Time iteration** explicit Runge-Kutta up to fourth order, explicit Strong Stability Preserving schemes up to third order. Optimized CFL time schemes: SSP(2,3) and SSP(3,4). CFL time stepping. Implicit integration with BDF schemes from 2nd to 6th order Newton method for stationary problems. Implicit unstationary time iterator non consistent in time for stationary problems. Implementation of in house GMRES and conjugate gradient based on Jacobian free iterations.
- **Validation** Poiseuille, Taylor-Green vortex. Laplace equation on a ring and Poiseuille flow on a ring. Volumic forcing based on wall dissipation. Turbulent channel flow.

In 2016, the following features have been added:

- Geometric multigrid methods: aggregation of the mesh based on PaMPA, definition of finite element basis on arbitrary shape cells. Definition of geometry, quadratures and numerical schemes on aggregated finite elements.
- Sutherland law in the Navier-Stokes equations.
- Mass matrix free implementation of discontinuous Galerkin methods.
- Improvement of installation documentation. Spack based installation.
- Implementation of Boussinesq type models and Shallow water discretizations with well balancing, positivity preserving, wet-dry handling, limiters based on entropy viscosity,
- Implementation of Barotropic Euler equations
- Implementation of Taylor-based basis on simplices.

5.2. CAKE

KEYWORDS: Moving bodies, Rarefied flows

- Contact: Luc Mieussens
- URL: <http://www.cake-solver.com/>

FUNCTIONAL DESCRIPTION

Cake (Cut cell Algorithm for Kinetic Equations) can simulate 2D plane rarefied flows around moving obstacles, by using an immersed boundary technique with Cartesian grids. This code can simulate flows induced by temperature gradients, like the thermal creep flow. It has for instance been applied to the simulation of the Crookes radiometer.

5.3. Crysa

KEYWORDS: Image processing, structural analysis, 2D crystallography

- Participants: Jean Mercat and Cécile Dobrzynski
- Partners: ISM - LCPO - LCTS (UMR 5801)
- Contact: Cécile Dobrzynski

Crysa is a library allowing to study the organization of objects once placed in an hexagonal grid thus allowing to analyze the crystal structure/organization of an image. The library allows to detect regions of coherence in an image of crystals, and it allows to determine e.g. the good separation of objects in an experiment (new polymeric materials, plasma, ...).

5.4. Cut-ANOVA

KEYWORDS: Stochastic models - Uncertainty quantification

- Participants: Pietro-Marco Congedo
- Contact: Pietro-Marco Congedo

SCIENTIFIC DESCRIPTION

An anchored analysis of variance (ANOVA) method is proposed to decompose the statistical moments. Compared to the standard ANOVA with mutually orthogonal component functions, the anchored ANOVA, with an arbitrary choice of the anchor point, loses the orthogonality if employing the same measure. However, an advantage of the anchored ANOVA consists in the considerably reduced number of deterministic solver's computations, which renders the uncertainty quantification of real engineering problems much easier. Different from existing methods, the covariance decomposition of the output variance is used in this work to take account of the interactions between non-orthogonal components, yielding an exact variance expansion and thus, with a suitable numerical integration method, provides a strategy that converges. This convergence is verified by studying academic tests. In particular, the sensitivity problem of existing methods to the choice of anchor point is analyzed via the Ishigami case, and we point out that covariance decomposition survives from this issue. Also, with a truncated anchored ANOVA expansion, numerical results prove that the proposed approach is less sensitive to the anchor point. The covariance-based sensitivity indices (SI) are also used, compared to the variance-based SI. Furthermore, we emphasize that the covariance decomposition can be generalized in a straightforward way to decompose higher-order moments. For academic problems, results show the method converges to exact solution regarding both the skewness and kurtosis. The proposed method can indeed be applied to a large number of engineering problems.

FUNCTIONAL DESCRIPTION

The Cut-ANOVA code (Fortran 90, MPI + OpenMP) is devoted to the stochastic analysis of numerical simulations. The method implemented is based on the spectral expansion of "anchored ANOVA", allowing the covariance-based sensitivity analysis. Compared to the conventional Sobol method, "Cut-ANOVA" provides three sensitivity indices instead of one, which allows a better analysis of the reliability of the numerical prediction. On the other hand, "Cut-ANOVA" is able to compute the higher order statistical moments such as the Skewness (3-rd order moment) and Kurtosis (4-th order moment). Several dimension reduction techniques have also been implemented to reduce the computational cost. Finally, thanks to the innovative method implemented into the Code Cut-ANOVA, one can obtain a similar accuracy for stochastic quantities by using a considerably less number of deterministic model evaluations, compared with the classical Monte Carlo method.

5.5. Fmg

KEYWORDS: Mesh adaptation, mesh deformation, elasticity, laplacian mesh equation

- Participants: Cécile Dobrzynski, Mario Ricchiuto, Leo Nouveau and Luca Arpaia
- Contact: Cécile Dobrzynski

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. This year a new semi-linear elasticity formulation has been implemented involving a constant coefficient PDE with a nonlinear *force* accounting for the smoothness of the target function. The advantage of this approach is that the non-linearity does not influence the elastic differential operator thus leading to a description of the deformation governed by a time-invariant matrix even in unsteady simulations. Other developments currently implemented in SLOWS are being imported in FMG.

5.6. MMG3D

KEYWORDS: Mesh - Anisotropic - Mesh adaptation

- Participants: Cécile Dobrzynski, Pascal Frey, Charles Dapogny and Algiane Froehly
- Partners: CNRS - IPB - Université de Bordeaux - UPMC
- Contact: Cécile Dobrzynski
- URL: <http://www.mmgttools.org>

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 of 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 reconstructed from the piecewise linear mesh using cubic Bezier triangular patches. The surface mesh is modified to respect a maximal Hausdorff distance between the ideal geometry and the mesh.

Inside the volume, the software performs 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. It is dedicated to the modification of 3D volume meshes. It performs the adaptation and the optimization of a tetrahedral mesh and allows to discretize an isovalue.

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

5.7. Mmg platform

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

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

SCIENTIFIC DESCRIPTION

The Mmg platform 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 of 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 patches. 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 platform 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.

5.8. NOMESH

- Participants: Cécile Dobrzynski and Algiane Froehly
- Partners: CNRS - IPB - Université de Bordeaux
- Contact: Cécile Dobrzynski

KEYWORDS: Mesh - Curved mesh - Tetrahedral mesh

FUNCTIONAL DESCRIPTION

NOMESH is a software allowing the generation of three order curved simplicial meshes. Starting from a "classical" mesh with straight elements composed by triangles and/or tetrahedra, we are able to curve the boundary mesh. Starting from a mesh with some curved elements, we can verify if the mesh is valid, that means there is no crossing elements and only positive Jacobian. If the curved mesh is non valid, we modify it using linear elasticity equations until having a valid curved mesh.

5.9. SLOWS

KEYWORDS: Free surface flows, Unstructured meshes, shallow water equations, Boussinesq equations

- Participants: Luca Arpaia, Andrea Filippini, Maria Kazolea, Mario Ricchiuto and Nikolaos Pattakos
- Contact: Mario Ricchiuto

FUNCTIONAL DESCRIPTION

SLOWS (Shallow-water fLOWS) 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. The kernel of the CODE is a shallow water solver based on second order residual distribution or second and third order finite volume schemes. Three different approaches are available to march in time, 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. Linear algebraic sparse systems arising in the discretization are solved with This year several enhancements have been implemented

- a correction of both the residual distribution and finite volume methods to solve the shallow water equations in spherical (or Mercator) curvilinear coordinates;
- mass-conserving mesh movement to adapt an initial grid to wet-dry interfaces as well as to other physical features of the flow;
- a new library has been developed to enhance the shallow water equations. This library computes an algebraic source term by inverting an elliptic (grad-div type) PDE. The addition of this term to the shallow water version of SLOWS allows to recover the a fully nonlinear weakly dispersive Green-Naghdi solver. The solution of the elliptic PDE is performed with a classical Galerkin FEM approach, and MUMPS is the MUMPS library is used to invert the resulting matrix;
- Initial optimization and OpenMP parallelization of the shallow water kernel.

SLOWS is our main simulation tool in both the TANDEM and Tides projects.

5.10. Sparse-PDD

Adaptive sparse polynomial dimensional decomposition for global sensitivity analysis

KEYWORDS: Stochastic models - Uncertainty quantification

- Participants: Pietro-Marco Congedo
- Contact: Pietro-Marco Congedo

SCIENTIFIC DESCRIPTION

The polynomial dimensional decomposition (PDD) is employed in this code for the global sensitivity analysis and uncertainty quantification (UQ) of stochastic systems subject to a moderate to large number of input random variables. Due to the intimate structure between the PDD and the Analysis of Variance (ANOVA) approach, PDD is able to provide a simpler and more direct evaluation of the Sobol sensitivity indices, when compared to the Polynomial Chaos expansion (PC). Unfortunately, the number of PDD terms grows exponentially with respect to the size of the input random vector, which makes the computational cost of standard methods unaffordable for real engineering applications. In order to address the problem of the curse of dimensionality, this code proposes essentially variance-based adaptive strategies aiming to build a cheap meta-model (i.e. surrogate model) by employing the sparse PDD approach with its coefficients computed by regression. Three levels of adaptivity are carried out in this code: 1) the truncated dimensionality for ANOVA component functions, 2) the active dimension technique especially for second- and higher-order parameter interactions, and 3) the stepwise regression approach designed to retain only the most influential polynomials in the PDD expansion. During this adaptive procedure featuring stepwise regressions, the surrogate model representation keeps containing few terms, so that the cost to resolve repeatedly the linear systems of the least-square regression problem is negligible. The size of the finally obtained sparse PDD representation is much smaller than the one of the full expansion, since only significant terms are eventually retained. Consequently, a much less number of calls to the deterministic model is required to compute the final PDD coefficients.

FUNCTIONAL DESCRIPTION

This code allows an efficient meta-modeling for a complex numerical system featuring a moderate-to-large number of uncertain parameters. This innovative approach involves polynomial representations combined with the Analysis of Variance decomposition, with the objective to quantify the numerical output uncertainty and its sensitivity upon the variability of input parameters.

5.11. TUCWave

KEYWORDS: free surface flows, Boussinesq equations, weakly nonlinear models, unstructured grids

- Participants: Maria Kazolea, Argiris Delis and Ioannis Nikolos
- Contact: Maria Kazolea

FUNCTIONAL DESCRIPTION

Fortran Planform which accounts for the study of near shore processes. 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. TUCWave is used in the TANDEM project to provide reference solutions with a weakly nonlinear and dispersive model.

6. New Results**6.1. High order discretizations on unstructured meshes**

- Participants: Héloïse Beaugendre, Cécile Dobrzynski, Léo Nouveau, Mario Ricchiuto, Quentin Viville
- Corresponding member: Héloïse Beaugendre

Our work on high order unstructured discretizations this year has pursued three main avenues:

- We have extended the team's previous work on the consistent residual based approximation of viscous flow equations to the framework of Immersed Boundary Methods (IBM). This is an increasingly popular approach in Computational Fluid Dynamics as it simplifies the mesh generation problem. In our work, we consider a technique based on the addition of a penalty term to the Navier-Stokes equations to account for the wall boundary conditions. To adapt the residual distribution method to the IBM, we developed a new formulation based on a Strang splitting approach in time. This approach, couples in a fully consistent manner an implicit asymptotically exact integration procedure of the penalization ODE, with the explicit residual distribution discretization for the Navier-Stokes equations, based on the method proposed in [122]. The ODE integrator provides an operator which is exact up to orders η^2 , with η the penalty parameter assuming values of the order of 10^{-10} . To preserve the accuracy of the spatial discretization in the Navier-Stokes step, we have introduced, in vicinity of the penalised region, a modification of the solution gradient reconstruction required for the evaluation of the viscous fluxes. We have shown formally and numerically that the approach proposed is second order accurate for smooth solutions, and shown its potential when combined with unstructured mesh adaptation strategies w.r.t. the (implicitly described) solid walls [16]. This approach has been combined with r -adaptation techniques to account for moving bodies and validated on simulations involving flapping wings, and computations of ices block trajectories in the framework of the STORM project [56], [46];

- Another research axis consists in proposing a novel approach that allows to use p-adaptation with continuous finite elements. Under certain conditions, primarily the use of a residual distribution scheme, it is possible to avoid the continuity constraint imposed to the approximate solution, while still retaining the advantages of a method using continuous finite elements. The theoretical material, the complete numerical method and practical results show as a proof of concept that p-adaptation is possible with continuous finite elements. This year, we extended the p-adaptation method to Navier-Stokes equations and coupled it with immersed boundary method.
- We have studied the high order approximation of problems with dispersion and suggested a route allowing to construct high order methods (up to order 4) allowing to obtain the same accuracy for the solution, and for its first and second order derivatives. Initial validation for the approach proposed has been shown for the time dependent KdV equations [14], [49].

6.2. High order mesh generation and mesh adaptation

- Participants: Luca Arpaia , Cécile Dobrzynski, Ghina El Jannoun, Léo Nouveau, Mario Ricchiuto
- Corresponding member: Cécile Dobrzynski

This year several new algorithmic improvements have been obtained which will allow to enhance our meshing tools:

- We have enhanced our work on r -adaptation techniques for time dependent equations. These techniques are based on mesh deformations obtained by solving continuous differential equations for the local displacements. These equations are controlled by an error monitor. Several improvements have been made. We have studied in depth the formulation of the coupling of the mesh movement with the flow solver. We have found that for both finite volume and residual distribution methods, a coupling of mesh and solution evolution (by means of an ALE method) provides accuracy enhancements, and is to be preferred to a simpler adapt-project-evolve approach. The method has been fully tested in two space dimensions and preliminary results have been performed in three dimensions. We have applied this technic to immersed boundary methods to compressible simulations. For problems with source terms, and in particular problems admitting some important physical invariants as the shallow water equations, we have solved the conflict between the conservation of either mass or the invariant, allowing for the conservation of both quantities up to machine accuracy. In parallel we have proposed a modified formulation of an elasticity equation allowing to reduce the nonlinearity of the mesh PDE to the force imposed in the right hand side. Initial validation has been shown in [56] and in the PhD of L. Nouveau ;

6.3. Uncertainty Quantification and robust design optimization

- Participants: Andrea Cortesi , Pietro Marco Congedo, Nassim Razaaly, Sanson Francois
- Corresponding member: Pietro Marco Congedo

We have developed an efficient sparse polynomial decomposition for sensitivity analysis and for building a surrogate in a problems featuring a large number of parameters. The Polynomial Dimensional Decomposition (PDD) is employed in this work for the global sensitivity analysis and uncertainty quantification (UQ) of stochastic systems subject to a moderate to large number of input random variables. Due to the intimate connection between the PDD and the Analysis of Variance (ANOVA) approaches, PDD is able to provide a simpler and more direct evaluation of the Sobol sensitivity indices, when compared to the Polynomial Chaos expansion (PC). Unfortunately, the number of PDD terms grows exponentially with respect to the size of the input random vector, which makes the computational cost of standard methods unaffordable for real engineering applications. In order to address the problem of the curse of dimensionality, this work proposes essentially variance-based adaptive strategies aiming to build a cheap meta- model (i.e. surrogate model) by employing the sparse PDD approach with its coefficients computed by regression. Three levels of adaptivity are carried out : 1) the truncated dimensionality for ANOVA component functions, 2) the active dimension technique especially for second- and higher-order parameter interactions, and 3) the stepwise regression

approach designed to retain only the most influential polynomials in the PDD expansion. During this adaptive procedure featuring stepwise regressions, the surrogate model representation keeps containing few terms, so that the cost to resolve repeatedly the linear systems of the least-squares regression problem is negligible. The size of the finally obtained sparse PDD representation is much smaller than the one of the full expansion, since only significant terms are eventually retained. Consequently, a much smaller number of calls to the deterministic model is required to compute the final PDD coefficients.

Concerning sensitivity analysis, we illustrate how third and fourth-order moments, i.e. skewness and kurtosis, respectively, can be decomposed mimicking the ANOVA approach. It is also shown how this decomposition is correlated to a Polynomial Chaos (PC) expansion leading to a simple strategy to compute each term. New sensitivity indices, based on the contribution to the skewness and kurtosis, are proposed. The outcome of the proposed analysis is depicted by considering several test functions. Moreover, the ranking of the sensitivity indices is shown to vary according to their statistics order. Furthermore, the problem of formulating a truncated polynomial representation of the original function is treated. Both the reduction of the number of dimensions and the reduction of the order of interaction between parameters are considered. In both cases, the impact on the reduction is assessed in terms of statistics, namely the probability density function. Feasibility of the proposed analysis in a real-case is then demonstrated by presenting the sensitivity analysis of the performances of a turbine cascade in an Organic Rankine Cycles (ORCs), in the presence of complex thermodynamic models and multiple sources of uncertainty.

Moreover, we have developed a new framework for performing robust design optimization. A strategy is developed to deal with the error affecting the objective functions in uncertainty-based optimization. We refer to the problems where the objective functions are the statistics of a quantity of interest computed by an uncertainty quantification technique that propagates some uncertainties of the input variables through the system under consideration. In real problems, the statistics are computed by a numerical method and therefore they are affected by a certain level of error, depending on the chosen accuracy. The errors on the objective function can be interpreted with the abstraction of a bounding box around the nominal estimation in the objective functions space. In addition, in some cases the uncertainty quantification methods providing the objective functions also supply the possibility of adaptive refinement to reduce the error bounding box. The novel method relies on the exchange of information between the outer loop based on the optimization algorithm and the inner uncertainty quantification loop. In particular, in the inner uncertainty quantification loop, a control is performed to decide whether a refinement of the bounding box for the current design is appropriate or not. In single-objective problems, the current bounding box is compared to the current optimal design. In multi-objective problems, the decision is based on the comparison of the error bounding box of the current design and the current Pareto front. With this strategy, fewer computations are made for clearly dominated solutions and an accurate estimate of the objective function is provided for the interesting, non-dominated solutions. The results presented in this work prove that the proposed method improves the efficiency of the global loop, while preserving the accuracy of the final Pareto front.

Concerning semi-intrusive methods, a novel multiresolution framework, namely the Truncate and Encode (TE) approach is generalized and extended for taking into account uncertainty in partial differential equations (PDEs). Innovative ingredients are given by an algorithm permitting to recover the multiresolution representation without requiring the fully resolved solution, the possibility to treat a whatever form of pdf and the use of high-order (even non-linear, i.e. data-dependent) reconstruction in the stochastic space. Moreover, the spatial-TE method is introduced, which is a weakly intrusive scheme for uncertainty quantification (UQ), that couples the physical and stochastic spaces by minimizing the computational cost for PDEs. The proposed scheme is particularly attractive when treating moving discontinuities (such as shock waves in compressible flows), even if they appear during the simulations as it is common in unsteady aerodynamics applications. The proposed method is very flexible since it can easily be coupled with different deterministic schemes, even with high-resolution features. Flexibility and performances of the present method are demonstrated on various numerical test cases (algebraic functions and ordinary differential equations), including partial differential equations, both linear and non-linear, in presence of randomness.

We applied a part of this method to a problem associated to the atmospheric reentry. In fact, an accurate determination of the catalytic property of thermal protection materials is crucial to design reusable atmospheric entry vehicles. This property is determined by combining experimental measurements and simulations of the reactive boundary layer near the material surface. The inductively-driven Plasmatron facility at the von Karman Institute for Fluid Dynamics provides a test environment to analyze gas-surface interactions under effective hypersonic conditions. In this study, we develop an uncertainty quantification methodology to rebuild values of the gas enthalpy and material catalytic property from Plasmatron experiments. A non-intrusive spectral projection method is coupled with an in-house boundary-layer solver, to propagate uncertainties and provide error bars on the rebuilt gas enthalpy and material catalytic property, as well as to determine which uncertainties have the largest contribution to the outputs of the experiments. We show that the uncertainties computed with the methodology developed are significantly reduced compared to those determined using a more conservative engineering approach adopted in the analysis of previous experimental campaigns.

6.4. Modelling of free surface flows

- Participants: Luca Arpaia , Stevan Bellec , Mathieu Collin , Sebastien De Brye , Andrea Filippini , Maria Kazolea, Luc Mieussens, and Mario Ricchiuto
- Corresponding member: Mario Ricchiuto

We have introduced a new systematic method to obtain discrete numerical models for incompressible free-surface flows. our approach allows to recover discrete asymptotic equations from a semi-discretized form (keeping the vertical z variable and time continuous) of the incompressible Euler equations with free surface. In particular, starting from a (continuous) Galerkin finite element discretization in the horizontal direction, we perform an asymptotic analysis of the resulting semi-discrete system. This has allowed to obtain new discrete equivalents of the Peregrine equations [5], as well as enhanced variants in the spirit of [115]. This has been done in the PhD of S. Bellec. We have demonstrated that the resulting discrete equations present dispersion characteristics much improved w.r.t. those obtained by directly discretizing the asymptotic Boussinesq equations with continuous finite elements. This has been confirmed by numerical experiments on long wave propagation benchmarks. Concerning more classical continuous Boussinesq models, additional work has been done to characterize some of their exact solutions. This has provided some improved solutions to benchmark our codes, as well as some additional knowledge on these models [4].

This year we extended our work on fully non-linear weakly dispersive wave models in two dimensional horizontal coordinates. The proposed framework in [11], to approximate the so-called Green-Naghdi equations is followed. The method proposed, while remaining unsplit in time, is based on a separation of the elliptic and hyperbolic components of the equations. This separation is designed to recover the standard shallow water equations in the hyperbolic step, so that the method can be written as an *algebraic* correction to an existing shallow water code. More precisely, we re-write the standard form of the equations by splitting the original system in its elliptic and hyperbolic parts, through the definition of a new variable, accounting for the dispersive effects and having the role of a non-hydrostatic pressure gradient in the shallow water equations. We consider a two-step solution procedure. In the first step we compute a source term by inverting the elliptic coercive operator associated to the dispersive effects; then in a hyperbolic step we evolve the flow variables by using the non-linear shallow water equations, with all nonhydrostatic effects accounted by the source computed in the elliptic phase. The advantages of this procedure are firstly that the GN equations are used for propagation and shoaling, while locally reverting to the non-linear shallow water equations to model energy dissipation in breaking regions. Secondly and from the numerical point of view, this strategy allows each step to be solved with an appropriate numerical method on arbitrary unstructured meshes. We propose a hybrid finite element (FE) finite volume (FV) scheme, where the elliptic part of the system is discretized by means of the continuous Galerkin FE method and the hyperbolic part is discretized using a third-order node-centered finite volume (FV) technique. This work was a part of Andrea Filippini's PhD and a research paper is under preparation.

We also continue our study on wave breaking techniques on unstructured meshes [55]. In particular, we evaluate the coupling of both a weakly and a fully non-linear Boussinesq system with a turbulence model. We reformulate an evolution model for the turbulent kinetic energy, initially proposed by Nwogu [115], and evaluate its capabilities to provide sufficient dissipation in breaking regions. We also compare this dissipation to the one introduced by the numerical discretization. A research paper on the topic, is under preparation. Further more we studied and tested the application and validation of TUCWave code on the transformation breaking and run-up of irregular waves. Its is the first time that an unstructured high-resolution FV numerical solver for the 2D extended BT equations of Nwogu is tested on the generation and propagation of irregular waves. A research paper is under preparation.

The tools developed have been also used intensively in funded research programs. Within the TANDEM project, several benchmarks relevant to tsunami modelling have been performed and several common publications with the project partners are submitted and/or in preparation [54], [45]. We also our code SLOWS, to study the conditions for tidal bore formation in convergent alluvial estuaries [7]. A new set of dimensionless parameters has been introduced to describe the problem, and the code SLOWS has been used to explore the space of these parameters allowing to determine a critical curve allowing to characterize an estuary as "bore forming" or not. Surprising physical behaviours, in terms of dissipation and nonlinearity of the tides, have been highlighted.

Finally, in collaboration with F. Veron (University of Delaware at Newark, USA), L. Mieussens has developed a model to describe the effect of rain falling on water waves [20]. This model is based on a kinetic description of rain droplets that is used to compute the induced pressure on a water wave. This allows to estimate the dissipation (or amplification) of the wave due to rainy conditions.

6.5. Wave energy conversion hydrodynamics

- Participants: Umberto Bosi, Mario Ricchiuto
- Corresponding member: Mario Ricchiuto

We have developed a prototype spectral element solver for a coupled set of differential equations modelling wave propagation (so-called outer domain), and the submerged flow under a floating body (inner domain). Both systems of equations are depth-averaged (Boussinesq type) systems involving some dispersive terms. They are further coupled to a force balance providing a (system of) ODE(s) for the floater. This model constitutes an intermediate fidelity approximation for the hydrodynamics of a wave energy converter. Differently from all industrial state of the art, it is a (fully) nonlinear model. However, its cost is extremely low when compared to full three-dimensional CFD analyses, due to the dimensional reduction brought from the depth averaged modelling. Last year we have shown the potential of this approach to predict the hydrodynamics of a floater in a simplified case [90], [91] (journal version to appear on *J. Ocean Eng. and Marine Energy*). This year we have further studied the issue of the coupling between domains with different PDE models (as in our case the inner and outer domains), and suggested an approach (based on a first order reformulation) allowing to coupled domains with different equations and with or without dispersive effects on either side. This work is done in the framework of the MIDWEST project funded by the EU OCEANERanet call.

7. Bilateral Contracts and Grants with Industry

7.1. Bilateral Contracts with Industry

Several contracts have been realized:

- SAFRAN-HERAKLES, 20Keuros for the development of a code for computing low-probability.
- CNES, 10 KEuros, for the technological transfer of Sparse-PDD code.
- CEA 2015 10237, 60 Keuro for the supervision of the post-doc of Maxence Clayes by P.M. Congedo
- CEA 16-CIFRE PELUCHON, 20 Keuro for the supervision by L. Mieussens of the PhD of Simon Peluchon at the CEA-CESTA (1/1/15 - 31/12/17)
- BGS IT&E (2016-2018), 20 Keuro for a consulting by M. Ricchiuto on the implantation of some of the technology in the code SLOWS in their in-house model.

8. Partnerships and Cooperations

8.1. Regional Initiatives

CRA 15/ THESE SANSON 10199

These co-funded by Airbus Safran Launchers and the Aquitaine Region during the period 2016-2019

Topic : uncertainty propagation approach in a system of codes

VIPER Projet

These co-funded by the Aquitaine Region and Inria. PhD student to recruit during the period 2017-2020

Topic : robust design of the EVE engine in collaboration with the SME EXOES.

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

Type: Apple à Projets Recherche du Conseil de la Région Aquitaine

Coordinator: M. Ricchiuto

Other partners: UMR EPOC (P. Bonneton)

Abstract: This project proposes to combine modern high order adaptive finite elements techniques with state of the art nonlinear and non-hydrostatic models for free surface waves to provide an accurate tool for the simulation of near shore hydrodynamics, with application to the study and prediction of tidal bores. The Garonne river will be used as a case study. This project co-funds (50%) the PhD of A. Filippini.

8.2. National Initiatives

8.2.1. ANR MAIDESC

Title: Maillages adaptatifs pour les interfaces instationnaires avec deformations, etirements, courbures.

Type: ANR

Duration: 48 months

Starting date : 1st Oct 2013

Coordinator: Dervieux Alain (Inria Sophia)

Abstract: Mesh adaptive numerical methods allow computations which are otherwise impossible due to the computational resources required. We address in the proposed research several well identified main obstacles in order to maintain a high-order convergence for unsteady Computational Mechanics involving moving interfaces separating and coupling continuous media. A priori and a posteriori error analysis of Partial Differential Equations on static and moving meshes will be developed from interpolation error, goal-oriented error, and norm-oriented error. From the minimization of the chosen error, an optimal unsteady metric is defined. The optimal metric is then converted into a sequence of anisotropic unstructured adapted meshes by means of mesh regeneration, deformation, high stretching, and curvature. A particular effort will be devoted to build an accurate representation of physical phenomena involving curved boundaries and interfaces. In association with curved boundaries, a part of studies will address third-order accurate mesh adaption. Mesh optimality produces a nonlinear system coupling the physical fields (velocities, etc.) and the geometrical ones (unsteady metric, including mesh motion). Parallel solution algorithms for the implicit coupling of these different fields will be developed. Addressing efficiently these issues is a compulsory condition for the simulation of a number of challenging physical phenomena related to industrial unsolved or insufficiently solved problems. Non-trivial benchmark tests will be shared by consortium partners and by external attendees to workshops organized by the consortium. The various advances will be used by SME partners and proposed in software market.

8.2.2. PIA TANDEM

Title: Tsunamis in the Atlantic and the English Channel: Definition of the Effects through numerical Modeling (TANDEM)

Type: PIA - RSNR (Investissement d'Avenir, "Recherches en matière de Sécurité Nucléaire et Radioprotection")

Duration: 48 months

Starting date : 1st Jan 2014

Coordinator: H. Hebert (CEA)

Abstract: TANDEM is a project dedicated to the appraisal of coastal effects due to tsunami waves on the French coastlines, with a special focus on the Atlantic and Channel coastlines, where French civil nuclear facilities have been operated since about 30 years. As identified in the call RSNR, this project aims at drawing conclusions from the 2011 catastrophic tsunami, in the sense that it will allow, together with a Japanese research partner, to design, adapt and check numerical methods of tsunami hazard assessment, against the outstanding observation database of the 2011 tsunami. Then these validated methods will be applied to define, as accurately as possible, the tsunami hazard for the French Atlantic and Channel coastlines, in order to provide guidance for risk assessment on the nuclear facilities.

8.2.3. APP Bordeaux 1

Title : Reactive fluid flows with interface : macroscopic models and application to self-healing materials

Type : Project Bordeaux 1

Duration : 36 months

Starting : September 2014

Coordinator : M. Colin

Abstract : 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. Though based on brittle ceramic components, these composites are not brittle due to the use of a fiber/matrix interphase that manages to preserve the fibers from cracks appearing in the matrix. The lifetime-determining part of the material is the fibers, which are sensitive to oxidation; when the composite is in use, it contains cracks that provide a path for oxidation. The obtained lifetimes can be of the order of hundreds of thousands of hours. These time spans make most experimental investigations impractical. In this direction, the aim of this project is to furnish predictions based on computer models that have to take into account: 1) the multidimensional topology of the composite made up of a woven ceramic fabric; 2) the complex chemistry taking place in the material cracks; 3) the flow of the healing oxide in the material cracks.

8.2.4. 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 air crash 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 environment : 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 platform, able to provide a complete design of these systems.

8.3. European Initiatives

8.3.1. FP7 & H2020 Projects

8.3.1.1. UTOPIA

Type: COOPERATION

Instrument: Specific Targeted Research Project

Objectif: The main objectives of this research programme are to develop, through the ESR's individual projects, fundamental mathematical methods and algorithms to bridge the gap between Uncertainty Quantification and Optimisation and between Probability Theory and Imprecise Probability Theory for Uncertainty Quantification, and to efficiently solve high-dimensional, expensive and complex engineering problems.

Duration: 2017 - 2021

Coordinator: University of Strathclyde (Scotland, UK)

Partner: University of Strathclyde (Scotland, UK), Inria Bordeaux Sud-Ouest (France), ESTECO (Italy), CIRA, Centro Italiano Aerospaziali (Italy), Politecnico di Milano (Italy), Jozef Stefan Institute (Slovenia), Cologne University of Applied Sciences (Germany), University of Durham (England, UK), Ghent University (Belgium), Von Karman Institute (Belgium), DLR, Institute of Aerodynamics and Flow Technology (Germany), National Physical Laboratory (England, UK), Leonardo Aircraft S.p.A (Italy), Airbus Operations GmbH (England, UK), Stanford University (USA)

Inria contact: Pietro Marco Congedo

Abstract: Research activities will be developed in the context of the European project - UTOPIAE <http://utopiae.eu> (520 K euros for Inria). The aim of this project is to develop, through the ESRs individual projects, fundamental mathematical methods and algorithms to efficiently solve high-dimensional, expensive and complex engineering problems. Two PhD thesis will be recruited at the beginning of 2017.

8.3.1.2. STORM

Type: COOPERATION

Instrument: Specific Targeted Research Project

Duration: October 2013 - September 2016

Coordinator: SNECMA (France)

Partner: SNECMA SA (FR), AEROTEX UK LLP (UK), AIRBUS OPERATIONS SL (ES), Airbus Operations Limites (UK), AIRCELLE SA (FR), ARTTIC (FR), CENTRO ITALIANO RICERCA AEROSPAZIALI SCPA (IT), CRANFIELD UNIVERSITY (UK), DEUTSCHES ZENTRUM FUER LUFT - UND RAUMFAHRT EV (DE), EADS DEUTSCHLAND GMBH (DE), ONERA (FR), TECHSPACE AERO SA (BE)

Inria contact: H eloise Beaugendre

Abstract: During the different phases of a flight, aircraft face severe icing conditions. When this ice then breaks away, and is ingested through the remainder of the engine and nacelle it creates multiple damages which have a serious negative impact on the operations costs and may also generate some incident issues. To minimise ice accretion, propulsion systems (engine and nacelle) are equipped with Ice Protection Systems (IPS), which however have themselves performance issues. Design methodologies used to characterise icing conditions are based on empirical methods and past experience. Cautious design margins are used non-optimised designs solutions. In addition, engine and nacelle manufacturers are now limited in their future architectures solutions development because of lack of knowledge of icing behaviour within the next generation of propulsive systems solutions, and of new regulations adopted that require aero engine manufacturers to address an extended range of icing conditions.

In this context that STORM proposes to: characterise ice accretion and release through partial tests ; Model ice accretion, ice release and ice trajectories ; Develop validated tools for runback ; characterise ice phobic coatings ; select and develop innovative low cost and low energy anti-icing and de-icing systems. Thus, STORM will strengthen the predictability of the industrial design tools and reduce the number of tests needed. It will permit lower design margins of aircraft systems, and thus reduce the energy consumption as well as prevent incidents and break downs due to icing issues.

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 - December 2018

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 International Labs

Inria@SiliconValley

Associate Team involved in the International Lab:

8.4.1.1. AQUARIUS2

Title: Advanced methods for uncertainty quantification in compressible flows

International Partner (Institution - Laboratory - Researcher):

Stanford (United States) - Department of Mechanical Engineering - Gianluca Iaccarino

Start year: 2014

See also: <http://www.stanford.edu/group/uq/aquarius/index3.html>

This research project deals with uncertainty quantification in computational fluid dynamics. Uncertainty Quantification (UQ) aims at developing rigorous methods to characterize the impact of limited knowledge on quantities of interest. Main objective of this collaboration is to build a flexible and efficient numerical platform, using intrusive methods, for solving stochastic partial differential equations. In particular, the idea is to handle highly non-linear system responses driven by shocks.

8.4.1.2. AMoSS

Title: Advanced Modeling on Shear Shallow Flows for Curved Topography : water and granular flows.

International Partner (Institution - Laboratory - Researcher):

Inria Sophia-Antipolis and University of Nice (France)

Inria Bordeaux and University of Bordeaux (France)

University of Marseille (France)

National Cheng Kung University, Tainan, Taiwan

National Taiwan University and Academia Sinica, Taipei, Taiwan

Duration: 2014 - 2016

See also: <https://team.inria.fr/amoss/>

Our objective is to generalize the promising modeling strategy proposed in G.L. Richard and S.L. Gavriluk 2012, to genuinely 3D shear flows and also take into account the curvature effects related to topography. Special care will be exercised to ensure that the numerical methodology can take full advantage of massively parallel computational platforms and serve as a practical engineering tool. At first we will consider quasi-2D sheared flows on a curve topography defined by an arc, such as to derive a model parameterized by the local curvature and the nonlinear profile of the bed. Experimental measurements and numerical simulations will be used to validate and improve the proposed modeling on curved topography for quasi-2D flows. Thereafter, we will focus on 3D flows first on simple geometries (inclined plane) before an extension to quadric surfaces and thus prepare the generalization of complex topography in the context of geophysical flows.

8.4.1.3. Informal International Partners

University of Zurich : R. Abgrall. Collaboration on penalisation on unstructured grids and high order adaptive methods for CFD and uncertainty quantification.

Politecnico di Milano, Aerospace Department (Italy) : Pr. A. Guardone. Collaboration on ALE for complex flows (compressible flows with complex equations of state, free surface flows with moving shorelines).

von Karman Institute for Fluid Dynamics (Belgium). With Pr. T. Magin we work on Uncertainty Quantification problems for the identification of inflow condition of hypersonic nozzle flows. With Pr. H. Deconinck we work on the design of high order methods, including goal oriented mesh adaptation strategies

NASA Langley: Dr. Alireza Mazaheri. Collaboration on high order schemes for PDEs with second and third order derivatives, with particular emphasis on high order approximations of solution derivatives.

Technical University of Crete, School of Production Engineering & Management : Pr. A.I. Delis. Collaboration on high order schemes for depth averaged free surface flow models, including robust code to code validation

Chalmers University (C. Eskilsson) and Technical University of Denmark (A.-P. Engsig-Karup) : our collaboration with Chalmers and with DTU compute in Denmark aims at developing high order non hydrostatic finite element Boussinesq type models for the simulation floating wave energy conversion devices such as floating point absorbers ;

University of Delaware: F. Veron. Collaboration on the modelling of rain effects on wave propagation.

8.5. International Research Visitors

8.5.1. Visits of International Scientists

- From 27/11 to 03/12/2016 Pascal POULLET (Université des Antilles) has visited M. Ricchiuto to work on nonlinear residual based approximations of free surface flows with moving bathymetries.
- From 21/11 to 09/12/2016 Luca CIRROTTOLA (Politecnico di Milano) has visited C. Dobrzinsky to work on parallel mesh adaptation.
- From 21/10 to 05/11/2016 François MORENCY (ETS, University of Québec, Montréal) has visited us to work on LESCAPE code with Héloïse, Léo and Aurore. The Spalart-Allmaras turbulent model has been validated using the periodic channel flow test case.
- From 01/10 to 29/10/2016 Claes ESKILSSON (Chalmers University of Technology, Sweden) has visited us to work with Mario Ricchiuto and U. Bosi on spectral element methods for Boussinesq models with floating structures.
- From 12/09 to 22/09/2016 Kazuo AOKI (University of Taiwan) has visited us to work with Luc Mieussens on models for reentry flows.
- From 07/07 to 09/07/2016 Volker ROEBER (Tohoku University, International Research Institute of Disaster Science) has visited us to work with Maria Kazolea and Mario Ricchiuto on robust code to code validation, on coastal engineering problems.
- From 27/03 to 01/04/2016 Alireza MAZAHARI (NASA Langley) came to visit Mario Ricchiuto and V. Perrier to work on the implementation of a hyperbolic formulation of the Navier-Stokes equations in the AeroSol platform.
- From 16/03/2016 Guglielmo SCOVAZZI (Duke University) has visited M. Ricchiuto to work on stabilized finite elements for geo-mechanics.
- From 1/01/2016 to 31/04/2016 Gianluca IACCARINO (Stanford University) has visited the Team in the context of AQUARIUS Team, collaborating actively with all the PhD student involved in uncertainty quantification research. All the students involved (Razaaly, Sanson and Cortesi) have then visited the group of G. Iaccarino in Stanford University in the fall 2016.
- From 15/05/2016 to 17/07/2016 Fabrice VERON (University of Delaware at Newark, USA) has visited us to work with Luc Mieussens on a project dedicated to the modelling and simulation of the interaction rain/water waves.
- From April 2015 to April 2016 : T. WATANABE, Department of Mathematics, Faculty of Science Kyoto Sangyo University visited M. Colin to work on the approximation of solitary wave solutions of nonlinear dispersive PDEs.

8.5.1.1. Internships

- From Feb 2016 to Jul 2016 Rama Ayoub (Inria, M. Sc. Student)
- From Apr 2016 to Sep 2016 Toufik Boubehziz (EDF, M. Sc. Student)
- From Jan 2016 to Mar 2016 Maxence Claey (CEA, Phd Student)
- From Feb 2016 to Jul 2016 Antoine Fondaneche (Inria, M. Sc. Student)
- From Oct 2016 to Feb 2016 Esben Grange (Inria, M. Sc. Student)
- From Jun 2016 to Sep 2016 Adrien Paumelle (Inria, Univ. Bordeaux)
- From May 2016 to Sep 2016 Raphael Robyn (Inria, Univ. Bordeaux)

9. Dissemination

9.1. Promoting Scientific Activities

9.1.1. Scientific Events Organisation

9.1.1.1. Member of the Organizing Committees

H. Beaugendre: Numerical workshop for the STORM European project, Inria Bordeaux, France, November 2016

M. Colin: Congress JEF, dedicated to young researchers in PDE analysis and applications, Bordeaux, France, March 2016

M. Ricchiuto : International workshop B' WAVES 2016, Bergen, Norway, June 2016 (<https://project.inria.fr/tsunamischool2016/>)

M. Ricchiuto : TANDEM and Defis Littoral Tsunami School, Bordeaux, France, April 2016 (<http://www.uib.no/en/bwaves2016>)

M. Ricchiuto : Verification, Validation et Quantification des incertitudes en simulation numerique (VVUQ), Aristote seminar cycles, Ecole Polytechnique, France, November 2016 (http://www.association-aristote.fr/doku.php/association-aristote_fr_doku.php_simulation)

9.1.2. Scientific Events Selection

9.1.2.1. Member of the Conference Program Committees

P.M. Congedo : NICFD 2016 Conference, Varenna, Italy, October 2016.

9.1.3. Journal

9.1.3.1. Member of the Editorial Boards

Mathieu Colin is a member of the board of the journal Applications and Applied Mathematics: An International Journal (AAM)

Mario Ricchiuto is member of the editorial board of *Computers & Fluids (Elsevier)*, and of *GEM - International Journal on Geomathematics (Springer)*

A special issue of the European Journal of Mechanics / B Fluids will be dedicated to the 2 editions of the international workshop B'Waves on wave breaking, held in 2014 in Bordeaux (M. Colin and M. Ricchiuto as co-organizers), and in 2016 in Bergen (M. Ricchiuto as co-organizer). M. Colin and M. Ricchiuto will be guest editors of this issue

9.1.3.2. Reviewer - Reviewing Activities

We reviewed papers for top international journals in the main scientific themes of the team : journal of Computational Physics, Computer Methods in Applied Mechanics and Engineering, Optimization and Engineering, International Journal of Numerical Methods in Fluids, Physics of Fluids, Journal of Marine Science and Technology, Engineering Applications of Computational Fluid Mechanics, Computers and Fluids, International Journal of Modelling and Simulation in Engineering Aircraft Engineering and Aerospace Technology, International Journal of Computational Fluid Dynamics, Applications and applied mathematics : An international journal, Discrete and Continuous Dynamical Systems - Series A, Electronic Journal of Differential Equations, Calculus of Variations and Partial Differential Equations, Nonlinear Analysis: Modelling and Control, Advanced Nonlinear Studies, Communications on Pure and Applied Analysis, Communications in Computational Physics, Nonlinearity, Applications and Applied Mathematics: An International Journal, Journal of Differential Equations, Analysis and Mathematical Physics.

9.1.4. Invited Talks

- P.M. Congedo, Presentation at Journées Scientifiques Inria, June 2016, Rennes
- P.M. Congedo, "General introduction to Uncertainty Quantification", CNES, March 2016, Toulouse
- M. Kazolea, "Wave breaking in Boussinesq free surface models", International Workshop B'Waves2016, Bergen (Norway)
- M. Ricchiuto, "Numerical issues in tsunami simulation: dispersion and diffusion ?scales?, what order of accuracy ?", TANDEM and Defis Littoral 2016 Tsunami school, Bordeaux

9.1.5. Leadership within the Scientific Community

P.M. Congedo has been appointed as the Co-Director of the Inria International Lab Inria-CWI.

9.2. Teaching - Supervision - Juries

9.2.1. Teaching

- Licence : Cécile Dobrzynski, Langages en Fortran 90, 54h, L3, ENSEIRB-MATMÉCA, FRANCE
- Master : Héloïse Beaugendre, TP langage 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, Initiation librairie MPI, 12h, M2, Ecole de Technologie Supérieure, Université du Québec, Montréal, Canada
- Master : Héloïse Beaugendre, Responsable de filière de 3ème année, 15h, M2, ENSEIRB-MATMÉCA, France
- Master : Héloïse Beaugendre, Calcul parallèle (MPI), 78h, M2, ENSEIRB-MATMÉCA, France
- Master : Héloïse Beaugendre, Encadrement de projets de la filière Calcul Haute Performance, 11h, M2, ENSEIRB-MATMÉCA, France
- Master : Héloïse Beaugendre, Projet fin d'études, 4h, M2, ENSEIRB-MATMÉCA, FRANCE
- Master : Mathieu Colin : Intégration, M1, 54h, ENSEIRB-MATMÉCA, FRANCE
- Master : Mathieu Colin : PDE, M2, 30h, ENSEIRB-MATMÉCA, FRANCE
- Master : Mathieu Colin : Fortran 90, M1, 44h, ENSEIRB-MATMÉCA, FRANCE
- Master : Mathieu Colin : PDE, M1, 28h, University of Bordeaux, FRANCE
- Master : Mathieu Colin : Analysis, L1, 47h, ENSEIRB-MATMÉCA, FRANCE
- Master: Luc Mieussens, Transport de particules : modèles, simulation, et applications, 24h, M2, ENSEIRB-MATMECA, France
- Master : Luc Mieussens, Projet fin d'études, 4h, M2, ENSEIRB-MATMÉCA, FRANCE
- Doctorat : P.M. Congedo, Uncertainty quantification, theory and application to algorithms, CFD and global change, Apr 2015, CERFACS, Toulouse, France, 4h.
- Master : Mario Ricchiuto : Fluid Dynamics II, 20h, ENSEIRB-MATMÉCA, FRANCE
- Master : Mario Ricchiuto, Encadrement de projets TER, 10h, ENSEIRB-MATMÉCA, FRANCE

9.2.2. Supervision

- HdR : Héloïse Beaugendre, Contributions à la simulation numérique des écoulements fluides : exemples en milieu poreux et en aéronautique, Bordeaux University, 18 March 2016.
- PhD : Fusi Francesca, Stochastic robust optimization of a helicopter rotor airfoil, March 2016.
- PhD : Bellec Stevan, Discrete asymptotic modelling of free surface flows, 5 October 2016.
- PhD : Viville Quentin, Construction d'une méthode hp-adaptative pour les schémas aux Résidus Distribués, Bordeaux University, 22 November 2016.
- PhD: Filippini Andrea, Nonlinear finite element Boussinesq modelling of non-hydrostatic free surface flows, 14 December 2016.
- PhD: Nouveau Léo, Adaptative Residual Based Schemes for Solving the Penalized Navier-Stokes Equations with Moving Bodies - Application to Ice Shedding Trajectories, Bordeaux University, 16 December 2016.
- PhD in progress : Arpaia Luca, Continuous mesh deformation and coupling with uncertainty quantification for coastal inundation problems, started in March 2014.
- PhD in progress : Bosì, Umberto, ALE spectral element Boussinesq modelling of wave energy converters, started in November 2015
- PhD in progress : Cortesi Andrea, Predictive numerical simulation for rebuilding freestream conditions in atmospheric entry flows, started in October 2014.

PhD in progress: Lin Xi, Asymptotic modelling of incompressible reactive flows in self-healing composites, started in October 2014.

PhD in progress: Perrot Gregory, Physico-chemical modelling of self-healing ceramic composites, started in October 2011.

PhD in progress : Peluchon Simon, Approximation numérique et modélisation de l'ablation différentielle de deux matériaux: application à l'ablation liquide. Started in December 2014. Advisor: Luc Mieussens. PhD hosted in CEA-CESTA.

PhD in progress: Aurore Fallourd, Modeling and Simulation of inflight de-icing systems, Started in October 2016.

PhD in progress: Guillaume Jeanmasson, Explicit methods with local time stepping for the simulation of unsteady turbulent flows. Started in October 2016. Advisor: Luc Mieussens. Hosted in ONERA Châtillon.

PhD in progress: Francois Sanson, Uncertainty propagation in a system of codes, started in February 2016.

PhD in progress: Nassim Razaaly, Robust optimization of ORC systems, started in February 2016.

9.2.3. *Juries*

P.M. Congedo : Rapporteur de thèse de Elio Bufi, ENSAM Paris Tech, December 2016.

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Publications of the year

Doctoral Dissertations and Habilitation Theses

- [1] H. BEAUGENDRE. *Contributions à la simulation numérique des écoulements fluides : exemples en milieu poreux et en aéronautique*, Université de Bordeaux, March 2016, Habilitation à diriger des recherches, <https://hal.inria.fr/tel-01315897>.

Articles in International Peer-Reviewed Journal

- [2] R. ABGRALL, H. ALCIN, H. BEAUGENDRE, C. DOBRZYNSKI, L. NOUVEAU. *Residual Schemes Applied to an Embedded Method Expressed on Unstructured Adapted Grids*, in "Acta Aerodynamica Sinica", 2016, vol. 34, n° 2, p. 214-223 [DOI : 10.7638/KQDLXXB-2016.0010], <https://hal.inria.fr/hal-01407945>.
- [3] R. ABGRALL, P. M. CONGEDO, G. GERACI. *Towards a unified multiresolution scheme for treating discontinuities in differential equations with uncertainties*, in "Mathematics and Computers in Simulation", February 2016, <https://hal.inria.fr/hal-01267140>.
- [4] S. BELLEC, M. COLIN. *On the existence of solitary waves for Boussinesq type equations and a new conservative model*, in "Advances in Differential Equations", 2016, vol. 21, n° 9,10, p. 945-976, <https://hal.inria.fr/hal-01378585>.
- [5] S. BELLEC, M. COLIN, M. RICCHIUTO. *Discrete asymptotic equations for long wave propagation*, in "SIAM Journal on Numerical Analysis", 2016, <https://hal.inria.fr/hal-01378612>.
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- [22] H. BEAUGENDRE. *Numerical simulation of ice block trajectories*, in "Conference LIAFSMA, Sino-French Conference on Applied Mathematics", Bordeaux, France, Bordeaux University, May 2016, <https://hal.inria.fr/hal-01409292>.
- [23] S. BRULL, L. FORESTIER-COSTE, L. MIEUSSENS. *Local velocity grids for deterministic simulations of rarefied flows*, in "European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS)", Crete, France, June 2016, <https://hal.archives-ouvertes.fr/hal-01397475>.
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- [27] P. M. CONGEDO. *Intrusive methods for Uncertainty Quantification*, in "Uncertainty quantification: theory and application to algorithms, CFD and geosciences", Toulouse, France, May 2016, <https://hal.inria.fr/hal-01378442>.
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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

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Keywords:

Computer Science and Digital Science:

- 6.2.1. - Numerical analysis of PDE and ODE
- 6.2.6. - Optimization
- 6.2.7. - High performance computing
- 6.3.1. - Inverse problems
- 6.3.2. - Data assimilation
- 6.3.4. - Model reduction

Other Research Topics and Application Domains:

- 2.2.1. - Cardiovascular and respiratory diseases
- 2.6.2. - Cardiac imaging

1. Members

Research Scientists

Jacques Henry [Inria, Senior Researcher, Emeritus, HDR]
Mark Potse [Inria, Advanced Research position]
Najib Zenzemi [Inria, Researcher]

Faculty Members

Yves Coudiere [Team leader, Professor, Univ. Bordeaux, HDR]
Mostafa Bendahmane [Univ. Bordeaux, Associate Professor]

Technical Staff

Julien Bouyssier [Inria, Engineer, until Sep 2016, granted by ANR REO-CARDIOXCOMP project]
Mehdi Juhoor [Inria, Engineer]
Pauline Migerditichan [Inria, Engineer, from Nov 2016]
Julien Pedron [Inria, Engineers, until Sep 2016]
Marc Fuentes [Inria, Ingénieur SED]

PhD Students

Andjela Davidovic [Inria, PhD Student]
Pierre-Elliott Bécue [Inria, Maison de la Simulation, PhD Student]
Charlie Douanla Lontsi [Inria, PhD Student]
Antoine Gérard [Univ. Bordeaux, PhD Student]

Post-Doctoral Fellows

Judit Chamorro Servent [Univ. Bordeaux, Post-Doctoral Fellow]
Michal Kania [Univ. Bordeaux, Post-Doctoral Fellow]

Visiting Scientists

Yassine Abidi [Ecole Nationale d'Ingénieurs de Tunis, PHD Student, Visiting Scientist, from May 2016 until Sep 2016]
Keltoum Chahour [Ecole Mohammadia d'ingénieurs - Université Mohammed V Rabat, PHD Student, Visiting Scientist]
Rabeb Chamekh [Ecole Nationale d'Ingénieurs de Tunis, PHD Student, Visiting Scientist]

Najib Fikal [Ecole Mohammadia d'ingénieurs - Université Mohammed V Rabat, PHD Student, Visiting Scientist]

Andres Fraguera Collar [Benemerita Universidad Autonoma de Puebla-Mexico, Professor, Visiting Scientist, until Jul 2016]

Anabel Hernandez Ramirez [Benemerita Universidad Autonoma de Puebla-Mexico, PHD Student, Visiting Scientist, from Dec 2016]

Ozkar Hernandez Romero [Benemerita Universidad Autonoma de Puebla-Mexico, PHD Student, Visiting Scientist, from Dec 2016]

Moncef Mahjoub [Ecole Nationale d'Ingénieurs de Tunis, Professor, Visiting Scientist, until Aug 2016]

Wajih Mbarki [Faculté des science de Tunis, PHD Student, Visiting Scientist, until May 2016]

David Andres Mora [Departamento de Matematica, Universidad del Bo-Bo, Casilla 5-C, Concepcion, Chile, Visiting Scientist, from 16 Jun 2016 until 13 Jul 2016]

Veronica Anaya Dominguez [Universidad del Bo-Bo, Casilla 5-C, Concepcion, Chile, Visiting Scientist, from 16 Jun 2016 until 13 Jul 2016]

Administrative Assistants

Catherine Cattaert Megrat [Inria, Assistant]

Anne-Laure Gautier [Inria, Assistant]

Chrystel Plumejeau [Inria, Assistant]

Others

Pierre-Yves Dulaurens [3rd-year *collège* pupil, Nov 2016]

Louis Giroux [3rd-year *collège* pupil, Nov 2016]

Corisande Lamy [Inria, Master 1 student, from Jun 2016 until Aug 2016]

Ronald Moussitou [Inria, Master 2 student, from Apr 2016 until Aug 2016]

Charles Pierre [CNRS, Ingénieur de recherche]

Simon Labarthe [INRA, Chargé de recherche]

Jason Bayer [Univ. Bordeaux, Post-Doctoral Fellow]

Florian Caro [Min. de l'Education Nationale, Researcher]

Gwladys Ravon [Univ. Bordeaux, Post-Doctoral Fellow]

Edward Vigmond [Univ. Bordeaux I, Professor]

2. Overall Objectives

2.1. Overall Objectives

The Carmen team develops and uses models and numerical methods in order 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, 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 arrhythmias 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 developed, based on previous work [44] and on the data available at IHU LIRYC:

- Enrichment of the current monodomain and bidomain models [44] [8] 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 [20] [46] and sudden-cardiac-death (SCD) syndromes [14], [51], [48]. 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 complex 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 dependence 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, both in the quasistatic and in the dynamic contexts.

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.

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

3.3. Numerical techniques

We want the numerical simulations of the previous direct or inverse models to be efficient and reliable with respect to the needs of the medical community. They should qualify and guarantee the accuracy and robustness of the numerical techniques and the efficiency of the resolution algorithms.

Based on previous work on solving the monodomain and bidomain equations [4], [5], [7], [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 parallelization, algebraic multigrid preconditioning, and a BiCGStab algorithm with adaptations to retain numerical accuracy while handling large underdetermined systems.

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. Existing models are two-dimensional or limited to idealized geometries, and use a linear (purely resistive) behaviour of the gap-junction channels that connect the cells. We propose a three-dimensional approach using realistic cellular geometry, 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).

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. 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.

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 aim at bringing applied mathematics and scientific computing closer to experimental and clinical cardiac electrophysiology. In collaboration with experimental and clinical researchers at Liry we aim at enhancing fundamental knowledge of the normal and abnormal cardiac electrical activity and of the patterns of the electrocardiogram, and we will 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 will help to write new concepts concerning the multiscale organisation of the cardiac action potentials and will serve our understanding in many electrical pathologies. For example, we will be modeling the structural heterogeneities at the cellular scale, 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 arrhythmias 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. They are supposed 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 and (2) modeling the heterogeneities related to the complex organization and disorganization of the myocytes and fibroblasts. Point (1) is supposed to play a major role in sudden cardiac death and point (2) 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.

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 (section 6.2).

5. Highlights of the Year

5.1. Highlights of the Year

5.1.1. Events

On 4 November 2016 the new building of the IHU Liryc was officially opened in the presence of representatives from the municipal, departmental, regional, and national authorities.

On 9 December 2016 A. Davidović defended her thesis *Multiscale Mathematical Modeling of Structural Heterogeneities in Cardiac Electrophysiology*.

5.1.2. Recruitments

M. Potse, whose work had been funded by IHU Liryc since 2013, has become a full-time member of the Carmen team and has won an Inria Advanced Research Position in June 2016. He will continue his numerical studies on cardiac sudden-death syndromes and atrial fibrillation and is developing a new project on the application of electrocardiographic inverse methods in the catheterization laboratory.

We recruited the engineer P. Migerditichan; she started working in November 2016 on a project named EPICARDial electrical signals VIZualisation (EPICARD-VIZ). The aim of this project is to build a software solution for the electrocardiographic inverse problem, coded in the MUSIC platform. The goal of the project is twofold: First, we aim at building a semi-automatic functionality that allows to obtain meshes of the epicardium, torso, lungs, liver, and skeletal muscle with minimal human interaction. Second, our aim is to include a dense linear algebra library and to construct a computational framework in which we will be able to compare different methods of solving the inverse problem.

After the completion of her PhD thesis A. Davidović was hired as an Engineer, granted by the ANR HR-CEM project. She continues her work on multiscale modelling of heterogeneities in cardiac tissue. She is going to use the experimental high-resolution MRI data on animal and human hearts that are provided by the imaging team of IHU Liryc. By means of image analysis and numerical simulations she is going to study the effects of fibrotic, fatty, and other kinds of tissue on AP propagation.

6. New Software and Platforms

6.1. CEPS: a Cardiac ElectroPhysiology Simulator

The Carmen team develops a software library to perform high-performance numerical simulations in cardiac electrophysiology using unstructured three-dimensional grids. The software, called CEPS (*Cardiac Electrophysiology Simulation*) is developed as a common tool for researchers in the Carmen team and for our partners and colleagues in scientific computing and biomedical engineering. The goal of CEPS is to facilitate the development of new numerical methods and new physical models.

Compared to other existing software, 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. The largest part of CEPS was developed by the Junior Engineer M. Juhoor, supervised by N. Zemzemi, during the CEPS ADT (*Action de Développement Technologique*).

To enforce a sound development process, some engineering and validation tools are used:

- Git hosted at the Inria GForge ([ceps](#)) to manage versions;
- Cmake for the building process
- [Jenkins](#), hosted at the Inria continuous integration service, which runs a test suite of about 200 tests after every commit.

Main users and developers of CEPS are the PhD students of Carmen, i.e.

- A. Gérard, who uses CEPS for patient-specific modeling, has implemented a bilayer model using coupled nodes.
- Charlie Douanla-Lountsi currently works on high-order temporal integration methods, for later integration in CEPS.
- P. E. Bécue is developing a code to run microscopic-scale models (section 3.4) and wrote a coupled node assembler to support this work.

Since January 2015, M. Fuentes from the *Service d'Experimentation et de Développement* (SED), is responsible for developing new features in CEPS, improve robustness, efficiency, and documentation. M. Juhoor, who has previously worked on CEPS, and works on the IDAM project, brings us from time to time his expertise. Actions done in 2016 include:

- support for P2 Lagrange finite Elements
- node partitioning using the PTScotch partitioner
- input files and VtkReader (M. Juhoor)
- code refactoring
- documentation writing

6.2. IDAM

The goal of the IDAM project is to define a collection of plugins in the MUSIC software in order to create realistic meshes for the CEPS code. MUSIC is a multimodal platform for cardiac imaging developed by the imaging team at IHU LIRYC (<https://bil.inria.fr/fr/software/view/1885/tab>). Information comes from magnetic resonance imaging and cardiac tomography performed in the clinic and in the LIRYC laboratories. Building complete cardiac models directly from imaging data requires expert knowledge and is time-consuming and error-prone: specific expertise and multiple software tools are often needed to process data stemming from medical imaging into realistic meshes and parameter distributions.

IDAM aims to streamline the workflow of a complete cardiac simulation: anatomical mesh generation from patient-specific data, description of simulation parameters, and eventually analysis of simulation results obtained by simulation packages like CEPS (<https://bil.inria.fr/fr/software/view/2630/tab>). IDAM integrates tools from other Inria teams by using specialized libraries, for example MMG (<https://bil.inria.fr/fr/software/view/2824/tab>) for high-quality mesh generation.

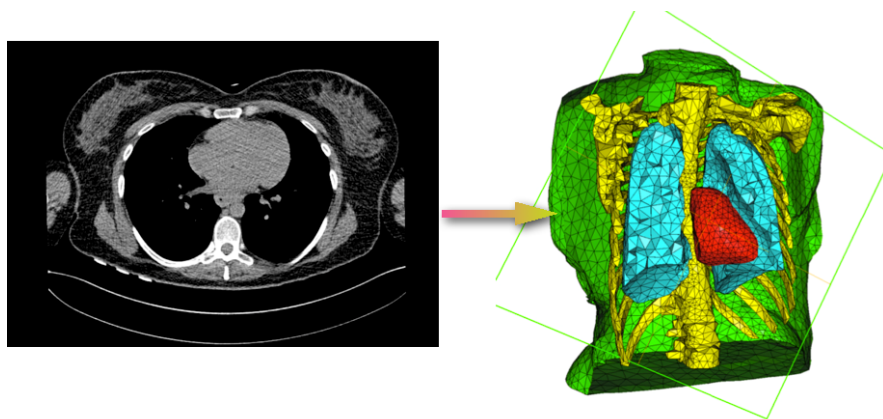


Figure 1. Mesh of a human torso and one of the X-ray computed-tomography slices on which it was based.

6.3. Platforms

6.3.1. Propag-5

Applied modeling studies performed by the Carmen team, especially M. Potse and M. Kania, in collaboration with IHU Liryc and foreign partners [39], [43], [18], [20], [14] [45], rely to a great extent on high-performance

computations on the national supercomputers Curie, Occigen, and Turing. While the newly developed CEPS code is not ready to run efficiently on these systems we rely on an older code named Propag-5. This code 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. Relatively small contributions to this code have been made by the Carmen team.

The predecessor of Propag-5, named Propag-4, was developed by M. Potse at the *Université de Montréal* [8]. It was based on earlier model code developed there by the team of Prof. R. Gulrajani [50], [53], and was parallelized with OpenMP to utilize the shared-memory SGI supercomputers available there at the time. Propag-4 was the first code ever able to run a bidomain reaction-diffusion model of the entire human ventricles; a problem 30 times larger than what had been reported before [8].

In order to utilize the more recent distributed-memory architectures Propag-4 was transformed into the hybrid MPI-OpenMP code Propag-5 at the Institute of Computational Science in Lugano by D. Krause and M. Potse [49]. The resulting code has been used for numerous applied studies. An important limitation of the Propag code is that it relies on a semi-structured mesh with a uniform resolution. On the other hand, 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, and only minor changes are being made currently. It can be considered the workhorse for our HPC work until CEPS takes over.

6.3.2. *Gepetto*

Gepetto, named after a famous model maker, is a software suite that 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 [52]. 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.

6.3.3. *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. The team also contributes a series of plugins for MUSIC through the IDAM project (section 6.2).

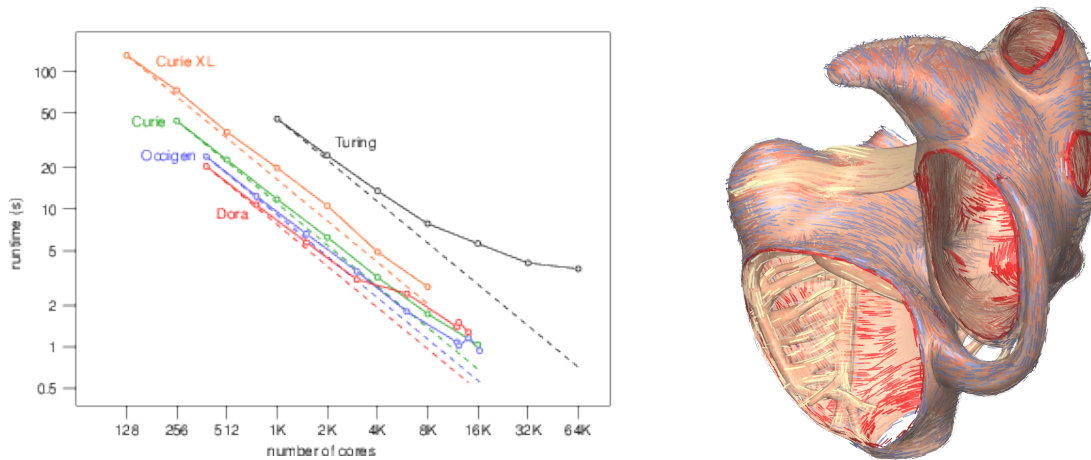


Figure 2. **Left:** Strong scaling of the Propag-5 code on a monodomain reaction-diffusion equation for four systems: The Bull clusters Curie (small nodes and large nodes, XL) and Occigen, The Cray XC30 “Piz Dora” at the Swiss supercomputing center CSCS and the IBM BlueGene/Q “Turing”. The graph shows the runtime needed for 10 ms of propagated activity using an explicit (forward) Euler integration. Dashed lines indicate the ideal scaling line with respect to the lowest number of cores measured. **Right:** Bundle structures and different layers of fiber orientation created by the Gepetto software.

7. New Results

7.1. Convergence analysis of a bidomain-bath model

M. Bendahmane and N. Chamakuri performed a convergence analysis for optimal control of a bidomain-bath model by using a finite-element scheme. The bidomain-bath model represents a commonly used experimental setup where a small piece of cardiac tissue is kept alive and studied for some time in a nutrient bath. The bidomain-bath model equations describe the cardiac bioelectric activity in the tissue and bath volumes where the control acts at the boundary of the tissue. The existence of the finite element scheme and convergence to a unique weak solution of the direct problem were established. The convergence proof was based on deriving a series of a-priori estimates and using a general L2-compactness criterion. Moreover, the well-posedness of the adjoint problem and the first order necessary optimality conditions were shown. Comparing to the direct problem, the convergence proof of the adjoint problem is based on using a general L1-compactness criterion. The model was used for a simulation of low-energy defibrillation.

7.2. An exponential Adams–Bashforth ODE solver for stiff problems

C. Douanla Lontsi, together with Y. Coudière and C. Pierre, obtained an important result on time integration of stiff differential problems. They considered Adams exponential integrators with general varying stabilizers. General stabilization brings flexibility and facilitates the integration of ODE systems and semilinear evolution PDEs coupled with ODE systems. They were able to prove the stability and convergence of this type of integrator by introducing a new framework that extends multistep linear methods. Dahlquist stability was numerically investigated. $A(\alpha)$ -stability was observed under a condition on the stabilizer, which is a singular property for explicit schemes. The method was numerically studied for two stiff models in electrophysiology. Its performance was compared with several classical methods. The authors concluded that for stiff ODE systems, it provides a cheaper way to compute accurate solutions at large time steps than implicit solvers.

7.3. Homogeneous Neumann condition on the torso for solving inverse problems

The electrical activity of the heart creates an electrical field in the body. This phenomenon is classically modelled in a quasistatic manner by Laplace's equation. The non-invasive electrocardiographic imaging (ECGI) problem consists in retrieving the best electrical map on the heart from given torso measurements. Classically, the solution is found as the best fit between data generated by a forward problem and the actual torso measurements, and it needs a regularization. Hence the inverse solution depends on the matrix of the forward problem, called the transfer matrix, and the choice of the regularization procedure. In 2006, a meshless method based on the method of fundamental solutions (MFS) was adapted by Y. Wang and Y. Rudy [54] to directly solve the inverse problem, combined with a 0-th order Tikhonov regularization. The MFS method is notably more robust than previous methods (e.g. BEM) to the uncertainties introduced by the segmentation of the geometries. In the MFS, the potential is expressed as summation of the fundamental solution of the Laplace equation over a discrete set of virtual point sources placed outside of the domain of interest. The inverse solution is searched as the set of sources that best fit the boundary conditions on the torso, up to the regularization term. This formulation yields a linear system, which matrix depends on the torso and heart geometries, and the boundary conditions at the torso surface. The regularization parameter also heavily depends on the properties of the transfer matrix. The boundary conditions considered in [54] are: i) the Dirichlet conditions, meaning that the potentials at the torso surface are fitted to the recorded ones, ii) homogeneous Neumann conditions (HNC) meaning that the normal flux of current is minimized.

Numerically, the HNC requires to build accurate directions at each measurement location of the body surface, which is a first difficulty. In addition, the body is cut at the top and the bottom where no-flux conditions are probably not relevant. Lastly, the matrix coefficients related to the HNC appears to be much smaller than the ones from the Dirichlet condition, due to the distance between the torso and the actual electrical source (the heart).

J. Chamorro-Servent, Y. Coudière and R. Dubois studied the effect of the HNC on the matrix. They showed that enforcing the Neumann condition has a negligible effect on the solution of the inverse problem. Reconstructed potentials and activation time maps were built for in-silico data. No major differences were found between the standard MFS and the MFS removing the HNC in terms of potentials and activation times. In addition, removing the HNC reduces the ill-conditioning of the problem and the computational burden: the normal at the torso surface is not required anymore, and the problem size is divided by 2. The results of this work were presented as a poster in CinC 2016, and collected in a proceeding for the same conference by J. Chamorro-Servent et al. [18].

7.4. Adaptive placement of the pseudo-boundaries improves the conditioning of the inverse problem

In order to complete the investigation concerning the MFS technique from [54], J. Chamorro-Servent, Y. Coudière and R. Dubois also studied the effect of the location of the virtual sources of the MFS method on the solutions of the inverse problem. Specifically, the regularization term spoils the biophysical content of the solution, and the regularization parameter must be chosen as small as possible. But the problem must be regularized enough to overcome its sensitivity to: i) noise on the measured potentials, ii) uncertainty in the location of measurement sites with respect to the surface on which the sources are distributed, iii) errors of segmentation of the geometries, iv) influence of cardiac motion, etc.

The regularization parameter can be studied in view of the singular values of the matrix, or for given measurements, the discrete Picart condition as defined by Hansen [47].

In the MFS problem, explained in section 7.3, the virtual sources are placed by inflating and deflating the heart and torso surfaces with respect to the heart's geometric center. However, for some heart-torso geometries, this geometrical center is a poor reference. Furthermore, it has been proved in other fields that the placement of the virtual sources influences the ill-posedness of the MFS problem. However, this has not been tested for the ECGI problem.

J. Chamorro-Servent, R. Dubois and Y. Coudière proposed a new method of placement of these virtual sources based on the minimal distance of each point considered on the heart surface to the torso electrodes. The singular value analysis and the discrete Picard condition were used to optimize the location of these sources. The new distribution of sources was compared with the standard one for a set of experimental data. These data consist of simultaneous acquisition of the cardiac (on a Langendorff perfusion of the heart) and body surface potentials, in a controlled experimental environment.

The results presented by J. Chamorro-Servent et al. at CinC2016 [24] showed that the new distribution of sources made the inverse problem less ill-posed and therefore, less sensitive to the regularization parameter chosen. This improved the reconstructed potentials on the heart surface, especially when artefact (as for example the baseline) or noise were present.

Further results from the combination of the works described here and in section 7.3 were presented in a poster in the Liryc workshop of October 2016 [33] by J. Chamorro-Servent et al. A journal manuscript is currently under preparation (to submit in 2017).

7.5. Reduced sodium current in the lateral ventricular wall induces J waves in the ECG

“J waves,” a particular abnormal waveform in electrocardiogram (ECG) leads, are associated with a higher risk for ventricular fibrillation. M. Potse has performed a series of simulations to investigate three possible mechanisms that could explain such waves and the associated arrhythmia risk. Out of these, a reduced sodium current in the lateral area of the left ventricular wall turned out to be the most powerful to cause J waves. The lateral area is particular because it is normally late activated, and a further delay due to regionally reduced sodium current can lead to J waves in the ECG. If the same occurs elsewhere in the heart, the resulting J waves would be masked by other ECG peaks. The simulations were supported, as far as possible, by experiments performed at the University of Amsterdam. The results have been published in the journal *Frontiers in Physiology*, and further refinements have recently been shown in a poster at the Annual workshop of IHU Liryc [14], [43].

7.6. Atrial fibrillation due to complex geometry

Atrial fibrillation (AF), a situation in which the electrical activation of the atria proceeds chaotically, is believed to be due to abnormal tissue structure (for example fibrosis), which slows propagation, and abnormalities in ionic currents, which make the action potential shorter. In collaboration with the Center for Computational Medicine in Cardiology in Lugano, Switzerland, we performed series of simulations in which we tried to reproduce these effects [20]. Rapid stimulation of the atria caused AF in some of the simulations, with a likelihood related to the severity of fibrosis. However, we also observed a 30 % likelihood of AF initiation in a model with no fibrosis at all. In these cases, the complex structure of our highly realistic models alone in combination with the rapid-pacing protocol sufficed to create situations of conditional propagation block, which led to a reentrant arrhythmia. These results may shed a new light on the course of new-onset AF. A manuscript on this topic is under preparation.

8. Partnerships and Cooperations

8.1. Regional Initiatives

8.1.1. IHU LIRYC

Our work is partially funded by the LIRYC project (ANR 10-IAHU 04).

- Until November 2016 the salary of M. Potse was funded by LIRYC.

8.2. National Initiatives

8.2.1. ANR HR-CEM

The project “High Resolution Cardiac Electrophysiology Models: HR-CEM” within the ANR call *Modèles Numériques* started in November 2013 and will last until November 2017.

It is an international project that involves three partners: Inria (coordinator), IHU LIRYC, and UMI-CRM in Montréal (Canada). The project has external collaborators in Univ. Bordeaux and Univ. Pau.

Based on these collaborations and new developments in structural and functional imaging of the heart available at LIRYC, we plan to reconsider the concepts behind the models in order to improve the accuracy and efficiency of simulations. Cardiac simulation software and high-resolution numerical models will be derived from experimental data from animal models. Validation will be performed by comparing of simulation output with experimentally recorded functional data. The validated numerical models will be made available to the community of researchers who take advantage of in-silico cardiac simulation and, hopefully, become references. In particular we shall provide the first exhaustive model of an animal heart including the four chambers coupled through the special conduction network, with highly detailed microstructure of both the atria and the ventricles. Such a model embedded in high-performance computational software will provide stronger medical foundations for in-silico experimentation, and elucidate mechanisms of cardiac arrhythmias.

8.2.2. ANR Labcom CardioXcomp

We are participant in the ANR Labcom project between Inria and the company Notocord (www.notocord.com). In this project, we propose a mathematical approach for the analysis of drug effects on the electrical activity of human induced pluripotent stem cell-derived cardiomyocytes (hiPSC-CMs) based on multi-electrode array (MEA) experiments. Our goal is to produce an *in-silico* tool able to simulate drug actions in MEA/hiPSC-CM assays. The mathematical model takes into account the geometry of the MEA and the electrode properties. The electrical activity of the stem cells at the ion-channel level is governed by a system of ordinary differential equations (ODEs). The ODEs are coupled to the bidomain equations, describing the propagation of the electrical wave in the stem cells preparation. The field potential (FP) measured by the MEA is modeled by the extra-cellular potential of the bidomain equations. First, we propose a strategy allowing us to generate a field potential in good agreement with the experimental data. We show that we are able to reproduce realistic field potentials by introducing different scenarios of heterogeneity in the action potential. This heterogeneity reflects the differentiation atria/ventricles and the age of the cells. Second, we introduce a drug/ion channels interaction based on a pore block model. We conduct different simulations for five drugs (mexiletine, dofetilide, bepridil, ivabradine and BayK). We compare the simulation results with the field potential collected from experimental measurements. Different biomarkers computed on the FP are considered, including depolarization amplitude, repolarization delay, repolarization amplitude and depolarization-repolarization segment. The simulation results show that the model reflect properly the main effects of these drugs on the FP.

8.2.3. REO

The CARMEN team is a partner with the REO team at Inria Paris Rocquencourt and the Notocord company in the CardioXcomp project.

8.2.4. MedicActiv

The CARMEN team cooperates in interaction with the MedicActiV project.

8.2.5. 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 October 2015, has been granted 9.4 million core-hours on the three major systems Curie, Occigen, and Turing. This compute time, to be used in the calendar year 2016, is primarily destined for our research into the interaction between ionic and structural heart disease in atrial fibrillation, Brugada syndrome, and early

repolarisation syndrome [51]. A renewal request has been submitted in October 2016 and was granted with 9.8 million core-hours.

8.3. European Initiatives

8.3.1. FP7 & H2020 Projects

The Carmen team is a core member of two H2020 proposals that are to be submitted in March 2017.

8.4. International Initiatives

8.4.1. Inria International Labs

8.4.1.1. EPICARD

Title: inversE Problems In CARDiac electrophysiology

International Partner (Institution - Laboratory - Researcher):

ENIT (Tunisia) – Department of Intelligence Science and Technology - Nabil Gmati

Start year: 2015

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

Improving the information that we can extract from electrical signals measured on patients with heart diseases is a major priority for the IHU LIRYC. We would like to non-invasively construct the electrical potential on the heart surface only from measurements of the potential on the chest of the patient. It is known that algorithms that have been used in the literature for solving this electrocardiography imaging (ECGI) problem, including those used in commercial medical devices, have several limitations. This problem could be mathematically seen as a boundary data completion problem for elliptic equations. Many studies have been carried out in order to solve this Cauchy problem, but have never been used for solving the ECGI problem. The goal of this Inria International Lab (IIL) is to develop an experimental platform allowing to test various methods and compare their performance on real life experimental data.

We describe here two projects that have been performed in the context of this IIL.

8.4.1.1.1. Mathematical analysis of the parameter estimation problem

N. Zemzemi, J. Lassoued, and M. Mahjoub worked on the mathematical analysis of a parameter identification problem in cardiac electrophysiology modeling. The work was based on a monodomain reaction-diffusion model of the heart. The purpose was to prove the stability of the identification of the parameter τ_{in} , which is the parameter that multiplies the cubic term in the reaction term. The proof of the result is based on a new Carleman-type estimate for both the PDE and ODE problems. As a consequence of the stability result they proved the uniqueness of the parameter τ_{in} giving some observations of both state variables at a given time t_0 in the whole domain and the PDE variable in a non empty open subset w_0 of the domain.

8.4.1.1.2. Uncertainty quantification in the electrocardiography problem

N. Zemzemi worked with N. Fikal, R. Aboulaich and EL.M. El Guarmah on uncertainty quantification in electrocardiography imaging. The purpose of this work was to study the influence of errors and uncertainties of the input data, like the conductivity, on the electrocardiographic imaging (ECGI) solution. They propose a new stochastic optimal control formulation to calculate the distribution of the electric potential on the heart from the measurement on the body surface. The discretization was done using a stochastic Galerkin method allowing to separate random and deterministic variables. The problem was discretized, in spatial part, using the finite element method and the polynomial chaos expansion in the stochastic part of the problem. The problem was solved using a conjugate gradient method where the gradient of the cost function was computed with an adjoint technique. The efficiency of this approach to solve the inverse problem and the usability to quantify the effect of conductivity uncertainties in the torso were demonstrated through numerical simulations on a 2D analytical geometry and on a 2D cross section of a real torso.

8.4.1.2. Informal International Partners

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 [20]. The Maastricht group was partially funded by the FP7 project EUTRAF and our simulations were supported by GENCI (section 8.2.5).

8.5. International Research Visitors

8.5.1. Visits of International Scientists

Professor Y. Bourgault (University of Ottawa) visited the team from 12 to 26 March.

Professor A. Fraguera Collar, from the *Benemerita Universidad Autonoma de Puebla-Mexico* visited us in July 2016.

8.5.2. Visits to International Teams

8.5.2.1. Other international activities

N. Zemzemi gave a course in the CIMPA research school: “Modelling and simulating the electrical activity of the heart Direct and Inverse problems.”

N. Zemzemi organized a mini-symposium intitled “Imaging and inverse modeling” in PICOF 2016: <https://picof.sciencesconf.org/resource/page/id/4#>. From 01/06/2016 to 03/06/2016. Autrans, France.

9. Dissemination

9.1. Promoting Scientific Activities

9.1.1. Scientific Events Organisation

9.1.1.1. Member of the Organizing Committees

- 6th international conference on “Computational Surgery,” Bordeaux, May 2016 (Y. Coudière).
- The annual workshop of IHU Liryc, Bordeaux, October 2016 (Y. Coudière).

N. Zemzemi organized a mini-symposium intitled “Imaging and inverse modeling” in PICOF 2016, from 01/06/2016 to 03/06/2016. Autrans, France.

9.1.2. Scientific Events Selection

9.1.2.1. Member of the Conference Program Committees

- 6th international conference on “Computational Surgery,” Bordeaux, May 2016 (Y. Coudière).
- CARI 2016 (N. Zemzemi)

9.1.3. Journal

9.1.3.1. Member of the Editorial Boards

M. Potse: associate editor of *Frontiers in Cardiac Electrophysiology*.

9.1.3.2. Reviewer - Reviewing activities

M. Potse: *Heart Rhythm*, *IEEE Transactions on Biomedical Engineering*, *Medical & Biological Engineering & Computing*, *Journal of Electrocardiology*.

Y. Coudière: *Journal of computational and applied mathematics*, *PLOS ONE*, *SMAI Journal of Computational Mathematics*

N. Zemzemi: *Inverse Problems*, *Europace*, *Inverse Problems in Science and Engineering*

9.1.4. Invited Talks

M. Bendahmane: Université Qadi Ayyad, IST d'Essaouira (Morocco), April 2016

M. Bendahmane: University of Oslo (Norway), October 2016.

Y. Coudière: University of Ottawa (Canada), February 2016.

N. Zemzemi gave a course in the CIMPA research school: "Modelling and simulating the electrical activity of the heart Direct and Inverse problems". From 04/10 to 10/10 2016. Tunis, Tunisia.

N. Zemzemi: Course on the electrophysiology modelling: Forward and Inverse problems. Ecole doctorale de mathématique. Faculté des sciences de Tunis. From 10/01/2016 to 15/01/2016. Tunis, Tunisia.

M. Potse gave an invited presentation titled "Visualization of 3D Lead Fields" at the [43rd International Congress on Electrocardiology](#).

9.1.5. Leadership within the Scientific Community

M. Potse is council member of the International Society of Electrocardiology.

9.1.6. Scientific Expertise

Y. Coudière:

- ATER committee for Université de Bordeaux
- Reviewer PhD Thesis of P.-L. Colin, Université Lille 1, 27/06/2016
- Reviewer HDR Thesis of M. Sermesant, Université de Nice Sophia-Antipolis, 09/06/2016
- SNF (Swiss National Science foundation)

9.1.7. Research Administration

Y. Coudière:

- Scientific responsibility of the IMB (CNRS UMR 5251) team "Calcul Scientifique et Modélisation," 60 persons.
- Responsible for the scientific communication (*Chargé de mission à l'animation scientifique*) of the IMB

N. Zemzemi: Administration of the Inria associated team Epicard (section [8.4.1.1](#)).

9.2. Teaching - Supervision - Juries

9.2.1. Teaching

DUT : P. E. Bécue, Introduction to modelling and Principal Component Analysis, 43 hours, level N/A, IUT Orsay, France

DUT : P. E. Bécue, Object Oriented Programming with java, 9 hours, level N/A, IUT Orsay, France

9.2.2. Supervision

PhD : A. Davidović, "Multiscale Mathematical Modeling of Structural Heterogeneities in Cardiac Electrophysiology," Université de Bordeaux, 9 December 2016, supervised by Y. Coudière.

PhD in progress: P. E. Bécue, "Modélisation et simulation numérique de l'électrophysiologie cardiaque à l'échelle microscopique," started 1 October 2014, supervised by F. Caro, M. Potse, and Y. Coudière.

PhD in progress: C. Douanla Lontsi, "Schémas d'ordre élevé pour des simulations réalistes en électrophysiologie cardiaque," started 1 November 2014, supervised by Y. Coudière.

PhD in progress: A. Gérard, "Modèles numériques personnalisés de la fibrillation auriculaire," started 1 September 2015, supervised by Y. Coudière.

9.2.3. Juries

M. Bendahmane was a jury member (*rapporteur*) for the PhD thesis of Jamila Lassoued (*Université de Tunis*).

9.3. Popularization

The Carmen team has responded to a call of Cap'Maths in 2014 on dissemination and popularization of mathematics destined for young pupils, the general public, and (future) mathematical professionals. For this project, G. Ravon and Y. Coudière developed a *serious game* called Heart Attack. The game is destined for middle and high school students as an introduction to mathematical modeling. The principal goal of the game is to illustrate the notion of numerical modeling in medical research, and in particular in cardiac rhythmology. The player takes the role of a scientist having developed a numerical model for the electrical activity of the heart and tries to learn how to prevent an arrhythmia. A secondary goal is to teach about the electrical activation mechanism of the heart.

Integrating scientific simulations in an interactive website is challenging because of the constraints imposed by a web-based framework. As a result of this project we have learned a great deal about such development and about the collaboration with professional web developers.

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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

Bordeaux - Sud-Ouest

THEME

Stochastic approaches

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Project-Team CQFD

Creation of the Project-Team: 2009 January 01

Keywords:

Computer Science and Digital Science:

- 1.1.6. - Cloud
- 1.2.4. - QoS, performance evaluation
- 1.3. - Distributed Systems
- 3.3. - Data and knowledge analysis
- 3.4.1. - Supervised learning
- 3.4.2. - Unsupervised learning
- 3.4.5. - Bayesian methods
- 3.4.6. - Neural networks
- 3.4.7. - Kernel methods
- 5.9.2. - Estimation, modeling
- 5.9.6. - Optimization tools
- 6.1.2. - Stochastic Modeling (SPDE, SDE)
- 6.1.3. - Discrete Modeling (multi-agent, people centered)
- 6.2.2. - Numerical probability
- 6.2.3. - Probabilistic methods
- 6.2.4. - Statistical methods
- 6.2.6. - Optimization
- 6.4.2. - Stochastic control
- 7.14. - Game Theory
- 8.2. - Machine learning
- 8.6. - Decision support

Other Research Topics and Application Domains:

- 2.2.4. - Infectious diseases, Virology
- 2.6.1. - Brain imaging
- 5.9. - Industrial maintenance
- 6.2. - Network technologies
- 6.3.3. - Network Management
- 6.5. - Information systems
- 9.2.3. - Video games
- 9.4.2. - Mathematics

1. Members

Research Scientists

Jonatha Anselmi [Inria, Researcher]

Pierre Del Moral [Inria, Senior Researcher, HDR]

Faculty Members

Francois Dufour [Team leader, INP Bordeaux, Professor, HDR]
Marie Chavent [Univ. Bordeaux, Associate Professor, HDR]
Alexandre Genadot [Univ. Bordeaux, Associate Professor]
Pierrick Legrand [Univ. Bordeaux, Associate Professor]
Jerome Saracco [INP Bordeaux, Professor, HDR]
Huilong Zhang [Univ. Bordeaux, Associate Professor]

PhD Students

Alizée Geeraert [Thales]
Christophe Nivot [Inria, until Aug 2016, granted by AIRBUS DEFENCE AND SPACE]
Chloe Pasin [Univ. Bordeaux]
Jessica Sodjo [Inria]
Adrien Todeschini [Inria, until november 2016, granted by EVOLLIS SAS]

Post-Doctoral Fellow

Solveig Badillo [Univ. Bordeaux, until Feb 2016]

Visiting Scientists

Oswaldo Luiz Do Valle Costa [Polytechnic School of the University of São Paulo]
Victor Raul Lopez Lopez [ITT (Instituto tecnologico de Tijuana), from Sep 2016 until Oct 2016]
Alexei Piunovskiy [University of Liverpool, until Jul 2016]

Administrative Assistant

Chrystel Plumejeau [Inria]

Others

Benoite de Saporta [Univ. Montpellier II, Professor, HDR]
Jose Enrique Hernandez Beltran [ITT (Instituto tecnologico de Tijuana), from Apr 2016 until Jul 2016]
Uriel Lopez Islas [Centro de Investigación y Desarrollo de Tecnología Digital (CITEDI), from Apr 2016 until Jul 2016]

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 mathematical representations which are in essence dynamic and stochastic with discrete and/or continuous variables. This increasing 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 and various probabilistic phenomena;
- Estimation: developing theoretical and computational procedures in order to estimate and evaluate the parameters and the performance of the system;
- Optimization: developing theoretical and numerical control tools to optimize the performance of complex systems such as computer systems and communication networks.

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. For example, in order to optimize the predictive maintenance of a system, it is necessary to choose the adequate model for its representation. The step of modeling is crucial before any estimation or computation of quantities related to its optimization. For this we have to represent all the different regimes of the system and the behavior of the physical variables under each of these regimes. Moreover, we must also select the dynamic variables which have a potential effect on the physical variable and the quantities of interest. The team CQFD works on the theory of Piecewise Deterministic Markov Processes (PDMP's) and on Markov Decision Processes (MDP's). These two classes of systems form general families of controlled stochastic processes suitable for the modeling of sequential decision-making problems in the continuous-time (PDMPs) and discrete-time (MDP's) context. They appear in many fields such as engineering, computer science, economics, operations research and constitute powerful class of processes for the modeling of complex system.

- 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. However, 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 $\theta = [\theta_1, \dots, \theta_d]$ (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 [44] and Duan and Li [42].

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 [43].

- Stochastic optimal control: optimal stopping, impulse control, continuous control, linear programming.

The first objective is to focus on the development of computational methods.

- In the continuous-time context, stochastic control theory has from the numerical point of view, been mainly concerned with Stochastic Differential Equations (SDEs in short). From the practical and theoretical point of view, the numerical developments for this class of processes are extensive and largely complete. It capitalizes on the connection between SDEs and second order partial differential equations (PDEs in short) and the fact that the properties of the latter equations are very well understood. It is, however, hard to deny that the development of computational methods for the control of PDMPs has received little attention. One of the main reasons is that the role played by the familiar PDEs in the diffusion models is here played by certain systems of integro-differential equations for which there is not (and cannot be) a unified theory such as for PDEs as emphasized by M.H.A. Davis in his book. To the best knowledge of the team, there is only one attempt to tackle this difficult problem by O.L.V. Costa and M.H.A. Davis. The originality of our project consists in studying this unexplored area. It is very important to stress the fact that these numerical developments will give rise to a lot of theoretical issues such as type of approximations, convergence results, rates of convergence,....
- Theory for MDP's has reached a rather high degree of maturity, although the classical tools such as value iteration, policy iteration and linear programming, and their various extensions, are not applicable in practice. We believe that the theoretical progress of MDP's must be in parallel with the corresponding numerical developments. Therefore, solving MDP's numerically is an awkward and important problem both from the theoretical and practical point of view. In order to meet this challenge, the fields of neural networks, neurodynamic programming and approximate dynamic programming became recently an active area of research. Such methods found their roots in heuristic approaches, but theoretical results for convergence results are mainly obtained in the context of finite MDP's. Hence, an ambitious challenge is to investigate such numerical problems but for models with general state and action spaces. Our motivation is to develop theoretically consistent

computational approaches for approximating optimal value functions and finding optimal policies.

- An effort has been devoted to the development of efficient computational methods in the setting of communication networks. These are complex dynamical systems composed of several interacting nodes that exhibit important congestion phenomena as their level of interaction grows. The dynamics of such systems are affected by the randomness of their underlying events (e.g., arrivals of http requests to a web-server) and are described stochastically in terms of queueing network models. These are mathematical tools that allow one to predict the performance achievable by the system, to optimize the network configuration, to perform capacity-planning studies, etc. These objectives are usually difficult to achieve without a mathematical model because Internet systems are huge in size. However, because of the exponential growth of their state spaces, an exact analysis of queueing network models is generally difficult to obtain. Given this complexity, we have developed analyses in some limiting regime of practical interest (e.g., systems size grows to infinity). This approach is helpful to obtain a simpler mathematical description of the system under investigation, which leads to the direct definition of efficient, though approximate, computational methods and also allows to investigate other aspects such as Nash equilibria.

The second objective of the team is to study some theoretical aspects related to MDPs such as convex analytical methods and singular perturbation. Analysis of various problems arising in MDPs leads to a large variety of interesting mathematical problems.

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 which gathers several topics of team is a collaboration started in September 2013 with Airbus Defence & Space. The goal of this project is the optimization of the assembly line of the future European launcher, taking into account several kinds of economical and technical constraints. We have started with a simplified model with five components to be assembled in workshops liable to breakdowns. We have modeled the problem using the Markov Decision Processes (MDP) framework and built a simulator of the process in order to run a simulation-based optimization procedure.

A second example concerns the optimization of the maintenance of a on board system equipped with a HUMS (Health Unit Monitoring Systems) in collaboration with THALES Optronique. 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.

However the spectrum of applications of the topics of the team is larger and may 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. Highlights of the Year

5.1. Highlights of the Year

Publication of the book: *Stochastic Processes. From Applications to Theory* written by P. Del Moral and S. Penev, CRC Press, 1290 pages, Jan 2017.

Pierre del Moral has been invited to the IMS World Congress in Toronto to give a Medallion lectures in May 2016.

6. New Software and Platforms

6.1. Package divclust

FUNCTIONAL DESCRIPTION

DIVCLUS-T is a divisive hierarchical clustering algorithm based on a monothetic bipartitional approach allowing the dendrogram of the hierarchy to be read as a decision tree. It is designed for numerical, categorical (ordered or not) or mixed data. Like the Ward agglomerative hierarchical clustering algorithm and the k-means partitioning algorithm, it is based on the minimization of the inertia criterion. However, it provides a simple and natural monothetic interpretation of the clusters. Indeed, each cluster is described by set of binary questions. The inertia criterion is calculated on all the principal components of PCAmix (and then on standardized data in the numerical case).

- Participants: Marie Chavent, Marc Fuentes
- Contact: Marie Chavent
- URL: <https://github.com/chavent/divclust>

6.2. Package ClustGeo

FUNCTIONAL DESCRIPTION

This R package is dedicated to the clustering of objects with geographical positions. The clustering method implemented in this package allows the geographical constraints of proximity to be taken into account within the ascendant hierarchical clustering.

- Marie Chavent, Amaury Labenne, Vanessa Kuentz, Jérôme Saracco
- Contact: Amaury Labenne
- URL: <https://cran.r-project.org/web/packages/ClustGeo/index.html>

6.3. PCAmixdata

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.

- Participants: Marie Chavent, Amaury Labenne, Jérôme Saracco
- Contact: Marie Chavent
- URL: <https://cran.r-project.org/web/packages/PCAmixdata/index.html>

6.4. QuantifQuantile

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.

- Isabelle Charlier, Jérôme Saracco
- Contact: Isabelle Charlier
- URL: <https://cran.r-project.org/web/packages/QuantifQuantile/index.html>

6.5. biips

Bayesian Inference with Interacting Particle Systems

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: Francois Caron and Adrien Todeschini
- Contact: Adrien Todeschini
- URL: <http://biips.gforge.inria.fr>

6.6. VCN: Software for analysis of VCN

FUNCTIONAL DESCRIPTION

VCN is a software for the analysis of the vigilance of the patient based on the analysis of the EEG signals. The code is written in Matlab and provides an interface easy to use for someone without informatics skills.

- Participants: Pierrick Legrand, Julien Clauzel, Laurent Vezard, Charlotte Rodriguez, Borjan Geshkovski.
- Contact: Pierrick Legrand

6.7. EMGView: Software for visualisation and time-frequency analysis of bio signals

FUNCTIONAL DESCRIPTION

EMGView is a software for the visualisation and the analysis of bio-signals. The code is written in Matlab and provides an interface easy to use for someone without informatics skills.

- Participants: Luis Herrera, Eric Grivel, Pierrick Legrand, Gregory Barriere
- Contact: Pierrick Legrand

7. New Results

7.1. Computable approximations for continuous-time Markov decision processes on Borel spaces based on empirical measures

The following result has been obtained by J. Anselmi (Inria CQFD), F. Dufour (Inria CQFD) and T. Prieto-Rumeau.

We propose an approach for approximating the value function and computing an ε -optimal policy of a continuous-time Markov decision processes with Borel state and action spaces, with possibly unbounded cost and transition rates, under the total expected discounted cost optimality criterion. Under the assumptions that the controlled process satisfies a Lyapunov type condition and the transition rate has a density function with respect to a reference measure, together with piecewise Lipschitz continuity of the elements of the control model, one can approximate the original controlled process by a sequence of models that are computationally solvable. Convergence of the approximations takes place at an exponential rate in probability.

7.2. Decentralized Proportional Load Balancing

The following result has been obtained by J. Anselmi (Inria CQFD) and N. Walton.

Load balancing is a powerful technique commonly used in communication and computer networks to improve system performance, robustness and fairness. In this paper, we consider a general model capturing the performance of communication and computer networks, and on top of it we propose a decentralized algorithm for balancing load among multiple network paths. The proposed algorithm is inspired by the modus operandi of the processor-sharing queue and on each network entry point operates as follows: every time a unit of load completes its service on a path, it increases by one unit the load of that path and decreases by one unit the load of a path selected at random with probability proportional to the amount of load on each of the available paths. We develop a dynamical system to argue that our load-balancer achieves a desirable network-wide utility optimization.

7.3. Constrained and Unconstrained Optimal Discounted Control of Piecewise Deterministic Markov Processes

The following result has been obtained by O. Costa, F. Dufour (Inria CQFD), and A. B. Piunovskiy.

The main goal of this paper is to study the infinite-horizon expected discounted continuous-time optimal control problem of piecewise deterministic Markov processes with the control acting continuously on the jump intensity λ and on the transition measure Q of the process but not on the deterministic flow ϕ . The contributions of the paper are for the unconstrained as well as the constrained cases. The set of admissible control strategies is assumed to be formed by policies, possibly randomized and depending on the history of the process, taking values in a set valued action space. For the unconstrained case we provide sufficient conditions based on the three local characteristics of the process ϕ , λ , Q and the semicontinuity properties of the set valued action space, to guarantee the existence and uniqueness of the integro-differential optimality equation (the so-called Bellman–Hamilton–Jacobi equation) as well as the existence of an optimal (and δ -optimal, as well) deterministic stationary control strategy for the problem. For the constrained case we show that the values of the constrained control problem and an associated infinite dimensional linear programming (LP) problem are the same, and moreover we provide sufficient conditions for the solvability of the LP problem as well as for the existence of an optimal feasible randomized stationary control strategy for the constrained problem.

7.4. Approximate Kalman-Bucy filter for continuous-time semi-Markov jump linear systems

The following result has been obtained by B. Saporta and E. F. Costa.

The aim of this paper is to propose a new numerical approximation of the Kalman-Bucy filter for semi-Markov jump linear systems. This approximation is based on the selection of typical trajectories of the driving semi-Markov chain of the process by using an optimal quantization technique. The main advantage of this approach is that it makes pre-computations possible. We derive a Lipschitz property for the solution of the Riccati equation and a general result on the convergence of perturbed solutions of semi-Markov switching Riccati equations when the perturbation comes from the driving semi-Markov chain. Based on these results, we prove the convergence of our approximation scheme in a general infinite countable state space framework and derive

an error bound in terms of the quantization error and time discretization step. We employ the proposed filter in a magnetic levitation example with Markovian failures and compare its performance with both the Kalman-Bucy filter and the Markovian linear minimum mean squares estimator.

7.5. Investigation of asymmetry in E. coli growth rate

The following result has been obtained by B. Saporta in collaboration with B. Delyon, N. Krell and Lydia Robert.

The data we analyze derives from the observation of numerous cells of the bacterium *Escherichia coli* (*E. coli*) growing and dividing. Single cells grow and divide to give birth to two daughter cells, that in turn grow and divide. Thus, a colony of cells from a single ancestor is structured as a binary genealogical tree. At each node the measured data is the growth rate of the bacterium. In this paper, we study two different data sets. One set corresponds to small complete trees, whereas the other one corresponds to long specific sub-trees. Our aim is to compare both sets. This paper is accessible to post graduate students and readers with advanced knowledge in statistics.

7.6. Impulsive Control for Continuous-Time Markov Decision Processes: A Linear Programming Approach

The following result has been obtained by F. Dufour (Inria CQFD) and A. B. Piunovskiy.

In this paper, we investigate an optimization problem for continuous-time Markov decision processes with both impulsive and continuous controls. We consider the so-called constrained problem where the objective of the controller is to minimize a total expected discounted optimality criterion associated with a cost rate function while keeping other performance criteria of the same form, but associated with different cost rate functions, below some given bounds. Our model allows multiple impulses at the same time moment. The main objective of this work is to study the associated linear program defined on a space of measures including the occupation measures of the controlled process and to provide sufficient conditions to ensure the existence of an optimal control.

7.7. Conditions for the Solvability of the Linear Programming Formulation for Constrained Discounted Markov Decision Processes

The following result has been obtained by F. Dufour (Inria CQFD) and T. Prieto-Rumeau.

We consider a discrete-time constrained discounted Markov decision process (MDP) with Borel state and action spaces, compact action sets, and lower semi-continuous cost functions. We introduce a set of hypotheses related to a positive weight function which allow us to consider cost functions that might not be bounded below by a constant, and which imply the solvability of the linear programming formulation of the constrained MDP. In particular, we establish the existence of a constrained optimal stationary policy. Our results are illustrated with an application to a fishery management problem.

7.8. Spatio-temporal averaging for a class of hybrid systems and application to conductance-based neuron models

The following result has been obtained by A. Genadot (Inria CQFD).

We obtain a limit theorem endowed with quantitative estimates for a general class of infinite dimensional hybrid processes with intrinsically two different time scales and including a population. As an application, we consider a large class of conductance-based neuron models describing the nerve impulse propagation along a neural cell at the scales of ion channels.

7.9. A comparison of fitness-case sampling methods for genetic programming

The following result has been obtained by Pierrick Legrand (Inria CQFD) in collaboration with Y. Martinez, E. Naredo, L. Trujillo, U. Lopez.

The canonical approach towards fitness evaluation in Genetic Programming (GP) is to use a static training set to determine fitness, based on a cost function averaged over all fitness-cases. However, motivated by different goals, researchers have recently proposed several techniques that focus selective pressure on a subset of fitness-cases at each generation. These approaches can be described as fitness-case sampling techniques, where the training set is sampled, in some way, to determine fitness. This paper shows a comprehensive evaluation of some of the most recent sampling methods, using benchmark and real-world problems for symbolic regression. The algorithms considered here are Interleaved Sampling, Random Interleaved Sampling, Lexicase Selection and a new sampling technique is proposed called Keep-Worst Interleaved Sampling (KW-IS). The algorithms are extensively evaluated based on test performance, overfitting and bloat. Results suggest that sampling techniques can improve performance compared with standard GP. While on synthetic benchmarks the difference is slight or none at all, on real-world problems the differences are substantial. Some of the best results were achieved by Lexicase Selection and KeepWorse-Interleaved Sampling. Results also show that on real-world problems overfitting correlates strongly with bloating. Furthermore, the sampling techniques provide efficiency, since they reduce the number of fitness-case evaluations required over an entire run.

7.10. Prediction of Expected Performance for a Genetic Programming Classifier

The following result has been obtained by Pierrick Legrand (Inria CQFD) in collaboration with Y. Martínez, L. Trujillo and E. Galván-López.

The estimation of problem difficulty is an open issue in genetic programming (GP). The goal of this work is to generate models that predict the expected performance of a GP-based classifier when it is applied to an unseen task. Classification problems are described using domain-specific features, some of which are proposed in this work, and these features are given as input to the predictive models. These models are referred to as predictors of expected performance. We extend this approach by using an ensemble of specialized predictors (SPEP), dividing classification problems into groups and choosing the corresponding SPEP. The proposed predictors are trained using 2D synthetic classification problems with balanced datasets. The models are then used to predict the performance of the GP classifier on unseen real-world datasets that are multidimensional and imbalanced. This work is the first to provide a performance prediction of a GP system on test data, while previous works focused on predicting training performance. Accurate predictive models are generated by posing a symbolic regression task and solving it with GP. These results are achieved by using highly descriptive features and including a dimensionality reduction stage that simplifies the learning and testing process. The proposed approach could be extended to other classification algorithms and used as the basis of an expert system for algorithm selection.

7.11. Evolving Genetic Programming Classifiers with Novelty Search

The following result has been obtained by Pierrick Legrand (Inria CQFD) in collaboration with E. Naredo, L. Trujillo, S. Silvac and Luis Muñoz.

Novelty Search (NS) is a unique approach towards search and optimization, where an explicit objective function is replaced by a measure of solution novelty. However, NS has been mostly used in evolutionary robotics while its usefulness in classic machine learning problems has not been explored. This work presents a NS-based genetic programming (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. These results are made possible by using a domain-specific behavior descriptor. 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. The paper also discusses the effects of NS on GP search dynamics and code growth. 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.

7.12. Regularity and Matching Pursuit Feature Extraction for the Detection of Epileptic Seizures

The following result has been obtained by Pierrick Legrand (Inria CQFD) in collaboration with E. Z-Flores, L. Trujillo, A. Sotelo and L. N. Coriaa.

The neurological disorder known as epilepsy is characterized by involuntary recurrent seizures that diminish a patient's quality of life. Automatic seizure detection can help improve a patient's interaction with her/his environment, and while many approaches have been proposed the problem is still not trivially solved.

In this work, we present a novel methodology for feature extraction on EEG signals that allows us to perform a highly accurate classification of epileptic states. 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 97.6% accuracy on the most difficult case. Comparison with existing methods: A comparison with recent literature, using a well known database, reveals that our proposal achieves state-of-the-art performance. The experimental results show that epileptic states can be accurately detected by combining features extracted through regularity analysis, the Matching Pursuit algorithm and simple time-domain statistical analysis. Therefore, the proposed method should be considered as a promising approach for automatic EEG analysis.

7.13. Probabilistic safety analysis of the collision between a space debris and a satellite with an island particle algorithm

The following result has been obtained by P. Del Moral (Inria CQFD) in collaboration with C. Verge, J. Morio and J.C Dolado Perez.

Collision between satellites and space debris seldom happens, but the loss of a satellite by collision may have catastrophic consequences both for the satellite mission and for the space environment. To support the decision to trigger off a collision avoidance manoeuvre, an adapted tool is the determination of the collision probability between debris and satellite. This probability estimation can be performed with rare event simulation techniques when Monte Carlo techniques are not enough accurate. In this chapter, we focus on analyzing the influence of different simulation parameters (such as the drag coefficient) that are set for to simplify the simulation, on the collision probability estimation. A bad estimation of these simulation parameters can strongly modify rare event probability estimations. We design here a new island particle Markov chain Monte Carlo algorithm to determine the parameters that, in case of bad estimation, tend to increase the collision probability value. This algorithm also gives an estimate of the collision probability maximum taking into account the likelihood of the parameters. The principles of this statistical technique are described throughout this chapter.

7.14. Particle association measures and multiple target tracking

The following result has been obtained by P. Del Moral (Inria CQFD) in collaboration with J. Houssineau.

In the last decade, the area of multiple target tracking has witnessed the introduction of important concepts and methods, aiming at establishing principled approaches for dealing with the estimation of multiple objects in an efficient way. One of the most successful classes of multi-object filters that have been derived out of these new grounds includes all the variants of the Probability Hypothesis Density (phd) filter. In spite of the attention that these methods have attracted, their theoretical performances are still not fully understood. In this chapter, we first focus on the different ways of establishing the equations of the phd filter, using a consistent set of notations. The objective is then to introduce the idea of observation path, upon which association measures are defined. We will see how these concepts highlight the structure of the first moment of the multi-object distributions in time, and how they allow for devising solutions to practical estimation problems.

7.15. Exponential mixing properties for time inhomogeneous diffusion processes with killing

The following result has been obtained by P. Del Moral (Inria CQFD) in collaboration with D. Villemonais.

We consider an elliptic and time-inhomogeneous diffusion process with time-periodic coefficients evolving in a bounded domain of \mathbb{R}^d with a smooth boundary. The process is killed when it hits the boundary of the domain (hard killing) or after an exponential time (soft killing) associated with some bounded rate function. The branching particle interpretation of the non absorbed diffusion again behaves as a set of interacting particles evolving in an absorbing medium. Between absorption times, the particles evolve independently one from each other according to the diffusion semigroup; when a particle is absorbed, another selected particle splits into two offsprings. This article is concerned with the stability properties of these non absorbed processes. Under some classical ellipticity properties on the diffusion process and some mild regularity properties of the hard obstacle boundaries, we prove a uniform exponential strong mixing property of the process conditioned to not be killed. We also provide uniform estimates w.r.t. the time horizon for the interacting particle interpretation of these non-absorbed processes, yielding what seems to be the first result of this type for this class of diffusion processes evolving in soft and hard obstacles, both in homogeneous and non-homogeneous time settings.

7.16. On particle Gibbs Markov chain Monte Carlo models

The following result has been obtained by P. Del Moral (Inria CQFD) in collaboration with R. Kohn and F. Patras.

This result analyses a new class of advanced particle Markov chain Monte Carlo algorithms recently introduced by Andrieu, Doucet, and Holenstein (2010). We present a natural interpretation of these methods in terms of well known unbiasedness properties of Feynman-Kac particle measures, and a new duality with Feynman-Kac models. This perspective sheds new light on the foundations and the mathematical analysis of this class of methods. A key consequence is their equivalence with the Gibbs sampling of a (many-body) Feynman-Kac target distribution. Our approach also presents a new stochastic differential calculus based on geometric combinatorial techniques to derive non-asymptotic Taylor type series for the semigroup of a class of particle Markov chain Monte Carlo models around their invariant measures with respect to the population size of the auxiliary particle sampler. These results provide sharp quantitative estimates of the convergence rate of the models with respect to the time horizon and the size of the systems. We illustrate the direct implication of these results with sharp estimates of the contraction coefficient and the Lyapunov exponent of the corresponding samplers, and explicit and non-asymptotic L^p -mean error decompositions of the law of the random states around the limiting invariant measure. The abstract framework developed in the article also allows the design of natural extensions to island (also called SMC²) type particle methodologies. We illustrate this general framework and results in the context of nonlinear filtering, hidden Markov chain problems with fixed unknown parameters, and Feynman-Kac path-integration models arising in computational physics and chemistry.

7.17. Sequential Monte Carlo with Highly Informative Observations

The following result has been obtained by P. Del Moral (Inria CQFD) in collaboration with L. Murray.

We propose sequential Monte Carlo (SMC) methods for sampling the posterior distribution of state-space models under highly informative observation regimes, a situation in which standard SMC methods can perform poorly. A special case is simulating bridges between given initial and final values. The basic idea is to introduce a schedule of intermediate weighting and resampling times between observation times, which guide particles towards the final state. This can always be done for continuous-time models, and may be done for discrete-time models under sparse observation regimes; our main focus is on continuous-time diffusion processes. The methods are broadly applicable in that they support multivariate models with partial observation, do not require simulation of the backward transition (which is often unavailable), and, where possible, avoid pointwise evaluation of the forward transition. When simulating bridges, the last cannot be avoided entirely without concessions, and we suggest an epsilon-ball approach (reminiscent of Approximate Bayesian Computation) as a workaround. Compared to the bootstrap particle filter, the new methods deliver substantially reduced mean squared error in normalising constant estimates, even after accounting for execution time. The methods are demonstrated for state estimation with two toy examples, and for parameter estimation (within a particle marginal Metropolis–Hastings sampler) with three applied examples in econometrics, epidemiology and marine biogeochemistry.

7.18. A duality formula for Feynman-Kac path particle models

The following result has been obtained by P. Del Moral (Inria CQFD) in collaboration with R. Kohn and F. Patras.

This result presents a new duality formula between genetic type genealogical tree based particle models and Feynman–Kac measures on path spaces. Among others, this formula allows us to design reversible Gibbs–Glauber Markov chains for Feynman–Kac integration on path spaces. Our approach yields new Taylor series expansions of the particle Gibbs–Glauber semigroup around its equilibrium measure w.r.t. the size of the particle system, generalizing the recent work of Andrieu, Doucet, and Holenstein [1]. We analyze the rate of convergence to equilibrium in terms of the ratio of the length of the trajectories to the number of particles. The analysis relies on a tree-based functional and combinatorial representation of a class of Feynman–Kac particle models with a frozen ancestral line. We illustrate the impact of these results in the context of Quantum and Diffusion Monte Carlo methods.

7.19. Non-Asymptotic Analysis of Adaptive and Annealed Feynman-Kac Particle Models

The following result has been obtained by P. Del Moral (Inria CQFD) in collaboration with F. Giraud.

Sequential and quantum Monte Carlo methods, as well as genetic type search algorithms can be interpreted as a mean field and interacting particle approximations of Feynman-Kac models in distribution spaces. The performance of these population Monte Carlo algorithms is strongly related to the stability properties of nonlinear Feynman-Kac semigroups. In this paper, we analyze these models in terms of Dobrushin ergodic coefficients of the reference Markov transitions and the oscillations of the potential functions. Sufficient conditions for uniform concentration inequalities w.r.t. time are expressed explicitly in terms of these two quantities. We provide an original perturbation analysis that applies to annealed and adaptive Feynman-Kac models, yielding what seems to be the first results of this kind for these types of models. Special attention is devoted to the particular case of Boltzmann-Gibbs measures' sampling. In this context, we design an explicit way of tuning the number of Markov chain Monte Carlo iterations with temperature schedule. We also design an alternative interacting particle method based on an adaptive strategy to define the temperature increments. The theoretical analysis of the performance of this adaptive model is much more involved as both the potential functions and the reference Markov transitions now depend on the random evolution on the particle model. The nonasymptotic analysis of these complex adaptive models is an open research problem. We initiate this study with the concentration analysis of a simplified adaptive models based on reference Markov transitions that coincide with the limiting quantities, as the number of particles tends to infinity.

7.20. Uniform stability of a particle approximation of the optimal filter derivative

The following result has been obtained by P. Del Moral (Inria CQFD) in collaboration with A. Doucet and S.S. Singh.

Particle methods, also known as Sequential Monte Carlo methods, are a principled set of algorithms used to approximate numerically the optimal filter in nonlinear non-Gaussian state-space models. However, when performing maximum likelihood parameter inference in state-space models, it is also necessary to approximate the derivative of the optimal filter with respect to the parameter of the model. References [G. Poyiadjis, A. Doucet, and S. S. Singh, Particle methods for optimal filter derivative: Application to parameter estimation, in Proceedings of IEEE International Conference on Acoustics, Speech, and Signal Processing (ICASSP) 5, Philadelphia, 2005, pp. 925–928 and G. Poyiadjis, A. Doucet, and S. S. Singh, Biometrika, 98 (2011), pp. 65–80] present an original particle method to approximate this derivative, and it was shown in numerical examples to be numerically stable in the sense that it did not deteriorate over time. In this paper we theoretically substantiate this claim. \mathbb{L}_p bounds and a central limit theorem for this particle approximation are presented. Under mixing conditions these \mathbb{L}_p bounds and the asymptotic variance are uniformly bounded with respect to the time index.

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

The following result has been obtained by M. Chavent, and J. Saracco in collaboration with R. Genuer.

High-dimensional data classification is a challenging problem. A standard approach to tackle this problem is to perform variables selection, e.g. using stepwise procedures or LASSO approaches. Another standard way is to perform dimension reduction, e.g. by Principal Component Analysis (PCA) or Partial Least Square (PLS) procedures. The approach proposed in this paper combines both dimension reduction and variables selection. First, a procedure of clustering of variables (CoV) is used to built groups of correlated variables in order to reduce the redundancy of information. This dimension reduction step relies on the R package ClustOfVar which can deal with both numerical and categorical variables. Secondly, the most relevant synthetic variables (which are numerical variables summarizing the groups obtained in the first step) are selected with a procedure of variable selection using random forests (VSURF), implemented in the R package VSURF. Numerical performances of the proposed methodology called CoV/VSURF are compared with direct applications of VSURF or random forests (RF) on the original p variables. Improvements obtained with the CoV/VSURF procedure are illustrated on two simulated mixed datasets (cases $n > p$ and $n \ll p$) and on a real proteomic dataset.

7.22. An innovative approach combining animal performances, nutritional value and sensory quality of meat

The following result has been obtained by M. Chavent and J. Saracco in collaboration with M.P. Ellies.

This work sets out a methodological approach to assess how to simultaneously control together animal performances, nutritional value, sensory quality of meat. Seventy-one young bulls were characterized by 97 variables. Variables of each element were arranged into either 5 homogeneous Intermediate Scores (IS) or 2 Global Indices (GI) via a clustering of variables and analysed together by Principal Component Analysis (PCA). These 3 pools of 5 IS (or 2 GI) were analysed together by PCA to established the links existing among the triptych. Classification on IS showed no opposition between animal performances and nutritional value of meat, as it seemed possible to identify animals with a high butcher value and intramuscular fat relatively rich in polyunsaturated fatty acids. Concerning GI, the classification indicated that animal performances were negatively correlated with sensory quality. This method appeared to be a useful contribution to the management of animal breeding for an optimal trade-off between the three elements of the triptych.

7.23. BIG-SIR: a Sliced Inverse Regression approach for massive data

The following result has been obtained by J. Saracco (Inria CQFD) in collaboration with B. Lique.

In a massive data setting, we focus on a semiparametric regression model involving a real dependent variable Y and a p -dimensional covariable X . This model includes a dimension reduction of X via an index $X'\beta$. The Effective Dimension Reduction (EDR) direction β cannot be directly estimated by the Sliced Inverse Regression (SIR) method due to the large volume of the data. To deal with the main challenges of analysing massive datasets which are the storage and computational efficiency, we propose a new SIR estimator of the EDR direction by following the “divide and conquer” strategy. The data is divided into subsets. EDR directions are estimated in each subset which is a small dataset. The recombination step is based on the optimisation of a criterion which assesses the proximity between the EDR directions of each subset. Computations are run in parallel with no communication among them. The consistency of our estimator is established and its asymptotic distribution is given. Extensions to multiple indices models, q -dimensional response variable and/or SIR α -based methods are also discussed. A simulation study using our `edrGraphicalTools` R package shows that our approach enables us to reduce the computation time and conquer the memory constraint problem posed by massive datasets. A combination of `foreach` and `bigmemory` R packages are exploited to offer efficiency of execution in both speed and memory. Finally, results are visualised using the `bin-summarise-smooth` approach through the `bigvis` R package

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

8.1.1. Airbus

Participants: Benoîte de Saporta, François Dufour, Christophe Nivot.

We are interested in the optimization of a launcher integration process. It comprises several steps from the production of the subassemblies to the final launch. The four subassemblies go through various types of operations such as preparation, integration, control and storage. These operations are split up into three workshops. Due to possible breakdowns or staff issues, the time spent in each workshop is supposed random. So is the time needed to deliver the subassemblies, for similar reasons including e.g. shipping delays. We also have to deal with constraints related to the architecture of the assembly process itself. Indeed, we have to take into account waiting policies between workshops. The workshops may work in parallel but can be blocked if their output is not transferred to the next workshop in line. Storage capacity of output products is limited.

Our goal is finding the best rates of delivery of the subassemblies, the best choice of architecture (regarding stock capacities) and the best times when to stop and restart the workshops to be able to carry out twelve launches a year according to a predetermined schedule at minimal cost. To solve this problem, we choose a mathematical model particularly suitable for optimization with randomness: Markov decision processes (MDPs).

We have implemented a numerical simulator of the process based on the MDP model. It provides the fullest information possible on the process at any time. The simulator has first been validated with deterministic histories. Random histories have then been run with exponentially distributed delivery times for the subassemblies and several families of random laws for the time spent in each workshop. Using Monte Carlo simulations, we obtain the distribution of the launch times. Preliminary optimization results allow choosing stock capacities and delivery rates that satisfy the launch schedule.

In this context, the PhD Thesis of Christophe Nivot (2013-2016) is funded by Chaire Inria-Astrium-EADS IW-Conseil régional d'Aquitaine.

8.1.2. Thales Optronique

Participants: Benoîte de Saporta, François Dufour, Alizée Geeraert.

Integrated maintenance, failure intensity, optimisation.

As part of optimizing the reliability, Thales Optronics includes systems that examine the state of their equipment. This function is performed by HUMS (Health Unit Monitoring Systems). The collaboration is the subject of the PhD of Alize Geeraert (CIFRE). The aim of this thesis is to implement in the HUMS a program based on observations that can determine the state of the system, optimize maintenance operations and evaluate the failure risk of a mission.

8.1.3. DCNS

Participants: Huilong Zhang, Jonatha Anselmi, François Dufour, Dann Laneuville.

This contract is with DCNS, a French industrial group specialized in naval defense and energy. In particular, DCNS designs and builds submarines and surface combatants, develops associated systems and infrastructure, and offers a full range of services to naval bases and shipyards, together with a focus into marine renewable energy. The main objective is to have robust algorithms able to build an accurate picture of the objects that are around a submarine by only using “passive sonar” information. This means that no information is transmitted by the submarine, which just listens to acoustic waves coming in, to the target. We estimate the position and the velocity of moving targets through noisy observations and a Kalman-type filter. Estimates become accurate depending on the type and the number of maneuvers done by the submarine. Our goal is to combine the filter that is currently used in DCNS with a Markov decision process. This provides a systematic framework to compute the best sequence of submarine maneuvers that allows the system to determine, as soon as possible, accurate target position and velocity. The current technological transfer to DCNS stands in a stochastic optimization framework developed in Matlab that operates under the hypothesis that the target follows a uniform linear motion with constant velocity or zero acceleration. The case where targets move in a more complex manner gives concrete perspectives for further transfers to DCNS.

9. Partnerships and Cooperations

9.1. Regional Initiatives

9.1.1. MATCHABLE project

Matchable is a startup incubated at IRA (Incubateur Régional d’Aquitaine) since Mars 2014. This startup predicts how players will behave, who is likely to spend money, who you should target with promotions/product placement, and who the developer has to pay attention to in order to prevent churners. The members of CQFD have supervised two masters internships and a postdoctoral researcher, granted by two PEPS contracts from AMIES.

9.1.2. project LabEx CPU TIMIC

The topic of the project is TIMIC is the multivariate treatment of human brain imaging and its application to the analysis of cerebral connectivity graph during rest. The project focuses on the analysis of variability of cerebral organisation on a large population using several methods of supervised and unsupervised classification. The volume of data and the iterative aspect of the methods will lead to implement the classification process on infrastructure of distributed computing.

Alexandre Laurent has been hired as full time research engineer this project for 12 months in 2016.

9.2. National Initiatives

9.2.1. ANR Piece

ANR Piece (2013-2016) of the program *Jeunes chercheuses et jeunes chercheurs* of the French National Agency of Research (ANR), lead by F. Malrieu (Univ. Tours). The Piecewise Deterministic Markov Processes (PDMP) are non-diffusive stochastic processes which naturally appear in many areas of applications as communication networks, neuron activities, biological populations or reliability of complex systems. Their

mathematical study has been intensively carried out in the past two decades but many challenging problems remain completely open. This project aims at federating a group of experts with different backgrounds (probability, statistics, analysis, partial derivative equations, modeling) in order to pool everyone's knowledge and create new tools to study PDMPs. The main lines of the project relate to estimation, simulation and asymptotic behaviors (long time, large populations, multi-scale problems) in the various contexts of application.

9.2.2. 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.

9.3. European Initiatives

9.3.1. FP7 & H2020 Projects

IRSES ACOBSEC

Project reference: 612689 Funded under: FP7-PEOPLE

Coordinator : Pierrick Legrand

Participants UNIVERSITE VICTOR SEGALEN BORDEAUX II Participation ended

UNIVERSITE DE BORDEAUX

FUNDAÇÃO DA FACULDADE DE CIÊNCIAS DA UNIVERSIDADE DE LISBOA Portugal

UNIVERSIDAD DE EXTREMADURA Spain

INESC ID - INSTITUTO DE ENGENHARIA DE SISTEMAS E COMPUTADORES, INVESTIGAÇÃO E DESENVOLVIMENTO EM LISBOA Participation ended

Over the last decade, Human-Computer Interaction (HCI) has grown and matured as a field. Gone are the days when only a mouse and keyboard could be used to interact with a computer. The most ambitious of such interfaces are Brain-Computer Interaction (BCI) systems. BCI's goal is to allow a person to interact with an artificial system using brain activity. A common approach towards BCI is to analyze, categorize and interpret Electroencephalography (EEG) signals in such a way that they alter the state of a computer. ACOBSEC's objective is to study the development of computer systems for the automatic analysis and classification of mental states of vigilance; i.e., a person's state of alertness. Such a task is relevant to diverse domains, where a person is required to be in a particular state. This problem is not a trivial one. In fact, EEG signals are known to be noisy, irregular and tend to vary from person to person, making the development of general techniques a very difficult scientific endeavor. Our aim is to develop new search and optimization strategies, based on evolutionary computation (EC) and genetic programming (GP) for the automatic induction of efficient and accurate classifiers. EC and GP are search techniques that can reach good solutions in multi-modal, non-differentiable and discontinuous spaces; and such is the case for the problem addressed here. This project combines the expertise of research partners from five converging fields: Classification, Neurosciences, Signal

Processing, Evolutionary Computation and Parallel Computing in Europe (France Inria, Portugal INESC-ID, Spain UNEX, Bordeaux university, Sciences University of Lisbon) and South America (Mexico ITT, CICESE). The exchange program goals and milestones give a comprehensive strategy for the strengthening of current scientific relations amongst partners, as well as for the construction of long-lasting scientific relationships that produce high quality theoretical and applied research.

9.3.2. Collaborations in European Programs, Except FP7 & H2020

Program: Direccion 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, Direccion 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 François 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

9.4. International Initiatives

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

9.4.1.1. CDSS

Title: Control of Dynamic Systems Subject to Stochastic Jumps

International Partner (Institution - Laboratory - Researcher):

Universidade de São Paulo (Brazil) - Departamento de Matemática Aplicada e Estatística (ICMC) - Costa Eduardo

Start year: 2014

See also: <https://team.inria.fr/cdss/fr/>

The main goals of this joint team CDSS is to study the control of dynamic systems subject to stochastic jumps. Three topics will be considered throughout the next 3 years. In the first topic we study the control problem of piecewise-deterministic Markov processes (PDMP?s) considering constraints. In this case the main goal is to obtain a theoretical formulation for the equivalence between the original optimal control of PDMP?s with constraints and an infinite dimensional static linear optimization problem over a space of occupation measures of the controlled process. F. Dufour (CQFD, Inria) and O. Costa (Escola Polit?cnica da Universidade de S?o Paulo, Brazil) mainly carry out this topic. In the second topic we focus on numerical methods for solving control and filtering problems related to Markov jump linear systems (MJLS). This project will allow a first cooperation between B. de Saporta (Univ. Montpellier II) and E. Costa (Universidade de S?o Paulo, Brazil). The third research subject is focused on quantum control by using Lyapunov-like stochastic methods conducted by P. Rouchon (Ecole des Mines de Paris) and P. Pereira da Silva (Escola Polit?cnica da Universidade de S?o Paulo, Brazil).

9.4.2. Inria International Partners

9.4.2.1. 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.

9.5. International Research Visitors

9.5.1. Visits of International Scientists

Oswaldo Costa (Escola Polit?cnica da Universidade de S?o 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 2016 supported by the Associate Team Inria: CDSS.

Alexey Piunovskiy (University of Liverpool) visited the team during 2 weeks in 2016. The main subject of the collaboration is the linear programming approach for Markov Decision Processes. This research was supported by the Clusters d'excellence CPU.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Selection

10.1.1.1. Member of the Conference Program Committees

J. Anselmi has been a member of the TPC of the international conferences: VALUETOOLS-2016, ASMTA-2016 and ECQT-2016.

F. Dufour is a member of the organizing committee of the international SIAM conference on Control & its Application, SIAM CT17.

M. Chavent has been vice-president of the program committee of the 5èmes Rencontres R in Toulouse in 2016.

10.1.2. Journal

10.1.2.1. Member of the Editorial Boards

F. Dufour is associate editor of the journal: SIAM Journal of Control and Optimization since 2009.

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

10.1.2.2. Reviewer - Reviewing Activities

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

10.1.3. Invited Talks

F. Dufour gave the following invited talks:

- *Unconstrained and Constrained Optimal Control of Piecewise Deterministic Markov Processes*, Workshop on switching dynamics & verification, Institut Henri Poincaré, Paris, France, January 28-29, 2016.
- *Stability of piecewise deterministic Markov processes*, Department of Statistics, Oxford University, United Kingdom, October 11, 2016.
- *Numerical Approximations for Average Cost Markov Decision Processes*, Inria Team TAO Seminar, February 9, 2016.

P. del Moral gave the following invited lectures:

- *An introduction to Feynman-Kac integration and genealogical tree based particle models*, Thematic Cycle on Monte-Carlo techniques, Labex Louis Bachelier, Institut Henri Poincaré, January 15, 22, 29, and February 12, 2016.
- *Mean Field Particle Samplers In Statistical Learning and Rare Event Analysis*, CFM-Imperial Distinguished Lecture Series, Imperial College, United Kingdom, October 18, 25, and November 1, 8, 2016.

A. Genadot gave the following talks:

- *Moyennisation à la mode de T. G. Kurtz pour des processus déterministes par morceaux*, Université de Lorraine, Nancy, January 14, 2016.
- *Averaging for some simple constrained Markov process*, Journées MAS, université Grenoble-Alpes, August 29, 30 and 31, 2016.

J. Saracco gave the following talks:

- *Analyse de la variance : une vision de type modèle linéaire gaussien ou comment expliquer une variable quantitative par un ou plusieurs facteurs qualitatifs*, University of Monastir (Tunisia), April 2016
- *Un exemple de régression semiparamétrique : l'approche SIR (sliced inverse regression)*, University of Monastir (Tunisia), April 2016
- *La régression par quantile non-paramétrique et semi-paramétrique*, "Les jeudis de Santé Publique", Paris, November 2016

J. Saracco was an invited professor at University of Monastir (Tunisia) in november 2016 and gave a course on Multidimensional Statistics.

Marie Chavent gave the following invited lecture :

- *Multivariate analysis of mixed data: The PCAmixdata R package*, CMStatistics, Seville, December 2016.

10.1.4. Research Administration

F. Dufour is member of the *Bureau du comité des projets*, Inria Bordeaux Sud-Ouest.

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 is member of the council of the Institut de Mathématique de Bordeaux.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

- Licence : J. Anselmi, Probabilités et statistiques, 13 heures, Institut Polytechnique de Bordeaux, école ENSEIRB-MATMECA, filiere telecom, France.
- Licence : J. Anselmi, Probabilités et statistiques, 13 heures, Institut Polytechnique de Bordeaux, école ENSEIRB-MATMECA, filiere electronique, France.
- Licence: M. Chavent, Analyse des données, 15 ETD, L3, Bordeaux university, France
- License: M. Chavent, Modélisation statistique, 15 ETD, niveau L3, Bordeaux university, France
- Master : M. Chavent, Apprentissage automatique, 50 ETD, niveau M2, Bordeaux university, France
- Licence : F. Dufour, Probabilités et statistiques, 16 heures, niveau L3, Institut Polytechnique de Bordeaux, école ENSEIRB-MATMECA, France.
- Master : F. Dufour, Méthodes numériques pour la fiabilité, 24 heures, niveau M1, Institut Polytechnique de Bordeaux, école ENSEIRB-MATMECA, France.
- Master : F. Dufour, Probabilités, 20 heures, niveau M1, Institut Polytechnique de Bordeaux, école ENSEIRB-MATMECA, France.
- P. Legrand, Algèbre (responsable de l'UE), Licence 1 SCIMS (108 heures)
- P. Legrand, Informatique pour les mathématiques (responsable de l'UE), Licence 1 et Licence 2 (36 heures)
- P. Legrand, Espaces Euclidiens. (responsable de l'UE), Licence 2 SCIMS (54 heures)
- P. Legrand, Formation Matlab pour le personnel CNRS (responsable de l'UE), (24 heures)
- Licence: J. Saracco, Probability and Descriptive statistics, 27h, L3, First year of ENSC - Bordeaux INP, France
- Licence: J. Saracco, Mathematical statistics, 20h, L3, First year of ENSC - Bordeaux INP, France
- Licence: J. Saracco, Data analysis (multidimensional statistics), 20h, L3, First year of ENSC - Bordeaux INP, France
- Master: J. Saracco, Statistical modeling, 27h, M1, Second year of ENSC - Bordeaux INP, France
- Master: J. Saracco, Applied probability and Statistics, 40h, M1, Second year of ENSCBP - Bordeaux INP, France
- Master: J. Saracco, Probability and Statistics, 12h, M2, Science Po Bordeaux, France
- A. Genadot, Probabilités de bases (18h), Licence MIASHS première année, Université de Bordeaux.
- A. Genadot, Statistiques de bases (18h), Licence MIASHS première année, Université de Bordeaux.
- A. Genadot, Probabilités (36h), Licence MIASHS deuxième année, Université de Bordeaux.
- A. Genadot, Processus (18h), Licence MIASHS troisième année, Université de Bordeaux.
- A. Genadot, Modélisation statistique (18h), Licence MIASHS troisième année, Université de Bordeaux.
- A. Genadot, Martingales (25h), Master MIMSE première année, Université de Bordeaux.

- A. Genadot, Probabilités (20h), Master MEEF première année, Université de Bordeaux.

10.2.2. Supervision

- PhD completed: Adrien Todeschini, Elaboration et validation d'un système de recommandation bayésien, supervised by F. Caron and M. Chavent.
- PhD completed: Christophe Nivot, Optimisation de la chaîne de montage du futur lanceur européen, May 2016, B. supervised by B. de Saporta and F. Dufour.
- PhD in progress : Alizé Geeraert, Contrôle optimal des processus Markoviens déterministes par morceaux et application à la maintenance, University of Bordeaux, supervised by B. de Saporta and F. Dufour (defense scheduled in June 2017).
- PhD in progress : Ines Jlassi, Contributions à la régression inverse par tranches et à l'estimation non para métrique des quantiles conditionnels, University of Monastir (Tunisia), September 2013, supervised by J. Saracco and L. Ben Abdelghani Bouraoui.
- PhD in progress : Hadrien Lorenzo, Analyses de données longitudinales de grandes dimensions appliquées aux essais vaccinaux contre le VIH et Ebola, University of Bordeaux, September 2016, supervised by J. Saracco and R. Thiebaut.

10.2.3. Juries

J. Saracco is vice president of the french statistical society (SFdS).

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- [2] J. ANSELM, N. S. WALTON. *Decentralized Proportional Load Balancing*, in "SIAM Journal on Applied Mathematics", 2016, vol. 76, n^o 1, p. 391-410 [DOI : 10.1137/140969361], <https://hal.archives-ouvertes.fr/hal-01415856>.
- [3] O. COSTA, F. DUFOUR, A. B. PIUNOVSKIY. *Constrained and Unconstrained Optimal Discounted Control of Piecewise Deterministic Markov Processes*, in "SIAM Journal on Control and Optimization", 2016, vol. 54, n^o 3, p. 1444 - 1474 [DOI : 10.1137/140996380], <https://hal.archives-ouvertes.fr/hal-01412604>.
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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

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- 5.1.2. - Evaluation of interactive systems
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- 5.1.5. - Body-based interfaces
- 5.1.6. - Tangible interfaces
- 5.1.7. - Multimodal interfaces
- 5.3.3. - Pattern recognition
- 5.4.1. - Object recognition
- 5.4.2. - Activity recognition
- 5.7.3. - Speech
- 5.8. - Natural language processing
- 5.10.5. - Robot interaction (with the environment, humans, other robots)
- 5.10.7. - Learning
- 5.10.8. - Cognitive robotics and systems
- 5.11.1. - Human activity analysis and recognition
- 6.3.1. - Inverse problems
- 8. - Artificial intelligence
- 8.2. - Machine learning
- 8.5. - Robotics
- 8.7. - AI algorithmics

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- 1.3.1. - Understanding and simulation of the brain and the nervous system
- 1.3.2. - Cognitive science
- 5.6. - Robotic systems
- 5.7. - 3D printing
- 5.8. - Learning and training
- 9. - Society and Knowledge
- 9.1. - Education
- 9.1.1. - E-learning, MOOC
- 9.2. - Art
- 9.2.1. - Music, sound
- 9.2.4. - Theater
- 9.5. - Humanities
- 9.5.1. - Psychology
- 9.5.8. - Linguistics
- 9.7. - Knowledge dissemination

1. Members

Research Scientists

Pierre-Yves Oudeyer [Team leader, Inria, Senior Researcher, HDR]
Anna-Lisa Vollmer [Inria, Starting Research position]
Manuel Lopes [Inria, Senior Researcher, HDR]

Faculty Members

David Filliat [ENSTA, Professor, HDR]
Alexander Gepperth [ENSTA, Associate Professor]
Freek Stulp [ENSTA, Associate Professor]

Technical Staff

Damien Caselli [Inria]
Yoan Mollard [Inria, until Nov 2016, granted by FP7 /13-3RDHAND project]
Stéphanie Noirpoudre [Inria]
Nicolas Rabault [Inria, until Oct 2016]
Matthieu Lapeyre [Inria]
Pierre Rouanet [Inria]
Didier Roy [Inria]
Théo Segonds [Inria]

PhD Students

Baptiste Busch [Inria]
Thibaut Munzer [Inria]
Thibault Desprez [Inria]
Benjamin Clément [Inria, granted by FP7 ERC/09-EXPLORERS project]
Céline Craye [Thales, granted by CIFRE]
Yuxin Chen [ENSTA]
Alexandra Delmas [ItWell SAS, granted by CIFRE]
Sébastien Forestier [Univ. Bordeaux]
Florian Golemo [Inria]
Clément Masson [ENSTA]
Adrien Matricon [Univ. Bordeaux]
Alvaro Ovalle Castaneda [Inria, from Oct 2016]
Gennaro Raiola [ENSTA]
William Schueller [Univ. Bordeaux]

Post-Doctoral Fellows

Cem Karaoguz [ENSTA, until Nov 2016]
Panagiotis Papadakis [ENSTA, until May 2016]

Administrative Assistant

Nicolas Jahier [Inria]

Others

Marie Demangeat [student, Master student]
Paul Ecoffet [student, Master student, Jul 2016]
Aurélien Lopes [student, Master student, from Sep 2016]
Sébastien Mick [student, Master student, until Jul 2016]

2. Overall Objectives

2.1. Overall Objectives

Can a robot learn like a child? Can it learn new skills and new knowledge in an unknown and changing environment? How can it 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. 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 approach is called developmental robotics, or epigenetic robotics, and imports concepts and theories from developmental psychology. As most of these theories 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.

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 in particular to self-organize developmental trajectories and collect efficiently learning data;
- Mechanisms of adequately constrained optimization and statistical inference for sensorimotor skill acquisition (e.g. for optimizing motor policies in real robots);
- 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;
- Maturation 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 robot 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 robots, 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 robots, 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;
- **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 (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.
- **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 [112] and neuroscience [22] 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 [124].

A grand challenge is thus to be able to build robotic 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” [174]. 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 [134], 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 [145] [178]. The approach of developmental robotics consists in importing and implementing concepts and mechanisms from developmental psychology [148], cognitive linguistics [123], and developmental cognitive neuroscience [139] 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 [116] [156], grounding [132], situatedness [105], self-organization [172] [158], enaction [176], and incremental learning [119].

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 [153]. 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 [148], 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" [108] [127]. 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 [112] [124] [126]. 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 [125] [136] [166]. Based on this, a number of researchers have began in the past few years to build computational implementation of intrinsic motivation [153] [154] [164] [111] [137] [146] [165]. 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 [154], [153], [155], [163]. 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 [120] [133] 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 [148]. 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 [107]. 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 [173], [113], motivated by the various mechanisms that allow humans to socially guide a robot [160]. In an interactive context the steps of self-exploration and social guidances are not separated and a robot learns by self exploration and by receiving extra feedback from the social context [173], [142] [147].

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 [150], [151]. We also work on developing perceptual capabilities by gradually segmenting the perceptual space and identifying objects and their characteristics through interaction with the user [32] and robots experiments [138]. 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 [144].

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

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 of 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

The Flowers team spin-off company Pollen Robotics was created in may 2016, targeting to develop and commercialize technologies for entertainment robotics: <http://pollen-robotics.com/en/>

Didier Roy was award the prize Serge Hocquenguem for his work on educational robotics, <http://psh.aid-creem.org/spip.php?rubrique1> et <http://binaire.blog.lemonde.fr/2016/12/09/pourquoi-didier-et-eva-jouent-avec-le-meme-robot/>

Sébastien Forestier, Yoan Mollard, Damien Caselli and Pierre-Yves Oudeyer obtained the notable mention demonstration award (2nd place) at the NIPS 2016 conference for their demonstration on Autonomous exploration, active learning and human guidance with open-source Poppy humanoid robot platform and Explauto library <https://hal.inria.fr/hal-01404399/document>

PY. Oudeyer and M. Lopes co-organized with J. Gottlieb and T. Gliga the Second Interdisciplinary Symposium on Information-Seeking, Curiosity and Attention (Neurocuriosity 2016) in London, gathering 150 researchers from neuroscience, psychology, education and machine learning/computational modelling. This was achieved in the context of the associated team Neurocuriosity. Web: <https://openlab-flowers.inria.fr/t/second-interdisciplinary-symposium-on-information-seeking-curiosity-and-attention-neurocuriosity-2016/187>

PY. Oudeyer and M. Lopes were awarded a 3 year-long HFSP grant with J. Gottlieb (Univ. Columbia, US) and C. Kidd (Univ. Rochester, US) for a research program targeting the understanding of active exploration in humans and monkeys through experimentation and modelling. Web: <https://flowers.inria.fr/neurocuriosityproject/>.

PY. Oudeyer was awarded the Lifetime Achievement Award from the Evolutionary Linguistics Association.

6. New Software and Platforms

6.1. Poppy project

6.1.1. HiPi Board

FUNCTIONAL DESCRIPTION

Hipi is a board to control robots on Raspberry Pi. It is an extension of the Pixl board with the following features:

- A DC/DC power converter from 12V (motor) to 5V (Raspberry Pi) at 3A.
- A stereo audio amplifier 3W.
- A MPU9250 central motion unit .
- A RS232 and a RS485 bus connected to the Raspberry Pi by SPI for driving MX and RX Dynamixel motor series.

This board will be integrated soon in the new head of the Poppy Humanoid and Poppy Torso.

Using the Raspberry Pi for every Poppy robots will simplify the hardware complexity (we maintain 4 types of embedded boards, with different Linux kernel and configurations) and improve the usage and installation of new robots.

- Contact: Theo Segonds
- URL: <https://forum.poppy-project.org/t/poppy-1-1-hipi/2137>

6.1.2. IKPy

Inverse Kinematics Python Library

FUNCTIONAL DESCRIPTION

IKPy is a Python Inverse Kinematics library, designed to be simple to use and extend. It provides Forward and Inverse kinematics functionality, bundled with helper tools such as 3D plotting of the kinematics chains. Being written entirely in Python, IKPy is lightweight and is based on numpy and scipy for fast optimization. IKPy is compatible with many robots, by automatically parsing URDF files. It also supports other (such as DH-parameters) and custom representations. Moreover, it provides a framework to easily implement new Inverse Kinematics strategies. Originally developed for the Poppy project, it can also be used as a standalone library.

- Contact: Pierre Manceron
- URL: <https://github.com/Phylliade/ikpy>

6.1.3. Pixl Board

FUNCTIONAL DESCRIPTION

Pixl is a tiny board used to create low cost robots based on Raspberry Pi board and Dynamixel XL-320 motors. This board has 2 main features:

- The power part, allowing the user to plug a 7.5V AC/DC converter or a battery directly into the Pixl. This power is distributed to all XL320 motors and is converted to 5V for the Raspberry Pi board.
- The communication part, which converts full duplex to half duplex and vice-versa. The half duplex part switch between RX and TX automatically. Another connector allows the user to connect his XL320 network.

The board is used in the Poppy Ergo Jr robot.

- Contact: Theo Segonds
- URL: <https://github.com/poppy-project/pixl>

6.1.4. Poppy

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

6.1.5. Poppy Ergo Jr

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.

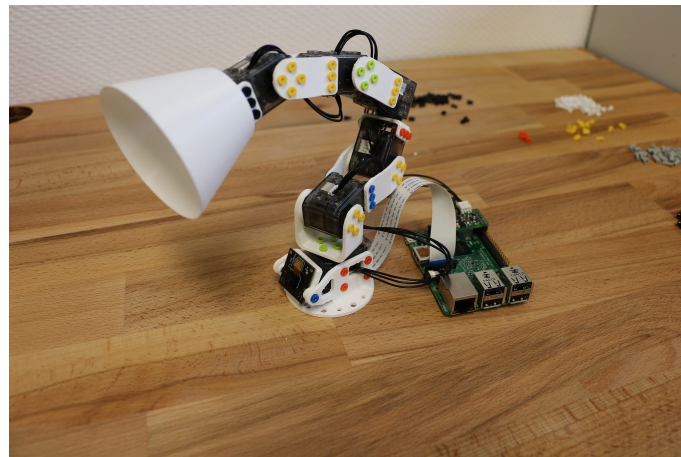


Figure 1. Poppy Ergo Jr; 6-DoFs arm robot for education

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

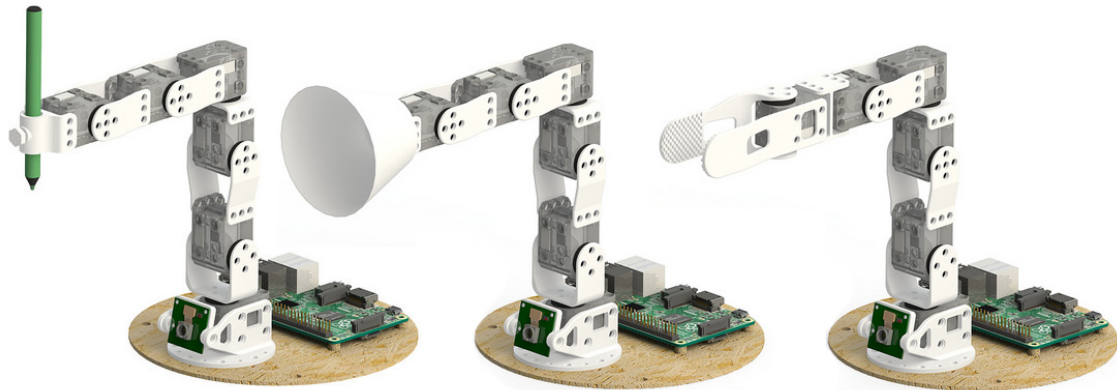


Figure 2. The available Ergo Jr tools: a pen holder, a lampshade and a gripper

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>

6.1.6. Poppy Ergo Jr Installer

FUNCTIONAL DESCRIPTION

An alternative way to install the Ergo Jr robot software is made available using containers.

Users can own their own operating system installation, then add the Ergo Jr required software in a sandboxed environment. This results in a non-intrusive installation on the host system.

Docker containers implementation were used, and image is hosted at Docker Hub.

- Contact: Damien Caselli
- URL: <https://hub.docker.com/r/poppycommunity/ergo-jr/>

6.1.7. Poppy Ergo Jr Simulator

FUNCTIONAL DESCRIPTION

Poppy Project, through Poppy Education, wants users to get used to robotics, even without owning a physical robot.

For that purpose, Poppy Project team created a dummy robot in Pypot that is meant to be used in conjunction with a consumer application. We choose to develop a web hosted application using a 3D engine (Threejs) to render the robot.

Our ambition is to have a completely standalone simulated robot with physics. Some prototypes were created to benchmark possible solutions.

- Contact: Damien Caselli
- URL: <https://github.com/poppy-project/poppy-simu>

6.1.8. PyPot

SCIENTIFIC DESCRIPTION

Pypot is a framework developed to make it easy and fast to control custom robots based on Dynamixel motors. This framework provides different levels of abstraction corresponding to different types of use. Pypot can be used to:

- control Robotis motors through a USB2serial device,
- define the structure of a custom robot and control it through high-level commands,
- define primitives and easily combine them to create complex behavior.

Pypot is part of the Poppy project. It is the core library used by the Poppy robots. This abstraction layer allows to seamlessly switch from a given Poppy robot to another. It also provides a common set of tools, such as forward and inverse kinematics, simple computer vision, recording and replaying moves, or easy access to the autonomous exploration library Explauto.

To extend pypot application domains and connection to outside world, it also provides an HTTP API. On top of providing an easy way to connect to smart sensors or connected devices, it is notably used to connect to Snap!, a variant of the well-known Scratch visual programming language.

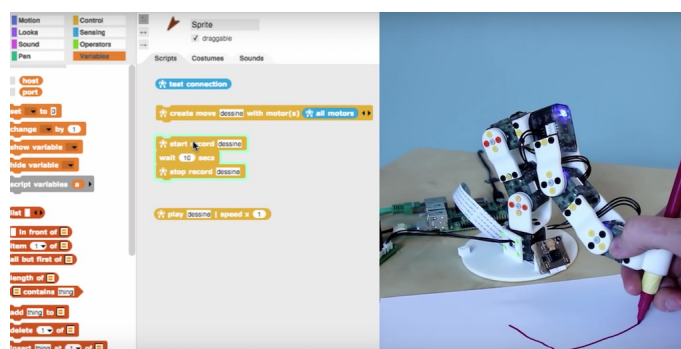


Figure 3. Example of using pypot to program a robot to reproduce a drawn shape

FUNCTIONAL DESCRIPTION

Pypot is entirely written in Python to allow for fast development, easy deployment and quick scripting by non-expert developers. It can also benefit from the scientific and machine learning libraries existing in Python. The serial communication is handled through the standard library and offers high performance (10ms sensorimotor loop) for common Poppy uses. It is cross-platform and has been tested on Linux, Windows and Mac OS.

Pypot is also compatible with the V-REP simulator. This allows the transparent switch from a real robot to its simulated equivalent with a single code base.

Finally, it has been developed to be easily and quickly extended for other types of motors and sensors.

It works with Python 2.7 or Python 3.3 or later, and has also been adapted to the Raspberry Pi board.

Pypot has been connected to Snap!, a variant of the famous Scratch visual language, developed to teach computer science to children. It is based on a drag-and-drop blocks interface to write scripts by assembling those blocks.

Thanks to the Snap! HTTP block, a connection can be made to pypot allowing users to directly control robots through their visual interfaces. A set of dedicated Snap! blocks have been designed, such as *set motor position* or *get motor temperature*. Thanks to the Snap! HTTP block, users can control robots through this visual interfaces connecting to Pypot. A set of dedicated Snap! blocks has been designed, such as *set motor position* or *get motor temperature*.



Figure 4. Using Snap! to program a robot by demonstration and create complex choreographies

Snap! is also used as a tool to program the robot by demonstration. Using the **record** and **play** blocks, users can easily trigger kinesthetic recording of the whole robot or only a specific subpart, such as an arm. These records can then be played or "mixed" - either played in sequence or simultaneously - with other recordings to compose complex choreographies. The moves are encoded as a model of mixture of gaussians (GMM) which allows the definition of clean mathematical operators for combining them.

This recording tool has been developed and used in collaboration with artists who show interest in the concept of robotic moves.

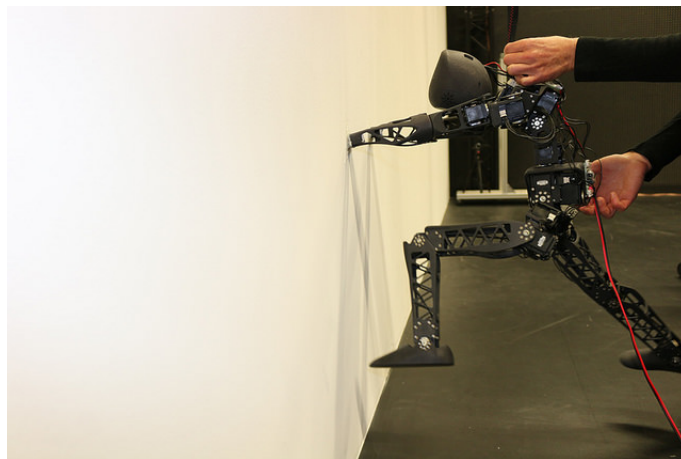


Figure 5. Artistic project exploring the concept of robotic move.

- Participants: Pierre Rouanet, Matthieu Lapeyre, Steve Nguyen, Damien Caselli and Theo Segonds
- Contact: Theo Segonds

- URL: <https://github.com/poppy-project/pypot>

6.1.9. PyQMC

Python library for Quasi-Metric Control

FUNCTIONAL DESCRIPTION

PyQMC is a python library implementing the control method described in <http://dx.doi.org/10.1371/journal.pone.0083411>. It allows to solve discrete markovian decision processes by computing a Quasi-Metric on the state space. This model based method has the advantage to be goal independant and thus can produce a policy for any goal with relatively few recomputation. New addition to this method is the possibility of online learning of the transition model and the Quasi-Metric.

- Participant: Steve Nguyen
- Contact: Steve Nguyen
- URL: <https://github.com/SteveNguyen/pyqmc>

6.2. Explauto

an autonomous exploration library

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 collect 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 [152], which has been extended to a more general family of autonomous exploration architectures by [3] and recently expressed as a compact and unified formalism [38]. The library is detailed in [39]. 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 [45]). 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 [152]. 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 [3].

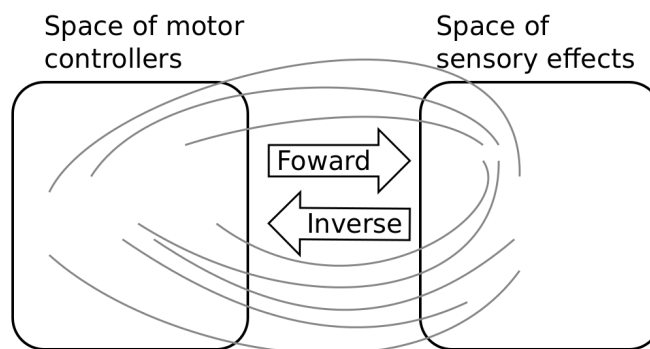


Figure 6. Complex parametrized policies involve high dimensional action and effect spaces. For the sake of visualization, the motor M and sensory S spaces are only 2D each in this example. The relationship between M and S is non-linear, dividing the sensorimotor space into regions of unequal stability: 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 the environment 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 cross-platform and has been tested on Linux, Windows and Mac OS. It has been released under the GPLv3 license.

- Contact: Sébastien Forestier
- URL: <https://github.com/flowersteam/explauto>

6.3. Tools for robot learning, control and perception

6.3.1. CARROMAN

FUNCTIONAL DESCRIPTION

This software implements a control architecture for the Meka humanoid robot. It integrates the Stanford Whole Body Control in the M3 architecture provided with the Meka robot, and provides clear and easy to use interfaces through the URBI scripting language. This software provides a modular library of control modes and basic skills for manipulating objects, detecting objects and humans which other research projects can reuse, extend and enhance. An example would be to locate a cylindrical object on a table using stereo vision, and grasping it using position and force control.

- Contact: David Filliat

6.3.2. Aversive++

FUNCTIONAL DESCRIPTION

Aversive++ is a C++ library that eases micro-controller programming. Its aim is to provide an interface simple enough to be able to create complex applications, and optimized enough to enable small micro-controllers to execute these applications. The other aspect of this library is to be multiplatform. Indeed, it is designed to provide the same API for a simulator (named SASIAE) and for AVR-based and ARM-based micro-controllers.

- Contact: Loïc Dauphin
- URL: <http://aversiveplusplus.com/>

6.3.3. DMP-BBO

Black-Box Optimization for Dynamic Movement Primitives

KEYWORD: -

FUNCTIONAL DESCRIPTION

The DMP-BBO Matlab library is a direct consequence of the insight that black-box optimization outperforms reinforcement learning when using policies represented as Dynamic Movement Primitives. It implements several variants of the PIBB algorithm for direct policy search. The dmp-bbo C++ library has been extended to include the “unified model for regression”. The implementation of several of the function approximators have been made real-time compatible.

- Participant: Freek Stulp
- Partner: ENSTA
- Contact: Freek Stulp
- URL: <https://github.com/stulp/dmpbbo>

6.3.4. *KERAS-QR*

KERAS with Quick Reset

KEYWORDS: Library - Deep learning

- Participant: Florian Golemo
- Contact: Florian Golemo
- URL: <https://github.com/fgolemo/keras>

6.3.5. *Multimodal*

FUNCTIONAL DESCRIPTION

The python code provides a minimum set of tools and associated libraries to reproduce the experiments in [98], together with the choreography datasets. The code is primarily intended for reproduction of the multimodal learning experiment mentioned above. It has already been reused in several experimentations by other members of the team and is expected to play an important role in further collaborations. It is also expected that the public availability of the code encourages further experimentation by other scientists with data coming from other domains, thus increasing both the impact of the aforementioned publication and the knowledge on the algorithm behaviors.

- Participant: Olivier Mangin
- Contact: Olivier Mangin
- URL: <https://github.com/omangin/multimodal>

6.3.6. *Of 3-D point cloud*

FUNCTIONAL DESCRIPTION

This software scans the 3-D point cloud of a scene to find objects and match them against a database of known objects. The process consists in 3 stages. The segmentation step finds the objects in the point cloud, the feature extraction computes discriminating properties to be used in the classification stage for object recognition.

- Participants: David Filliat, Alexander Geppert and Louis-Charles Caron
- Contact: Alexander Geppert

6.3.7. *PEDDETECT*

FUNCTIONAL DESCRIPTION

PEDDETECT implements real-time person detection in indoor or outdoor environments. It can grab image data directly from one or several USB cameras, as well as from pre-recorded video streams. It detects multiple persons in 800x600 color images at frame rates of >15Hz, depending on available GPU power. In addition, it also classifies the pose of detected persons in one of the four categories "seen from the front", "seen from the back", "facing left" and "facing right". The software makes use of advanced feature computation and nonlinear SVM techniques which are accelerated using the CUDA interface to GPU programming to achieve high frame rates. It was developed in the context of an ongoing collaboration with Honda Research Institute USA, Inc.

- Participant: Alexander Geppert
- Contact: Alexander Geppert

6.3.8. *ThifloNet*

KEYWORDS: Deep learning - Policy Learning

SCIENTIFIC DESCRIPTION

We created a software architecture that combines a state-of-the-art computer vision system with a policy learning framework. This system is able to perceive a visual scene, given by a still image, extract facts (“predicates”), and propose an optimal action to achieve a given goal. Both systems are chained into a pipeline that is trained by presenting images and demonstrating an optimal action. By providing this information, both the predicate recognition model and the policy learning model are updated.

Our architecture is based on the recent works of Lerer, A., Gross, S., & Fergus, R., 2016 ("Learning Physical Intuition of Block Towers by Example"). They created a large network able to identify physical properties of stacked blocks. Analogously our vision system utilizes the same network layout (without the image prediction auxiliary output), with an added output layer for predicates, based on the expected number and arity of predicates. The vision subsystem is not trained with a common cross-entropy or MSE loss function, but instead receives its loss from the policy learning subsystem. The policy learning module calculates the loss as optimal combination of predicates for the given expert action.

By using this combination of systems, the architecture as a whole requires significantly fewer data samples than other systems (which exclusively utilize neural networks). This makes the approach more feasible to real-life application with actual live demonstration.

FUNCTIONAL DESCRIPTION

The neural network consists of ResNet-50 (the currently best-performing computer vision system), with 50 layers, 2 layers for converting the output of ResNet to predicates and a varying amount of output neurons, corresponding to the estimated number of n-arity predicates. The network was pretrained on the ImageNet dataset. The policy learning module incorporates the ACE tree learning tool and a wrapper in Prolog.

Our example domain consists of 2-4 cubes colored in red, blue, green, and yellow and randomly stacked on top of each other in a virtual 3D environment. The dataset used for training and testing contains a total of 30000 elements, each with an image of the scene, the correct predicates, a list of blocks that are present and the corresponding expert action, that would lead to stacking the blocks to a tower.

- Participants: Florian Golemo, Thibaut Munzer and Manuel Lopes
- Contact: Florian Golemo

6.4. Tools for education

6.4.1. *KidLearn*

KEYWORD: Automatic Learning

FUNCTIONAL DESCRIPTION

KidLearn is a software which adaptively personalizes 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. The library regrouping the different developed technologies is available on [github](#).

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

6.4.2. *KidBreath*

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>

6.4.3. 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 7). 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.

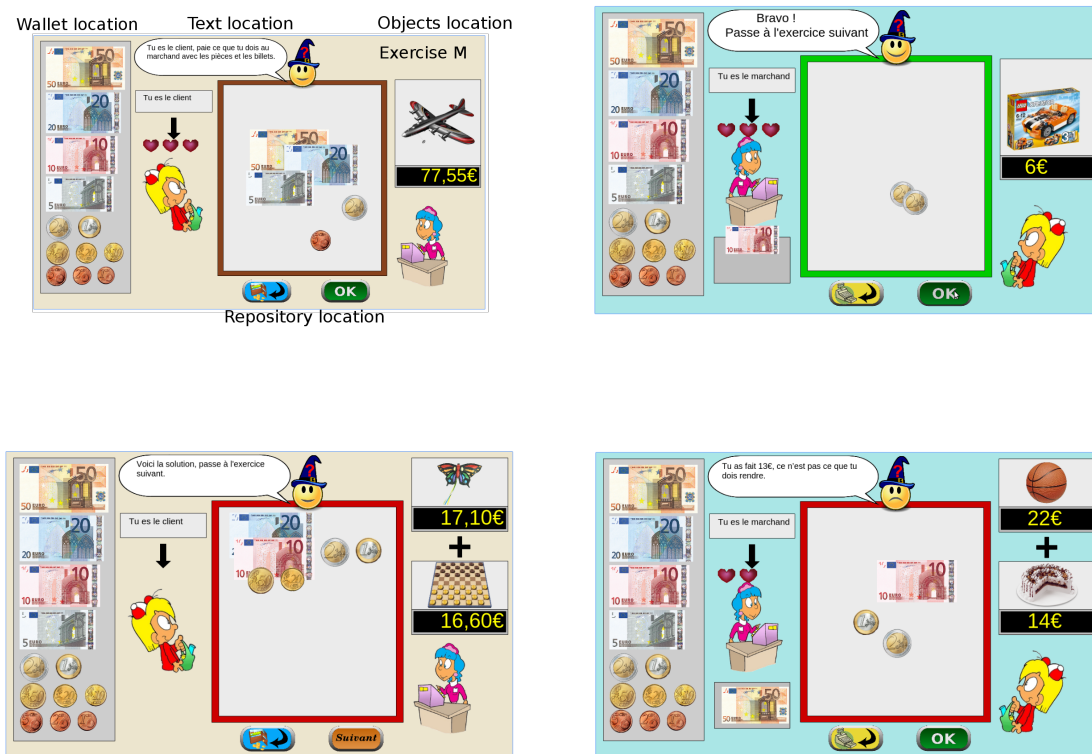


Figure 7. Four principal regions are defined in the graphical interface. The first is the wallet location where users can pick and drag the money items and drop them on the repository location to compose the correct price. The object and the price are present in the object location. Four different types of exercises exist: M : customer/one object, R : merchant/one object, MM : customer/two objects, RM : merchant/two objects.

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

6.4.4. Kidlearn: script for Kidbreath use

FUNCTIONAL DESCRIPTION

A new way to test Kidlearn algorithms is to use them on Kidbreath Platform. The Kidbreath Platform 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.

Github link to explanation about it : https://github.com/flowersteam/kidlearn/tree/feature/kidbreath/module_php.

- Contact: Benjamin Clement
- URL: https://github.com/flowersteam/kidlearn/tree/feature/kidbreath/module_php

6.5. 3rdHand Project

6.5.1. 3rdHand Infrastructure

KEYWORDS: Interaction - Robotics - Infrastructure software - Framework - Robot Operating System (ROS)

FUNCTIONAL DESCRIPTION

The infrastructure is predicate-based to handle relational actions and covers perception (scene description generation, human actions recognition), decision making (teleoperated, scripted or learning from demonstrations), interaction with end users (GUI, voice, gestures) and parallel executions of robotic actions (hold, pick, grasp, bring, ...).

- Contact: Yoan Mollard
- https://github.com/3rdHand-project/thr_infrastructure

6.5.2. Kinect 2 Server

Kinect 2 server

KEYWORDS: Depth Perception - Speech recognition - Gesture recognition - Kinect

FUNCTIONAL DESCRIPTION

The server written in C# uses the Kinect SDK v2 to get the RGBD raw image, skeleton tracking information, recognized speech. It also uses the text-to-speech from Microsoft. Then it streams JSON data over the network using the Publisher/Subscriber pattern from the ZeroMQ network library. A Linux client has been written in Python but it can be written in any other language that is compatible with ZeroMQ. Features are controllable through a Graphical User Interface on Windows, or through the code from any Linux/Windows client. The clients can for instance enable features (speech recognition on, skeleton tracking off, ...) and parameters (set new speech to recognize, change language, ...) from remote.

- Contact: Yoan Mollard
- URL: https://github.com/baxter-flowers/kinect_2_server/

6.5.3. ProMP

Probabilistic Movement Primitives

KEYWORDS: Interaction - Robotics - Probability - Motion model - Robot Operating System (ROS)

FUNCTIONAL DESCRIPTION

Joint-space primitives with a task-space constraint: The primitives are stored in joint-space but demonstrations are provided both in joint space and task space, context. Thanks to this context, task-space goals can be requested to these joint-space primitives. The benefit is that requesting a new task-space goal does not require to call an IK method which would return demonstrations-agnostic joint configurations.

Vocal interactive learning and clustering: This work includes an interactive learning aspect which allows to automatically cluster motor primitives based on the standard deviation of their demonstrations. A new primitive is created automatically if the provided demonstration is out of 2 standard deviation of the existing primitives, otherwise the demonstration is distributed to an existing one.

- Contact: Yoan Mollard
- URL: <https://github.com/baxter-flowers/promplib>

6.5.4. ROS Optitrack Publisher

KEYWORDS: Target tracking - Robot Operating System (ROS)

FUNCTIONAL DESCRIPTION

This package allows to publish optitrack markers declared as rigid bodies as TF transforms. Data is gathered through the embedded VRPN server of Motive/Arena. Only rigid bodies are requested to the server, thus single points in 2D/3D are ignored. VRPN server can be enable in View > Data streaming in Motive.

- Contact: Yoan Mollard
- URL: https://github.com/baxter-flowers/optitrack_publisher

7. New Results

7.1. Robotic And Computational Models Of Human Development and Cognition

7.1.1. Computational Models Of Information-Seeking, Curiosity And Attention in Humans and Animals

Participants: Manuel Lopes, Pierre-Yves Oudeyer [correspondant], Jacqueline Gottlieb, Celeste Kidd, Alvaro Ovalle, William Schueller, Sebastien Forestier, Nabil Daddaouda, Nicholas Foley.

This project involves a collaboration between the Flowers team, the Cognitive Neuroscience Lab of J. Gottlieb at Columbia Univ. (NY, US), and the developmental psychology lab of Celeste Kidd at Univ. Rochester, US, on the understanding and modeling of mechanisms of curiosity, attention and active intrinsically motivated exploration that until now have been little explored in neuroscience, machine learning and cognitive robotics.

It is organized around the study of the hypothesis that information gain (or control gain) 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 (Gottlieb's lab) and children (Kidd's lab) together with computational modeling of curiosity/intrinsic motivation and learning in the Flowers team.

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 [29], [155], [162]. Therefore we hypothesize that, rather than using a single optimization process as it has been the case in most previous theoretical work [131], 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 [153] [110], [149]. 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. We will quantitatively characterize this dynamic, multi-dimensional system in the framework of Bayesian Reinforcement Learning, as described below.

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 [143], [161], and rats show individual variation in learning styles and novelty seeking behaviors [128], 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 [159], [171], [106], [175]. 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 model based on Bayesian reinforcement learning.

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 [143], [141] 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 Bayesian Reinforcement 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

In particular, new results in 2015 include:

7.1.1.4. *Intrinsically motivated oculomotor exploration guided by uncertainty reduction and conditioned reinforcement in non-human primates*

Using a novel oculomotor paradigm, combined with reinforcement learning (RL) simulations, we show that monkeys are intrinsically motivated to search for and look at reward-predictive cues, and that their intrinsic motivation is shaped by a desire to reduce uncertainty, a desire to obtain conditioned reinforcement from positive cues, and individual variations in decision strategy and the cognitive costs of acquiring information. The results suggest that free-viewing oculomotor behavior reveals cognitive and emotional factors underlying the curiosity driven sampling of information. These results were published in [66].

7.1.1.5. *Experiments in Active Categorization*

An ongoing effort to characterize curiosity and exploration in an experimental setting consists in evaluating the manner in which diverse tasks or goals are selected. This would include monitoring what does a test subject decide to learn, in what order and how is it done. This has been referred to as strategic learning [31]. Accordingly, it is of particular interest for the project to observe the type of learning dynamics in relation to their learning progress [153]. This principle tries to establish links between the selection and ordering of tasks and the speed or the rate of improvement a subject may achieve. This implies that during free exploration the subject would focus on tasks that are considered of certain complexity and where it makes consistent progress. At the same time the subject would avoid: (1) trivial tasks that do not offer much learning due to their simplicity or (2) very complicated tasks where little or no progress is achieved.

We have been working on prototyping an experiment where the subject is presented with different stimuli classification tasks of varying difficulty. The goal for each of the tasks is to correctly predict and differentiate between different classes of stimuli. Two main aspects of the task are under the control of the subject: (1) the task that he/she wants to learn and (2) once selected a task, what elements to explore in order to subsequently being able to predict future stimuli. Essentially the subject autonomously organizes which tasks to focus on and in what order. Therefore one of the objectives of this investigation is to analyze if the learning dynamics are guided by the amount of progress the subject achieves in the tasks.

7.1.2. ***Computational Models Of Tool Use and Speech Development: the Roles of Active Learning, Curiosity and Self-Organization***

Participants: Pierre-Yves Oudeyer [correspondant], Clement Moulin-Frier, Sébastien Forestier, Linda Smith.

7.1.2.1. *Modeling Cognitive Development and Tool Use in Infants*

A scientific challenge in developmental and social robotics is to model how autonomous organisms can develop and learn open repertoires of skills in high-dimensional sensorimotor spaces, given limited resources of time and energy. This challenge is important both from the fundamental and application perspectives. First, recent work in robotic modeling of development has shown that it could make decisive contributions to improve our understanding of development in human children, within cognitive sciences [131]. Second, these models are key for enabling future robots to learn new skills through lifelong natural interaction with human users, for example in assistive robotics [157].

In recent years, two strands of work have shown significant advances in the scientific community. On the one hand, algorithmic models of active learning and imitation learning combined with adequately designed properties of robotic bodies have allowed robots to learn how to control an initially unknown high-dimensional body (for example locomotion with a soft material body [3]). On the other hand, other algorithmic models have shown how several social learning mechanisms could allow robots to acquire elements of speech and language [118], allowing them to interact with humans. Yet, these two strands of models have so far mostly remained disconnected, where models of sensorimotor learning were too “low-level” to reach capabilities for language, and models of language acquisition assumed strong language specific machinery limiting their flexibility. Preliminary work has been showing that strong connections are underlying mechanisms of hierarchical sensorimotor learning, artificial curiosity, and language acquisition [49].

Recent robotic modeling work in this direction has shown how mechanisms of active curiosity-driven learning could progressively self-organize developmental stages of increasing complexity in vocal skills sharing many properties with the vocal development of infants [37]. Interestingly, these mechanisms were shown to be exactly the same as those that can allow a robot to discover other parts of its body, and how to interact with external physical objects [152].

In such current models, the vocal agents do not associate sounds to meaning, and do not link vocal production to other forms of action. In other models of language acquisition, one assumes that vocal production is mastered, and hand code the meta-knowledge that sounds should be associated to referents or actions [118]. But understanding what kind of algorithmic mechanisms can explain the smooth transition between the learning of vocal sound production and their use as tools to affect the world is still largely an open question.

The goal of this work is to elaborate and study computational models of curiosity-driven learning that allow flexible learning of skill hierarchies, in particular for learning how to use tools and how to engage in social interaction, following those presented in [152],[3], [43], [37]. The aim is to make steps towards addressing the fundamental question of how speech communication is acquired through embodied interaction, and how it is linked to tool discovery and learning.

A first question that we study in this work is the type of mechanisms that could be used for hierarchical skill learning allowing to manage new task spaces and new action spaces, where the action and task spaces initially given to the robot are continuous and high-dimensional and can be encapsulated as primitive actions to affect newly learnt task spaces.

We presented firsts results on that question at the 38th Annual Meeting of the Cognitive Science Society, Philadelphia, Pennsylvania, USA, August 10-13th [80]. In this work, we presented the HACOB (Hierarchical Active Curiosity-driven mOdel Babbling) architecture of algorithms that actively chooses which sensorimotor model to train in a hierarchy of models representing the environmental structure. We studied this architecture using a simulated robotic arm interacting with objects in a 2D environment (See Fig. 8). Studies of child development of tool use precursors showed successive but overlapping phases of qualitatively different types of behaviours [167]. We hypothesized that two mechanisms in particular play a role in the structuring of these phases: the intrinsic motivation to explore and the representation used to encode sensorimotor experience.

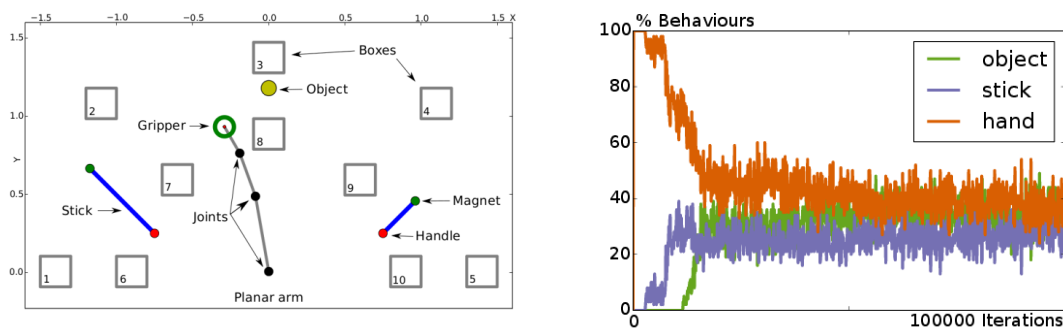


Figure 8. Left: simulated robotic environment with a 4 DOF robotic arm, 2 tools and a toy. Right: Observed behaviours of an agent: it first explores its arm to move its hand, then also explore to move the stick and the toy.

We showed that using a hierarchical structure of sensorimotor models and active model babbling as an intrinsic motivation to explore sensorimotor models that have a high learning progress, then overlapping phases of behaviours are autonomously emerging in the developmental trajectories of agents. To our knowledge, this is the first model of curiosity-driven development of simple tool use and of the self-organization of overlapping phases of behaviours. In particular, our model explains why and how intrinsically motivated exploration of

non-optimal methods to solve certain sensorimotor problems can be useful to discover how to solve other sensorimotor problems, in accordance with Siegler's overlapping waves theory, by scaffolding the learning of increasingly complex affordances in the environment.

In computational models of strategy selection for the problem of integer addition, Shrager and Siegler proposed a mechanism that maintains the concurrent exploration of alternative strategies with use frequencies that are proportional to their performance for solving a particular problem. This mechanism was also used by Chen and Siegler to interpret an experiment with 1.5- and 2.5-year-olds that had to retrieve an out-of-reach toy, and where they could use one of several available strategies that included leaning forward to grasp a toy with the hand or using a tool to retrieve the toy.

In a paper that we presented at the The Sixth Joint IEEE International Conference on Developmental Learning and Epigenetic Robotics, Cergy-Pontoise, France, September 19-22nd [82], we studied tool use discovery and considered other mechanisms of strategy selection and evaluation. In particular, we presented models of curiosity-driven exploration where strategies are explored according to the learning progress/information gain they provide (as opposed to their current efficiency to actually solve the problem). In these models, we defined a curiosity-driven agent learning a hierarchy of different sensorimotor models in a simple 2D setup with a robotic arm, a stick and a toy. In a first phase, the agent learns from scratch how to use its robotic arm to control the tool and to catch the toy, and in a second phase with the same learning mechanisms, the agent has to solve three problems where the toy can only be reached with the tool (See Fig. 9). We showed that agents choosing strategies based on learning progress also display overlapping waves of behavior compatible with the one observed in infants, and we suggested that curiosity-driven exploration could be at play in Chen and Siegler's experiment, and more generally in tool use discovery.

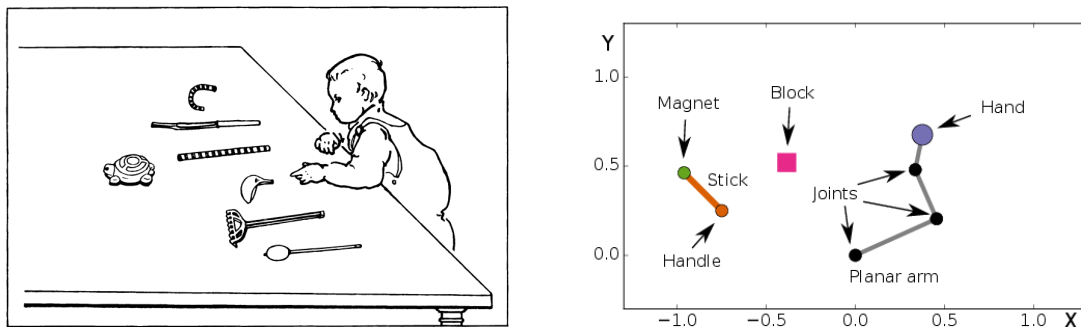


Figure 9. Left: Chen and Siegler's experimental setup with 1.5 and 2.5 years old babies who have to pick the good toy to retrieve an interesting toy. Right: Simulated robotic setup with a 3 DOF robotic arm that has 2 strategies to retrieve a toy: either grasp it with the hand, or use the stick to pull the toy.

7.1.2.2. Curiosity-driven developmental processes and their role in development and evolution of language

Infants' own activities create and actively select their learning experiences. In a collaboration with Linda Smith, we have analyzed recent models of embodied information seeking and curiosity-driven learning and have showed that these mechanisms have deep implications for development and evolution. In [69], we have discussed how these mechanisms yield self-organized epigenesis with emergent ordered behavioral and cognitive developmental stages. We described a robotic experiment that explored the hypothesis that progress in learning, in and for itself, generates intrinsic rewards: the robot learners probabilistically selected experiences according to their potential for reducing uncertainty. In these experiments, curiosity-driven learning led the robot learner to successively discover object affordances and vocal interaction with its peers. We explain how a learning curriculum adapted to the current constraints of the learning system automatically

formed, constraining learning and shaping the developmental trajectory. The observed trajectories in the robot experiment share many properties with those in infant development, including a mixture of regularities and diversities in the developmental patterns. Finally, we argued that such emergent developmental structures can guide and constrain evolution, in particular with regards to the origins of language.

7.1.3. Computational Models Of Developmental Exploration Mechanisms in Vocal Babbling and Arm Reaching in Infants

Participants: Pierre-Yves Oudeyer [correspondant], Clement Moulin-Frier, Freek Stulp, Jules Borchard.

7.1.3.1. Proximodistal Freeing of DOFs in Motor Learning as an Emergent Property of Stochastic Optimization Principles

To harness the complexity of their high-dimensional bodies during sensorimotor development, infants are guided by patterns of freezing and freeing of degrees of freedom. We have formulated and studied computationally the hypothesis that such patterns, such as the proximodistal freeing of degrees of freedom when learning to reach, can emerge spontaneously as the result of a family of stochastic optimization processes, without an innate encoding of a maturational schedule. In particular, we present simulated experiments with a 6-DOF arm where a computational learner progressively acquires reaching skills through adaptive exploration, and we show that a proximodistal organization appears spontaneously, which we denote PDFF (ProximoDistal Freezing and Freeing of degrees of freedom). We also compare the emergent structuration as different arm structures are used – from human-like to quite unnatural ones – to study the effect of different kinematic structures on the emergence of PDFF.

7.1.3.2. Emergent Jaw Predominance in Vocal Development through Stochastic Optimization

Infant vocal babbling is strongly relying on jaw oscillations, especially at the stage of canonical babbling, which underlies the syllabic structure of world languages. We have proposed, modelled and analyzed an hypothesis to explain this predominance of the jaw in early babbling. This hypothesis states that general stochastic optimization principles, when applied to learning sensorimotor control, automatically generate ordered babbling stages with a predominant exploration of jaw movements in early stages, just like they generate proximo-distal organization of exploration in arm reaching as described in the paragraph above. In particular, such stochastic optimization principles predominantly explore jaw movement at the beginning of vocal learning, and when close to the rest position of the vocal tract, as it impacts the auditory effects more than other articulators.

7.1.4. Learning and Teaching in Adult-Child and Human-Robot Interaction

Participants: Anna-Lisa Vollmer [correspondant], Pierre-Yves Oudeyer.

7.1.4.1. Pragmatic Frames

One of the big challenges in robotics today is to learn from human users that are inexperienced in interacting with robots but yet are often used to teach skills flexibly to other humans and to children in particular. A potential route toward natural and efficient learning and teaching in Human-Robot Interaction (HRI) is to leverage the social competences of humans and the underlying interactional mechanisms. In this perspective, we propose ‘pragmatic frames’ as flexible interaction protocols that provide important contextual cues to enable learners to infer new action or language skills and teachers to convey these cues. Following the concept developed in the field of developmental linguistics [117], we define a pragmatic frame to be an interaction protocol negotiated over time between interaction partners. We further specify a Pragmatic Frame to especially involve an observable **coordinated sequence of behaviors** and also relevant **cognitive operations**.

Figure 10 depicts the book reading frame Bruner observed in his studies on word learning.

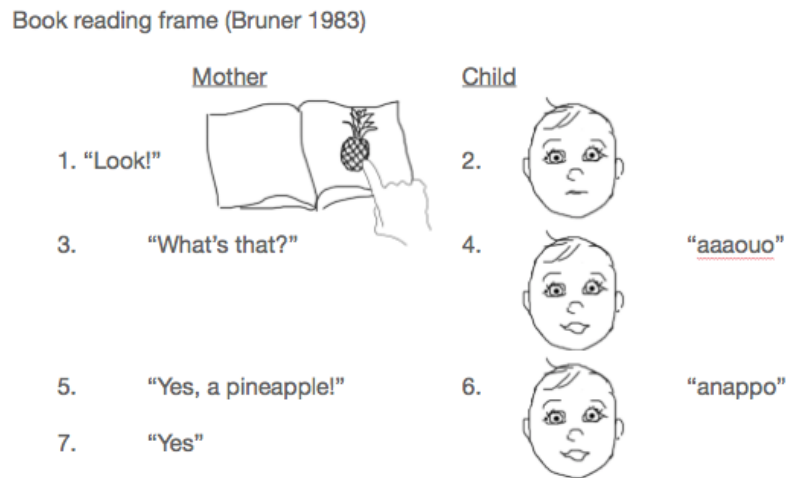


Figure 10. Example of a learning/teaching pragmatic frame.

At home, a mother is sitting on the sofa with her child on her lap and she is holding a picture book in front of them. The mother points to the book and says “look!” to direct the child’s attention. The child then gazes to the image. And the mother asks “What’s that?”, prompting the child’s performance. The child answers with babble strings and smiles, maybe “auo”. “Yes, a pineapple!” The mother gives positive feedback and the correct label. “Anappo”, again babble strings and smiles. And the mother gives positive feedback. This stable sequence that the child is familiar with helps the child to participate and to pick up the only variable information he or she is supposed to learn. We argue that this frame also triggers the relevant cognitive functions to process the information.

Our results in 2016 have been twofold. First, in a paper published in *Frontiers in Psychology* [70], we have given a theoretical account of pragmatic frames as an alternative to the mapping metaphor which posits that children learn a word by mapping it onto a concept of an object or event. However, we believe that a mapping metaphor cannot account for word learning, because even though children focus attention on objects, they do not necessarily remember the connection between the word and the referent unless it is framed pragmatically, that is, within a task. Word learning with pragmatic frames occurs as children accomplish a goal in cooperation with a partner. We elaborate on pragmatic frames, offer some initial parametrizations of the concept, and embed it in current language learning approaches.

Second, aiming at leveraging the concept of pragmatic frames for Human-Robot Interaction, we published an article in *Frontiers in Neurorobotics* [71] in which we study a selection of HRI work in the literature which has focused on learning–teaching interaction and analyze the interactional and learning mechanisms that were used in the light of pragmatic frames. This allows us to show that many of the works have already used in practice, but not always explicitly, basic elements of the pragmatic frames machinery. However, we also show that pragmatic frames have so far been used in a very restricted way as compared to how they are used in human–human interaction and argue that this has been an obstacle preventing robust natural multi-task learning and teaching in HRI. In particular, we explain that two central features of human pragmatic frames, mostly absent of existing HRI studies, are that (1) social peers use rich repertoires of frames, potentially combined together, to convey and infer multiple kinds of cues; (2) new frames can be learnt continually, building on existing ones, and guiding the interaction toward higher levels of complexity and expressivity. To conclude, we give an outlook on the future research direction describing the relevant key challenges that need to be solved for leveraging pragmatic frames for robot learning and teaching.

7.1.5. Models of Self-organization of lexical conventions: the role of Active Learning and Active Teaching in Naming Games

Participants: William Schueller [correspondant], Pierre-Yves Oudeyer.

How does language emerge, evolve and gets transmitted between individuals? What mechanisms underlie the formation and evolution of linguistic conventions, and what are their dynamics? Computational linguistic studies have shown that local interactions within groups of individuals (e.g. humans or robots) can lead to self-organization of lexica associating semantic categories to words [168]. However, it still doesn't scale well to complex meaning spaces and a large number of possible word-meaning associations (or lexical conventions), suggesting high competition among those conventions.

In statistical machine learning and in developmental sciences, it has been argued that an active control of the complexity of learning situations can have a significant impact on the global dynamics of the learning process [30], [131], [140]. This approach has been mostly studied for single robotic agents learning sensorimotor affordances [153], [38]. However active learning might represent an evolutionary advantage for language formation at the population level as well [49], [170].

Naming Games are a computational framework, elaborated to simulate the self-organization of lexical conventions in the form of a multi-agent model [169]. Through repeated local interactions between random couples of agents (designated *speaker* and *hearer*), shared conventions emerge. Interactions consist of uttering a word – or an abstract signal – referring to a topic, and evaluating the success or failure of communication.

However, in existing works processes involved in these interactions are typically random choices, especially the choice of a communication topic.

The introduction of active learning algorithms in these models produces significant improvement of the convergence process towards a shared vocabulary, with the speaker [53], [46], [122] or the hearer [90] actively controlling vocabulary growth.

We study here how the convergence time and the maximum level of complexity scale with population size, for three different strategies (one with random topic choice and two with active topic choice) detailed in table 11.

Naive (random)	Success Threshold	Minimal counts
$m \leftarrow \text{random}(\mathcal{M})$	if $\text{mean} \left(\frac{\text{succ}(i)}{\text{succ}(i) + \text{fail}(i)} \right)_{i \in \mathcal{LM}} \geq \alpha$: $m \leftarrow \text{random}(\mathcal{LM})$ else: $m \leftarrow \text{argmin}_{i \in \mathcal{LM}} \left(\frac{\text{succ}(i)}{\text{succ}(i) + \text{fail}(i)} \right)$	if $\forall i \in \mathcal{LM} \text{ succ}(i) > n$: $m \leftarrow \text{random}(\mathcal{LM})$ else: $m \leftarrow \text{argmin}_{i \in \mathcal{LM}} (\text{succ}(i))$
\mathcal{M} : all meanings, \mathcal{LM} : labeled meanings, \mathcal{UM} : unlabeled meanings, μ : vocabulary size (# word-meaning associations) succ : # successful interactions per meaning, fail : # failed interactions per meaning		

Figure 11. Strategies: Choice of meaning m . Both active strategies use a parameter (α and n), which is each time chosen optimal in our simulations.

As for the version of the Naming Game used in our work, the scenario of the interaction is described in [90]. Vocabulary is updated as described in the Minimal Naming Game, detailed in [177]. In our simulations, we choose to set $N = M = W$, where N is the population size, M the number of meanings, and W the number of possible words. The computed theoretical success ratio of communication is used to represent the degree of convergence toward a shared lexicon for the whole population. A value of 1 means that the population reached full convergence. Complexity level of an individual lexicon is measured as the total number of distinct associations between meanings and words in the lexicon, or in other words: memory usage.

We show here (see figures 12,13) that convergence time and maximum complexity are reduced with active topic choice, a behavior that is amplified as larger populations are considered. The minimal counts strategy yields a strictly minimum complexity (equal to the complexity of a completed lexicon), while converging as

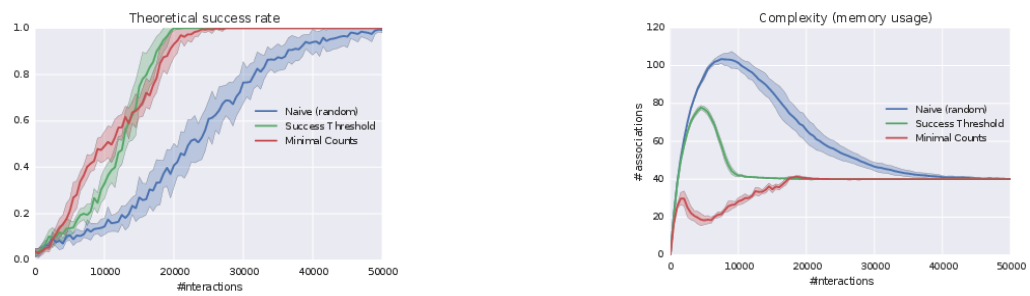


Figure 12. Strategy comparisons, in terms of convergence time (theoretical success ratio) and complexity level (memory usage). In this case, the hearer is the one choosing the topic. $M=W=N=40$, averaged over 8 trials

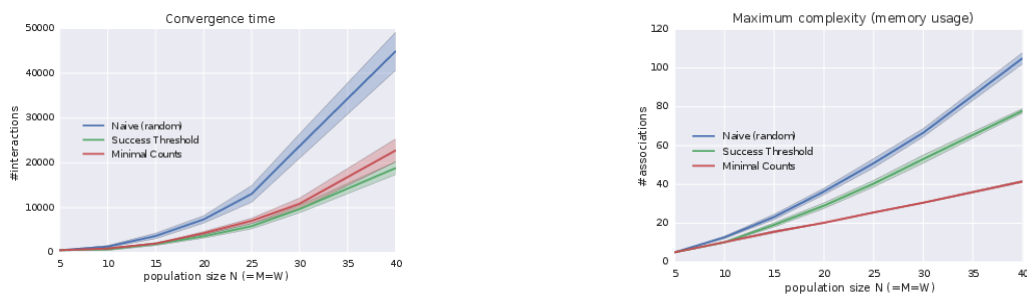


Figure 13. Scaling of maximum memory usage and convergence time for the different strategy, in function of population size. In this case, the hearer is the one choosing the topic. $M=W=N$, averaged over 8 trials.

fast as the success threshold strategy. Further work will deal with other variants of the Naming Game (with different vocabulary update, population replacement, and different ratio for N , M and W). For the moment only the hearer's choice scenario is studied, because of its high robustness to changes in parameter values for the different strategies [90].

7.2. Lifelong Robot Learning And Development Of Motor And Social Skills

7.2.1. Intrinsically Motivated Multitask Reinforcement Learning

Participants: Sébastien Forestier [correspondant], Pierre-Yves Oudeyer, Fabien Benureau.

7.2.1.1. Intrinsically Motivated Exploration of Spaces of Parameterized Skills/Tasks and Application to Robot Tool Learning

A major challenge in robotics is to learn 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 problems 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 [109].

In this work we study algorithms used by a learner to explore high-dimensional structured sensorimotor spaces such as in tool use discovery. We consider goal babbling architectures that were designed to explore and learn solutions to fields of sensorimotor problems, i.e. to acquire inverse models mapping a space of parameterized sensorimotor problems/effects to a corresponding space of parameterized motor primitives. However, so far these architectures have not been used in high-dimensional spaces of effects. Here, we show the limits of existing goal babbling architectures for efficient exploration in such spaces, and introduce a novel exploration architecture called Model Babbling (MB). MB exploits efficiently a modular representation of the space of parameterized problems/effects. We also study an active version of Model Babbling (the MACOB architecture). We compared those architectures in a simulated experimental setup with an arm that can discover and learn how to move objects using two tools with different properties, embedding structured high-dimensional continuous motor and sensory spaces (See Fig. 14).

7.2.1.2. Transfer Learning through Measures of Behavioral Diversity Generation in Autonomous Exploration

The production of behavioral diversity – producing a diversity of effects – is an essential strategy for robots exploring the world when facing situations where interaction possibilities are unknown or non-obvious. It allows to discover new aspects of the environment that cannot be inferred or deduced from available knowledge. However, creating behavioral diversity in situations where it is most crucial – new and unknown ones – is far from trivial. In particular in large and redundant sensorimotor spaces, only small areas are interesting to explore for any practical purpose. When the environment does not provide clues or gradient toward those areas, trying to discover those areas relies on chance. To address this problem, we introduce a method to create behavioral diversity in a new sensorimotor task by re-enacting actions that allowed to produce behavioral diversity in a previous task, along with a measure that quantifies this diversity. We have showed that our method can learn how to interact with an object by reusing experience from another, that it adapts to instances of morphological changes and of dissimilarity between tasks, and how scaffolding behaviors can emerge by simply switching the attention of the robot to different parts of the environment. Finally, we show that the method can robustly use simulated experiences and crude cognitive models to generate behavioral diversity in real robots. This work was published in [62].

We presented the results at the IEEE/RSJ International Conference on Intelligent Robots and Systems, Daejeon, Korea, October 9-14th [81].

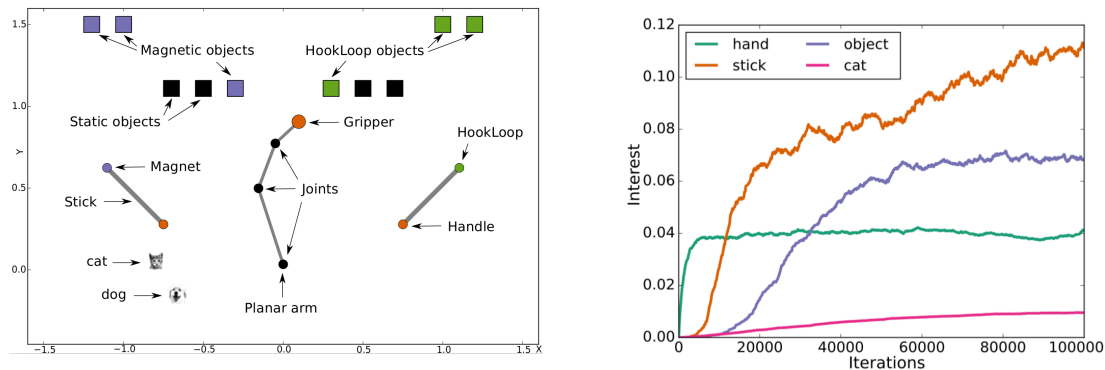


Figure 14. Left: Simulated robotic setup with a robotic arm that can grab tools to retrieve some interesting objects among a set of controllable and non-controllable (cat and dog) objects. Right: Evolution of the self-measured learning progress to move objects, with the MACOB active exploration architecture. The learning progress to explore objects is increasing for the tool and toy objects and stays low for the uncontrollable animals.

7.2.2. Social Learning of Interactive Skills

Participants: Manuel Lopes [correspondant], Thibaut Munzer, Marc Toussaint, Li Wang Wu, Yoan Mollard, Baptiste Busch, Jonathan Grizou, Marie Demangeat, Freek Stulp.

7.2.2.1. Relational Activity Processes for Modeling Concurrent Cooperation

In human-robot collaboration, multi-agent domains, or single-robot manipulation with multiple end-effectors, the activities of the involved parties are naturally concurrent. Such domains are also naturally relational as they involve objects, multiple agents, and models should generalize over objects and agents. We propose a novel formalization of relational concurrent activity processes that allows us to transfer methods from standard relational MDPs, such as MonteCarlo planning and learning from demonstration, to concurrent cooperation domains. We formally compare the formulation to previous propositional models of concurrent decision making and demonstrate planning and learning from demonstration methods on a real-world human-robot assembly task. A paper summarizing this research has been published to the *International Conference on Robotics and Automation (ICRA) 2016* [84].

7.2.2.2. Interactive Behavior Learning for Cooperative Tasks

This work goal is to propose a method to learn cooperative behavior to solve a task while performing the task with the user. The proposed approach reuses previous work on learning policy for RAP. The main differences are: i) formulate the problem as a cooperative process. In MDP and RAP, it is assumed that there is one central decision maker. However, in a cooperative both the robot and the operator are taking decisions. ii) estimating the confidence. A Query by Bagging approach has been used where many policies are learned from a subset of the data. Their potential disagreement allows quantifying the confidence. iii) Using the confidence for autonomous acting and for query making. Based on the confidence, the robot either act before acting or ask confirmation before acting.

Results show that using an interactive approach require less instruction from the user while producing a policy that makes fewer mistakes. We developed a robotic implementation 15 using a Baxter robot. A first article resulting from this work focusing on interactive preferences learning have been submitted to the *International Conference on Robotics and Automation (ICRA) 2017* and a video demonstration can be view at : <https://vimeo.com/182913540>. A broader journal article is in preparation. We also conducted a user study to evaluate the impact of interactive learning on naïve users acceptance and performances.

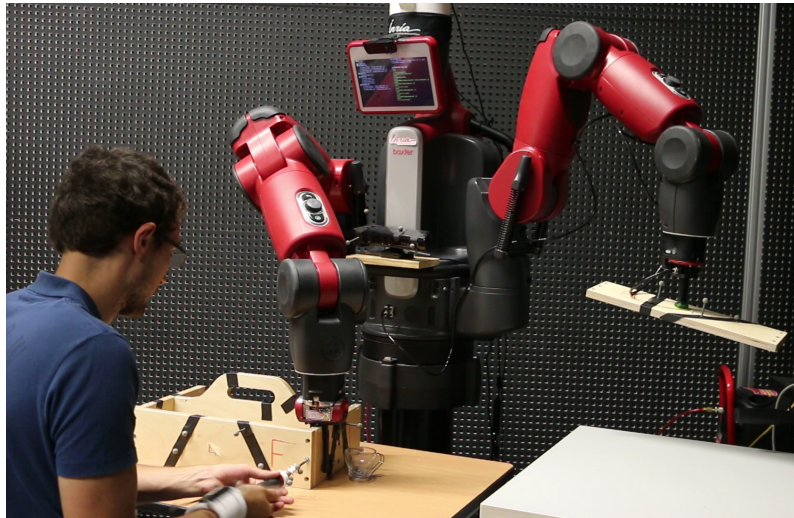


Figure 15. Interactive cooperative task learning.

7.2.2.3. Legible Motion

In a human-robot collaboration context, understanding and anticipating the robot intentions ease the completion of a joint-task. Whereas previous work has sought to explicitly optimize the legibility of behavior, we investigate legibility as a property that arises automatically from general requirements on the efficiency and robustness of joint human-robot task completion.

Following our previous work on legibility of robot motions [56], we have conducted several user experiments to analyze the effects of the policy representation on the universality of the legibility.

This work lead to a submission of a journal article to the International Journal of Social Robotics (IJSR) under the special issue: Towards a Framework for Joint Action. The article has been accepted with minor revisions and is currently in the final stage of the review process.

7.2.2.4. Postural optimization for a safe and comfortable human-robot interaction

When we, humans, accomplish a task our body posture is (partially) constrained. For example, acting on an object constrains the pose of the hand relatively to the object, and the head faces the object we are acting upon. But due to the large number of degrees of freedom (DOF) of the human body, other body parts are unconstrained and several body postures are viable with respect to the task. However, not all of them are viable in terms of ergonomics. Using a personalized human model, observational postural assessment techniques can be automatized. Optimizing the model body posture is then the logical next step to find an ergonomically correct posture for the worker to accomplish a specific task.

To optimize the subject's model to achieve a specific task, we define an objective function that minimizes the efforts of the whole body posture, based on the Rapid Entire Body Assessment (REBA) technique [135]. The objective function also account for visibility of the target object and worker's laterality. We have also implemented an automatic assessment of the worker's body posture based on the REBA method.

Using a spherical object, carried by a Baxter humanoid robot as illustrated in Fig. 16, we mimic an industrial scenario where the robot helps the worker by positioning and orienting an object in which the worker has to insert specific shapes. In a user-study with forty participants, we compare three different robot's behaviors, one of them being the result of the postural optimization of the subject's personalized model. By the mean of

a survey session, and the online assessment of the subject's posture during the interaction, we prove that our method leads to a safer posture, and is perceived as more comfortable.

This work has been submitted to the IEEE Robotics and Automation Letters (RA-L) with the ICRA conference option and is currently under review.

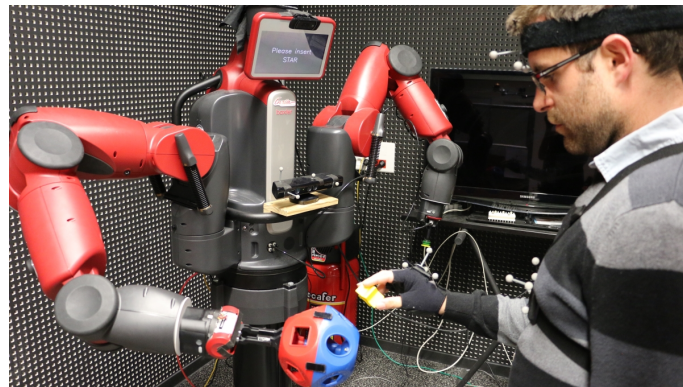


Figure 16. Representation of the setup considered in the user study. The robot presents to the user a spherical ball in which multiple shapes can be inserted. Final pose of the object is calculated from the user posture at his current location. Body motions during the insertion are recorded using a suit made from OptiTrack markers.

7.3. Representation Learning

Participants: David Filliat [correspondant], Celine Craye, Yuxin Chen, Clement Masson, Adrien Matricon, Freck Stulp.

7.3.1. Incremental Learning of Object-Based Visual Saliency

Searching for objects in an indoor environment can be drastically improved if a task-specific visual saliency is available. We describe a method to learn such an object-based visual saliency in an intrinsically motivated way using an environment exploration mechanism. We first define saliency in a geometrical manner and use this definition to discover salient elements given an attentive but costly observation of the environment. These elements are used to train a fast classifier that predicts salient objects given large-scale visual features. In order to get a better and faster learning, we use intrinsic motivation to drive our observation selection, based on uncertainty and novelty detection. Our approach has been tested on RGB-D images, is real-time, and outperforms several state-of-the-art methods in the case of indoor object detection. We published these results in two conferences [78],[77].

7.3.2. Cross-situational noun and adjective learning in an interactive scenario

Learning word meanings during natural interaction with a human faces noise and ambiguity that can be solved by analysing regularities across different situations. We propose a model of this cross-situational learning capacity and apply it to learning nouns and adjectives from noisy and ambiguous speeches and continuous visual input. We compared two different topic models for this task: Non Negative Matrix Factorization and Latent Dirichlet Association. We present experiments on learning object names and color names showing the performance of these model on realistic data and show how active learning can be used to speed-up learning by letting the learner choose the objects to be described. We published these results in a conference paper [75]

7.3.3. Learning representation with gated auto-encoders

We investigated algorithms that would be able to learn relevant visual or multi-modal features from data recorded while the robot performed some task. Representation learning is a currently very active research field, mainly focusing on deep-learning, which investigates how to compute more meaningful features from the raw high dimensional input data, providing a more abstract representation from which it should be easier to make decision or deduction (e.g classification, prediction, control, reinforcement learning). In the context of robotics, it is notably interesting to apply representation learning in a temporal and multi-modal approach exploiting vision and proprioception so as to be able to find feature that are relevant for building models of the robot itself and of its actions and their effect on the environment. Among the many existing approaches, we decided to explore the use of gated auto-encoders [104], a particular kind of neural networks including multiplicative connections, as they seem well adapted to this problem. Preliminary experimentations have been carried out with gated auto-encoders to learn transformations between two images. We observed that Gated Auto-Encoders (GAE) can successfully find compact representations of simple transformations such as translations, rotation or scaling between two small images. This is however not directly scalable to realistic images such as ones acquired by a robot's camera because of the number of parameters, memory size and computational power it would require (unless drastically downsampling the image which induces sensible loss of information). In addition, the transformation taking an image to the next one can be the combination of transformations due to the movement of several object in the field of view, composed with the global movement of the camera. This induces the existence of an exponential number of possible transformations to model, for which the basic GAE architecture is not suited.

7.3.4. Incremental Learning in high dimensions

Participants: Alexander Gepperth [correspondant], Cem Karaoguz.

7.3.4.1. Incremental learning in data spaces of high dimensionality

Currently existing incremental learning algorithms in robotics have achieved a relatively high degree of usability due to the reduction of free model parameters in such approaches LWPR. Indeed, such algorithms are usually applied to low-dimensional tasks such as graspin with very good success, as the incremental learning paradigm is very appropriate to the robotics domain in general, especially in interactive scenarios. On the other hand, the partitioning of input space that is performed by LWPR and related approaches fails to be applicable if data dimension exceeds 50 elements since the used covariance matrices grow quadratically in size w.r.t. data dimensionality. Therefore, especially the incremental treatment of visual information is difficult, particularly for recognition and classification of objects or obstacles in general. To remedy this, we developed the incremental learning algorithm PROPRES [130] of fixed model complexity that can easily deal with data dimensionalities of 10.000 and beyond, where the only assumption is the same that is explicitly made for LWPR: that the data has structure, i.e., lies on a low-dimensional sub-manifold. We demonstrated the feasibility of the algorithm on several realistic datasets, on the one hand MNIST and on the other hand a much more challenging visual pedestrian pose recognition task from the intelligent vehicle domain[65].

7.3.4.2. Incremental learning with two memory systems

In order to increase PROPRES's ability to react quickly to changes in data statistics (e.g., a newly added visual class) while at the same time avoiding fast forgetting, a second, short-term memory system was proposed for PROPRES in [65]. This short-term memory is filled when task failures occur and is used to re-train the incremental long-term memory at a later time and on a slower time scale. In this way, abrupt changes in data statistics maybe immediately reacted upon, whereas the long-term memory can retain its stability that ensures that any forgetting happens gradually, on a determined time scale.

7.3.4.3. Steps towards incremental deep learning

Since PROPRES is a neural architecture with just one hidden layer, its capacity is limited. This is why steps were taken to create deeper hierarchies with PROPRES in afashion totally analogous to current deep learning approaches. First of all, it was shown that a deep PROPRES architecture can achieve the same classification accuracy on MNIST as a shallow one but at a significantly lower computational cost [86]. Furthermore, it was

shown that a deep PROPRES architecture is capable of change detection at multiple levels, a prerequisite for incremental learning [87]. Next steps will consist of creating regular deep PROPRES architectures and testing them on currently accepted machine learning benchmark tasks.

7.3.4.4. Real-world application of incremental learning

In [88], the incremental PROPRES algorithm was applied to object recognition and detection problems in the domain of intelligent vehicles. It was shown that, by re-casting pedestrian detection as an incremental learning problem where the background class is added only after learning the pedestrian class, the number of required model resources for representing the background is reduced, and better accuracy can be obtained.

7.3.5. Measuring Uncertainty in Deep Learning Networks

Participants: Florian Golemo [correspondant], Manuel Lopes.

As precursor to the main objective of the IGLU project, we investigated methods that would enable deep neural networks to judge their knowledge about a domain.

Neural networks, especially deep ones, have been shown to be able to model arbitrarily complex problems, and thus offer powerful tools for machine learning. Yet they come with a significant flaw of not being inherently able to represent certainty of their predictions. By adding a measure of uncertainty to neural networks, this technology could be applied to autonomous exploration and open-ended learning tasks.

Thus the goal of this project was to find a method to measure how much knowledge a neural network has about an unlabeled data item (measure of uncertainty), and to apply this new measure in an active learning context. The objective of the latter was to demonstrate the efficiency in handpicking interesting data, to optimally extend the system's own capabilities.

We were successful in finding a measure of uncertainty that would reliably distinguish data that the network has seen before, from data that was generally unfamiliar to the network. This measure was created by measuring the entropy of the network's last layer across a batch of stochastic samples generated by adding Poisson noise to the inputs.

The measure failed however to outperform random sampling in several active learning scenarios. Yarín Gal published related work as part of his dissertation [129] after this project was concluded. He elaborated that deep neural networks are very effective in canceling out input noise. The author suggested to use existing "Dropout" layers instead for stochastic sampling, but he reaches the same conclusion of using the last layer entropy as measure of uncertainty.

7.3.6. Learning models by minimizing complexity

We introduce COCOTTE (CONstrained Complexity Optimization Through iterative merging of Experts), an iterative algorithm for discovering discrete, meaningful parameterized skills and learning explicit models of them from a set of behaviour examples. We show that forward-parameterized skills can be seen as smooth components of a locally smooth function and, framing the problem as the constrained minimization of a complexity measure, we propose an iterative algorithm to discover them. This algorithm fits well in the developmental robotics framework, as it does not require any external definition of a parameterized task, but discovers skills parameterized by the action from data. An application of our method to a simulated setup featuring a robotic arm interacting with an object is shown. This work was published in a conference paper [83]

7.4. Applications for Robotic myoelectric prostheses: co-adaptation algorithms and design of a 3D printed robotic arm prosthesis

Participants: Pierre-Yves Oudeyer [correspondant], Manuel Lopes, Mathilde Couraud, Sebastien Mick, Aymar de Rugy, Daniel Cattaert, Florent Paclet.

Together with the Hybrid team at INCIA, CNRS, the Flowers team continued to work on establishing the foundations of a long-term 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. In particular, in 2016 two lines of work were achieved, concerning two important scientific challenges, and in the context of one PEPS CNRS projects:

First, a new version of the experimental setup was designed to allow fast prototyping of 3D printed robotic prostheses. This work was based on the use of the Poppy open-source modular platform, and resulted in a functional prototype. A video demonstrations is available at: <https://github.com/s-mick>

Second, we have designed various control models allowing to transform signals coming from the human arm (either measured through EMGs or direct force sensors) and we have studied the influence of control modes on usability in the operation of a robotic arm prosthesis. In this context, we designed an experimental framework centered on a target-reaching task, and carried out tests with healthy subjects. The usability assessment relies on performance metrics on one hand, and a post-experiment questionnaire on another hand, in order to explore the multiple dimensions of the system's usability rather than focus only on measurements evaluating skills and performances. The code associated to this experimental setup is open-source and available at <https://github.com/s-mick>.

7.5. Applications for Educational Technologies

7.5.1. Multi-Armed Bandits for Adaptive Personalization in Intelligent Tutoring Systems

Participants: Manuel Lopes [correspondant], Pierre-Yves Oudeyer, Didier Roy, Alexandra Delmas, Benjamin Clement.

7.5.1.1. 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 present 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 introduce 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 is evaluated in a scenario where 7-8 year old schoolchildren learn how to decompose numbers while manipulating money. Systematic experiments are presented with simulated students, followed by results of a user study across a population of 400 school children. [14]

7.5.1.2. A Comparison of Automatic Teaching Strategies for Heterogeneous Student Populations

Online planning of good teaching sequences has the potential to provide a truly personalized teaching experience with a huge impact on the motivation and learning of students. In this work we compare two main approaches to achieve such a goal, POMDPs that can find an optimal long-term path, and Multi-armed bandits that optimize policies locally and greedily but that are computationally more efficient while requiring a simpler learner model. Even with the availability of data from several tutoring systems, it is never possible to have a highly accurate student model or one that is tuned for each particular student. We study what is the impact of the quality of the student model on the final results obtained with the two algorithms. Our hypothesis is that the higher flexibility of multi-armed bandits in terms of the complexity and precision of the student model will compensate for the lack of longer term planning featured in POMDPs. We present several simulated results showing the limits and robustness of each approach and a comparison of heterogeneous populations of students.

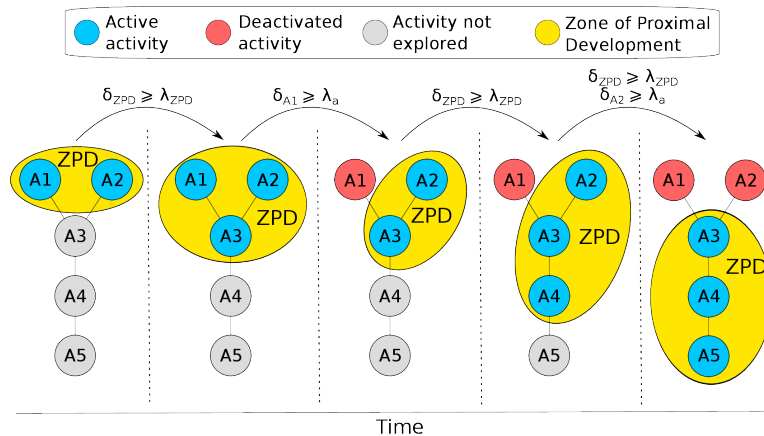


Figure 17. ZPDES exploration of an activity graph, with δ_{ZPD} the success rate over all active activities, λ_{ZPD} the threshold to expand the ZPD, δ_{Ax} the success rate for the activity Ax , and λ_a the threshold to reach to deactivate an activity.

This work has been published and presented at Educational Data Mining 2016 conference in Raleigh, USA [76].

Github link of the experiments paper code : <https://github.com/flowersteam/kidlearn/tree/edm2016>

7.5.1.3. The KidBreath project

To create learning contents linked to asthma to personalize it like mathematics activities in Kidlearn project [14] we used recommendation criterias in Therapeutic Education Program for asthma kids made by Health High Authority. Following an approach of participatory design [114], contents were validated by medical experts like health educators, pulmonologists and pediatrics. Then, we conducted a workshop with forty kids aged 8 in order to iterate over the application interfaces and evaluate enjoy about it with observations. Finally, we realized a focus group with 5 asthma kids to validate the global comprehension of a part of the content. It revealed that children wanted more contents about the crisis treatment and how the asthma works in the human system (verbatim).

In a preliminary study, we experimented two conditions in 20 control children (with 3 asthma kids), one giving the possibility of choosing activities like the child wants, and one no giving this choice (activities displayed in random). No significative difference between the two groups, but results showed KidBreath was easy to use with scores > 75 using System Usability Scale [115]. Based on Cordova and Lepper works to evaluate

motivation and knowledge with similar system and population [121], children had their disease knowledge increased with just one week use and were motivated using it. Finally, asthma kids showed they were more engaged than healthy kids and used KidBreath more seriously (stayed in breaks). These results were presented in the 5th edition of Serious Games in Medicine Conference in Nice.

We presented Thesis project in some events this year, with one publication submitted and validated:

- 2nd Meeting for Aquitaine and Euskadi companies in Biology and Health Between, February 11th 2016 in San Sebastian (poster),
- Hackathon of innovation in pulmonary diseases, Respirhacktion, September 16th to 18th 2016 in Paris (project development in hackathon),
- 5th Conference in Health Ergonomics and Patient Safety, October 5th to 7th 2016 (poster) [102],
- Learning Lab day, November 16th in Inria Paris (oral presentation of project),
- 5th edition of Serious Games in Medicine Conference, December 2nd to 3rd 2016 in Nice Sophia-Antipolis University (oral presentation).

7.5.2. *Poppy Education: Designing and Evaluating Educational Robotics Kits*

Participants: Pierre-Yves Oudeyer [correspondant], Didier Roy, Théo Segonds, Stéphanie Noirpoudre, Marie Demangeat, Thibault Desprez, Matthieu Lapeyre, Pierre Rouanet, Nicolas Rabault.

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.

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, engineer schools, ...). For secondary education and higher education, scientific literacy centers, Fablabs.

Poppy Education is based on the robotic platform poppy (open-source platform for the creation, use and sharing of interactive 3D printed robots), including:

- Poppy Humanoid, a robust and complete robotics platform designed for genuine experiments in the real world and 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. 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, which is a variant of Scratch. Its features allow a thorough introduction of information technology.
- 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. It is possible in the classroom to work on the simulated model and then allow students to run their program on the physical robot.

7.5.2.1. *Pedagogical experimentations : Design and experiment robots and the pedagogical activities in classroom*

This project is user centred design. The pedagogical tools of the project (real and virtual robots, pedagogical activities, etc.) are being created directly with the users and evaluated in real life by experiments. For our experimentations in the classroom we are mainly using the robot Poppy Ergo Jr (real and virtual) and Snap! Our purpose is to improve these pedagogical tools and to create pedagogical activities and resources for teachers.

- A pedagogical working group:



Figure 18. Experiment robots and pedagogical activities in classroom

At the beginning of the project, we established a pedagogical working group of 12 volunteers, teachers from different level (mainly high school teachers of the Aquitaine region) to help to design educational activities in line with the needs of the school curriculum and to test them in the classroom.

At the beginning of the second year of the project we added 7 other teachers from different background (middle-school and high school teachers) into the group to add more diversity.

We organised some training to help them to discover and learn how to use the robotics platform, then we met monthly to exchange about the project and to get some feedbacks from them.

You can see the videos of pedagogical robotics activities here:

https://www.youtube.com/playlist?list=PLdX8RO6QsgB7hM_7SQNLvyp2QjDAkkzLn

- Experiment and Evaluate the pedagogical kits:

Some engineer of the Poppy Education team went to visit the teachers in their school to see and to evaluate the pedagogical tools (robot and activities) in real contexts of use.

In addition to the observations in classroom, two trainee students of Master 2 in cognitive sciences (M. Demangeat, D. Thibaut) have established an experimental protocol to evaluate the utility and the integration of the pedagogical kits in class. They created and filled out questionnaires by teachers and students. The analyzes of the results are presented in their paper thesis.

This experimentations are helping us to understand the educational needs, to create and improve the pedagogical tools.

7.5.2.2. 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.

Last year student of "bachelor degree" (ENSAM-Talence) have designed, manufactured, assembled and programmed 4 different solutions to replace the fixed hand of Poppy by a gripper device:

<https://www.youtube.com/watch?v=DZjGaJk2fQk>

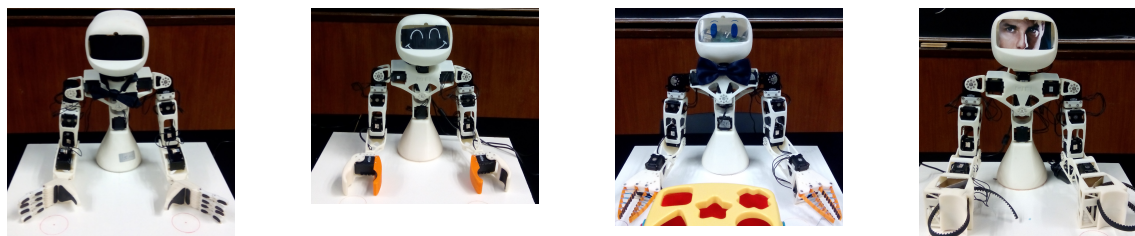


Figure 19. 4 grippers hands designed by students

- Audiovisual Students project

Students from the BTS audiovisual of Saint-Genes La Salle have created a complete video report on the Poppy project to highlight the use in education and art:

<https://www.youtube.com/watch?v=NMwwH7AWO2Q>

- Poppy entre dans la danse (Poppy enters the dance)

The project "Poppy enters the dance" (Canope 33) uses the humanoid robot Poppy, 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 an overview of the project with kindergarten students :

<https://www.youtube.com/watch?v=XB9IXwcfJo0>

7.5.2.3. Created pedagogical documents and resources

- Rebuilt the documentation of Poppy-project

It was necessary for us to have an accessible and clear documentation to help teachers to use and create projects with the robots in the classroom so we rebuilt the existing documentation of the robotics platform Poppy. We added and improve the contents and we used the platform gitbook :

<https://docs.poppy-project.org/en/>

- Pedagogical booklet

The pedagogical booklet [96] brings together all the pedagogical activities and project testing in the classroom. It provides guided activities, small challenges and projects to become familiar with the Poppy Ergo Jr robot and the Programming language Snap!

<https://drive.google.com/file/d/0B2jV8VX-IQHwTUxXZjF3OGxHVGM/view>

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>

- Guide on the pedagogical use of the kit Poppy Ergo Jr in classroom

We wrote an article [95] to explain how to use the Robot Ergo Jr in a classroom. It includes a summary of the characteristics of the robots, activities example and give all the necessary resources:

<https://pixees.fr/dans-la-famille-poppy-je-voudrais-le-robot-ergo-jr>



Figure 20. Pedagogical booklet: learn to program the robot Poppy Ergo Jr in Snap!

- Demonstration guide to introduce the project

This document is for people who already have a little experience with the Poppy Ergo Jr robot and snap! and wishing to present the project (i.e: to a colleague/acquaintance, on a exhibition stand, during a conference).

The purpose of this document is to provide the necessary elements to enable the Poppy Education project to be presented through the use of Poppy Ergo Jr. robot. The key points of the Poppy Education project and the features of Poppy Ergo Jr kit are presented as well as examples of demonstrations of educational activities (videos and snap! projects) and educational projects (videos). An example of structuring a demo is provided at the end of the document.

<https://forum.poppy-project.org/t/guide-de-demo-du-kit-pedagogique-poppy-ergo-jr-version-beta/2698>

- Model of pedagogical activities sheet

We designed a model of pedagogical activity sheet. It helps us to get back the various activities and allows to have a homogeneous presentation. It is simpler to share and get back the creations of each.

<https://forum.poppy-project.org/t/modele-de-fiche-pedagogique-telechargeable-pour-les-activites-robotiques/2706>

7.5.2.4. Scientific mediation

To promote educational uses of the platform, we participated in events (conference, seminar etc.).

We participated as well at some workshops to introduce students to robotics and programming.

7.5.2.5. Symposium robotics

We organized a symposium robotics (<http://dm1r.fr/colloque-robotique-education/>) that present research results and feedback on the use of Poppy and Thymio robots in education (other robots have been discussed, such as BeeBot and Metabot), from kindergarten to higher education, The Centers for Scientific and Technical Culture.

It was a 2 day event : 200 participants, 40 speakers (conferences and workshops).

Poppy Education team and the working group teachers helped with the organisation of the event and during the event (talk and workshops).

All conference videos are available on the web :

https://www.youtube.com/watch?v=prFmC-BpdY8&index=1&list=PL9T8000j7sJBC_H3L_hS-i4Lth1Fz2FY

7.5.3. *IniRobot: Educational Robotics in Primary Schools*

Participants: Didier Roy [correspondant], Pierre-Yves Oudeyer.

IniRobot (a project done in collaboration with EPFL/Mobsya) aims to create, evaluate and disseminate a pedagogical kit which uses Thymio robot, open-source and low cost, for teaching computer science and robotics.

IniRobot Project consists to produce and diffuse a pedagogical kit for teachers and animators, to help 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 enquiry-based educational approach, where kids are led to construct their understanding through practicing an active investigation methodology within teams. It is based on the use of the Thymio II robotic platform. More details about this projects were published in RIE 2015 [50] , which presents the detailed pedagogical objectives and a first measure of results showing that children acquired several robotics-related concepts. See also <http://www.inirobot.fr>.

Deployment: After 24 months of activity, IniRobot is used by about 1400 adults and 16 000 children in 54 cities of France. Example of action in university: MEEF teacher training for the hope of Aquitaine. Example of action in school: training of all Gironde Pedagogical ICT Advisors, covering nearly 1000 schools. Example of action in the extracurricular time: training 82 facilitators TAP cities of Talence, Pessac, Lille, ..., CDC Gates of inter-seas. Example of national action: Training of the digital mediators of the 8 Inria centers.

7.5.3.1. *Partnership*

The project is carried out in main collaboration with the LSRO Laboratory from EPFL (Lausanne) and others collaborations with French National Education/Rectorat d'Aquitaine, with Canopé Educational Network, with ESPE (teacher's school) Aquitaine, ESPE Martinique, ESPE Poitiers, National Directorate of Digital Education

7.5.3.2. *Created pedagogical documents and resources*

- IniRobot pedagogical kit [94]: This pedagogical booklet provides activities scenarized as missions to do. A second pedagogical booklet has been also created by three pedagogical advisers for primary school, with pedagogical instructions and aims, under ou supervision. <http://tice33.ac-bordeaux.fr/Ecolien/ASTEP/tabid/5953/language/fr-FR/Default.aspx> A new pedagogical kit is in progress, Inirobot Scratch, which will propose activities with Scratch and Snap! and Thymio robot.
- Inirobot website and forum <http://www.inirobot.fr> With this website, teachers, animators and general public can download documents, exchange about their use of inirobot' kit.
- Publication about Inirobot and Poppy Education A poster and talk were produced in Didapro-Didastic 6 Conference in Namur (Belgium) on 2016 January. [99]

7.5.3.3. *Scientific mediation*

Inirobot is very popular and often presented in events (conferences, workshops, ...) by us and by others.

7.5.3.4. *Symposium robotics*

With Poppy Education, Inirobot is a main line in our colloquium "Robotics and Education" (<http://dm1r.fr/colloque-robotique-education/>)

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 further developed a planning algorithm for a autonomous electric car for Renault SAS in the continuation of the previous PAMU 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, and with multiple lane roads (overtake, insertion...).

8.2. Bilateral Grants with Industry

8.2.1. Curiosity and visual attention

Participants: David Filliat [correspondant], Celine Craye.

Financing of the CIFRE PhD grant of Celine Craye by Thales S.A. with the goal of developing a mechanism of visual attention guiding the exploration of a robot.

8.2.1.1. Adaptive device for disease awareness and treatment adherence of asthma in children

Participants: Manuel Lopes [correspondant], Alexandra Delmas, Pierre-Yves Oudeyer.

Financing of the CIFRE PhD grant of Alexandra Delmas by Itwell with the goal of developing a tool for self-learning for patients to improve their compliance to treatment.

9. Partnerships and Cooperations

9.1. Regional Initiatives

9.1.1. Poppy Education

Poppy Education

Program: Feder - Région Aquitaine

Duration: January 2014 - December 2017

Coordinator: PY Oudeyer, Inria Flowers

Partners: Inria Flowers

Funding: 1 million euros (co-funded by Feder/EU Commission, Region Aquitaine and Inria)

Poppy Education aims to create, evaluate and disseminate pedagogical kits “turnkey solutions” complete, open-source and low cost, for teaching computer science and robotics. 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/Rectorat, Highschools, engineering schools, ...). It targets secondary education and higher education, scientific literacy centers, Fablabs.

Poppy robotic platform used in the project is free hardware and software, printed in 3D, and is intended primarily for:

- learning of computer science and robotics,
- introduction to digital manufacturing (3D printing ...)
- initiation to the integration of IT in physical objects in humanoid robotics, mechatronics.
- artistic activities.

Educational sectors covered by the project are mainly: Enseignement d'exploration ICN en seconde, enseignement ISN en terminale S et bientôt en 1ère , filière STI2D, MPS seconde. Web: <http://www.poppy-project.org/education> .

9.1.2. ENSAM

The orientation of a (high school) student, choosing a career, is often based on an imagined representation of a discipline, sector of activity or training. Moreover, higher education is sometimes for a college student or a student a self centered universe, with inaccessible teaching methodologies and level of competence.

The Arts and Métiers campus at Bordeaux-Talence in partnership with Inria contributes with 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. These teaching sequences will be built and tailored to different levels of training, from high schools to Engineer schools.

The new formation "Bachelor of Technology", started in September 2014 at Ensam Bordeaux, is resolutely turned towards a project based pedagogy, outlining concepts from concrete situations. 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 formation: mechanics, manufacturing (3D printing), electrical, mechatronics, computer sciences, design. . .

For the 1st and 2nd year of the ENSAM Engineer cursus, the Poppy robot is now used to support the teaching and to conduct further investigation.

9.1.3. KidLearn and Region Aquitaine

A Conseil Régional d'Aquitaine Project (KidLearn, 2015-) began, coordinated by Manuel Lopes entitled KidLearn. Will fund 50% of a 3 years PhD student.

We propose here a research project that aims at elaborating algorithms and software systems to help humans learn efficiently, at school, at home or at work, by adapting and personalizing sequences of learning activities to the particularities of each individual student. This project leverages recent innovative algorithmic models of human learning (curiosity in particular, developed as a result of ERC European project of the Flowers team), and combines it with state-of-the-art optimization algorithms and an original integration with existing expert knowledge (human teachers). Given a knowledge domain and a set of possible learning activities, it will be able to propose the right activity at the right time to maximize learning progress. It can be applied to many learning situations and potential users: children learning basic knowledge in schools and with the support of their teachers, older kids using educational software at home, of adults needing to acquire new skills through professional training ("formation professionnelle"). Because it combines innovations in computational sciences (machine learning and optimization) with theories of human cognition (theories of human learning and of education), this project is also implementing a strong cross-fertilization between technology and human sciences (SHS).

9.1.4. Comacina Capsule Creative Art/Science project and Idex/Univ. Bordeaux

The artist community is a rich source of inspiration and can provide new perspectives to scientific and technological questions. This complementarity is a great opportunity that we want to enforce in the Poppy project by making the robot accessible to non-robotic-expert users. The Comacina project, in collaboration with the Flowers team and supported by funding from Idex/Univ. Bordeaux, explored the role of movements and light in expressing emotions. This project was implemented through several residencies during the year, and several performances at various cultural places in Aquitaine, including at Pole Evasion in Ambares-et-Lagrave. a report is available at <https://flowers.inria.fr/RencontreAutourDuGeste.pdf> . It benefitted from funding from the Art/Science Idex call for project.

9.2. National Initiatives

PY Oudeyer and M Lopes collaborated with Aymar de Rugy, Daniel Cattaert and Florent Paclet (INRIA, 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.

D. Roy is the Inria leader of project "Ecole du code" <http://www.ecoleducode.net/> which provides teachers and animators formations and learning games to initiate young people to computer science and robotics.

D. Roy is member of the Class'code team (Inria is member of the consortium of this project) <https://pixees.fr/classcode/accueil/>. Class'code is a blended formation for teachers and animators who aim to initiate young people to computer science and robotics. D. Roy has in charge the robotics module of the project.

D. Roy is member of the organization of computer science exhibition in "Palais de la découverte" which will begin on 2017 September for three years. He participates for robotics part.

D. Roy is member of the Scratch Conference (Bordeaux, 2017 July) organization team.

D. Roy is member of the team "Education en Scène" which organize educational activities with robotics in Bordeaux Digital City (2017 July).

D. Roy is member of "CRIC" Project, about Robotics in Vocational Schools, with Canope Ile de France, Lutin Userlab (Cité des Sciences), CNAM.

D. Roy is project leader of Thymio Simulator for Classcode project. Specifications and coordination of work.

D. Roy is project leader of Thymio Scratch and Thymio Snap! development, with D. Sherman. Inria, EPFL and Mobsya collaboration.

Around Robotics for education, many collaborations were put in place. With the LSRO Laboratory from EPFL (Lausanne) and others collaborations with French National Education/Rectorat d'Aquitaine, with Canopé Educational Network, with ESPE (teacher's school) Aquitaine, ESPE Martinique, ESPE Poitiers, National Directorate of Digital Education, Fondation "La Main à la Pâte", Maison for Science in Bordeaux University, Orange Fondation.

9.3. European Initiatives

9.3.1. FP7 & H2020 Projects

9.3.1.1. 3rd HAND

Title: Semi-Autonomous 3rd Hand

Programm: FP7

Duration: October 2013 - September 2017

Coordinator: Inria

Partners:

Technische Universität Darmstadt (Germany)

Universität Innsbruck (Austria)

Universität Stuttgart (Germany)

Inria contact: Manuel Lopes

Robots have been essential for keeping industrial manufacturing in Europe. Most factories have large numbers of robots in a fixed setup and few programs that produce the exact same product hundreds of thousands times. The only common interaction between the robot and the human worker has become the so-called 'emergency stop button'. As a result, re-programming robots for new or personalized products has become a key bottleneck for keeping manufacturing jobs in Europe. The core requirement to date has been the production in large numbers or at a high price. Robot-based small series production requires a major breakthrough in robotics: the development of a new

class of semi-autonomous robots that can decrease this cost substantially. Such robots need to be aware of the human worker, alleviating him from the monotonous repetitive tasks while keeping him in the loop where his intelligence makes a substantial difference. In this project, we pursue this breakthrough by developing a semi-autonomous robot assistant that acts as a third hand of a human worker. It will be straightforward to instruct even by an untrained layman worker, allow for efficient knowledge transfer between tasks and enable an effective collaboration between a human worker with a robot third hand. The main contributions of this project will be the scientific principles of semi-autonomous human-robot collaboration, a new semi-autonomous robotic system that is able to: i) learn cooperative tasks from demonstration; ii) learn from instruction; and iii) transfer knowledge between tasks and environments. We will demonstrate its efficiency in the collaborative assembly of an IKEA-like shelf where the robot acts as a semi-autonomous 3rd-Hand .

9.3.1.2. DREAM

Title: Deferred Restructuring of Experience in Autonomous Machines

Programm: H2020

Duration: January 2015 - December 2018

Coordinator: UPMC

Partners:

Armines (ENSTA ParisTech)

Queen Mary University London (England)

University of A Coruna (Spain)

Vrije University Amsterdam (Holland)

Contact: David Filliat

Abstract: A holy grail in robotics and artificial intelligence is to design a machine that can accumulate adaptations on developmental time scales of months and years. From infancy through adulthood, such a system must continually consolidate and bootstrap its knowledge, to ensure that the learned knowledge and skills are compositional, and organized into meaningful hierarchies. Consolidation of previous experience and knowledge appears to be one of the main purposes of sleep and dreams for humans, that serve to tidy the brain by removing excess information, to recombine concepts to improve information processing, and to consolidate memory. Our approach – Deferred Restructuring of Experience in Autonomous Machines (DREAM) – incorporates sleep and dream-like processes within a cognitive architecture. This enables an individual robot or groups of robots to consolidate their experience into more useful and generic formats, thus improving their future ability to learn and adapt. DREAM relies on Evolutionary Neurodynamic ensemble methods (Fernando et al, 2012 *Frontiers in Comp Neuro*; Bellas et al., *IEEE-TAMD*, 2010) as a unifying principle for discovery, optimization, re- structuring and consolidation of knowledge. This new paradigm will make the robot more autonomous in its acquisition, organization and use of knowledge and skills just as long as they comply with the satisfaction of pre-established basic motivations. DREAM will enable robots to cope with the complexity of being an information-processing entity in domains that are open-ended both in terms of space and time. It paves the way for a new generation of robots whose existence and purpose goes far beyond the mere execution of dull tasks. <http://www.robotsthatdream.eu>

9.3.2. Collaborations in European Programs, except FP7 & H2020

9.3.2.1. 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: Manuel Lopes

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) - __DEPARTMENT???)__ - JACQUELINE
GOTTLIEB

Start year: 2016

See also: <https://flowers.inria.fr/neurocuriosity>

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. Informal International Partners

Benjamin Clement and Manuel Lopes just begin a collaboration with Joseph Jay Williams (Harvard University), Douglas Selent and Neil Heffernan (Worcester Polytechnic Institute) to use Kidlearn algorithm and contextual multi-armed bandit to recommend explanation on ASSISTments online tutoring system. Joseph Jay Williams and Neil Heffernan used multi-armed bandit algorithm on ASSISTments platform [179] to provide efficient explanation, and now we are looking to use new algorithm to provide a more personal and relevant feedback.

Pierre-Yves Oudeyer and Didier Roy have create 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.

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.

9.5. International Research Visitors

9.5.1. Visits of International Scientists

- Lauriane Rat-Fisher, IAST, Toulouse (November 23-25th)
- Fumihide Tanaka, ISI Lab, University of Tokyo, Japan (November 9th)
- Romain Brette, Institut de la Vision, Paris (February, 12th)
- Tony Belpaeme, Univ. Plymouth, UK (January)
- Tobjorn Dahl, Univ. Plymouth, UK (January)
- Jens Moenig, SAP Research, Germany (June)
- Stéphane Magnégnat, ETH Zurich, Switzerland (June)
- Francesco Mondada, EPFL, Lausanne, Switzerland (June)

9.5.1.1. Internships

- Yasmin Ansari, The Biorobotics Institute, Scuola Superiore S. Anna, Pontedera, Italy (January to May, 2016)

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

10.1.1.1. General Chair, Scientific Chair

- PY. Oudeyer and M. Lopes have been general co-chair of Second Interdisciplinary Symposium on Information Seeking, Curiosity and Attention (Neurocuriosity 2016), London, UK (150 participants). <https://goo.gl/BYL0h4>
- D. Roy has been general chair of the colloquium "Robotique et Education" in Bordeaux, June 2016, <http://dm1r.fr/colloque-robotique-education/>.

10.1.1.2. Member of the Organizing Committees

- Manuel Lopes co-organized the R:SS 2016 workshop on Bootstrapping Manipulation Skills 06.2016 <http://www.bootstrapping-manipulation.com/>
- Alexander Gepperth co-organized a special session ("Incremental learning algorithms and application") on ESANN 2016, together with Barbara Hammer of Bielefeld university (Germany).
- PY. Oudeyer has been member of the steering committee of the IEEE ICDL-Epirob conference.
- PY. Oudeyer has been member of the steering committee of the fOSSa conference.
- PY. Oudeyer has been "Robotics Liaison" of IJCNN 2017, Anchorage, Alaska.

10.1.2. Scientific Events Selection

10.1.2.1. Member of the Conference Program Committees

- David Filliat was Associate Editor for IROS.
- PY. Oudeyer has been member of the PC committee of IEEE ICDL-Epirob 2016.
- Alexander Gepperth was member of the program committee for IJCNN 2016, ECAI 2016 and ESANN 2016.

10.1.2.2. Reviewer

- David Filliat was reviewer for the IFAC, IV, RFIA, ICRA conferences.
- Sébastien Forestier was reviewer for IEEE ICDL-Epirob
- Manuel Lopes was reviewer for IEEE IROS, IEEE ICDL-EPIROB, IEEE ICRA, IJCAI, NIPS
- Thibaut Munzer was reviewer for IEEE IJCAI.
- Baptiste Busch reviewer for IEEE RO-MAN.
- PY. Oudeyer has been a reviewer for the conferences IEEE ICDL-Epirob and Humanoids 2016.
- Alexander Gepperth was reviewer for ESANN 2016, IJCNN2016, IEEE Symposium on Intelligent Vehicles (IV) and ECAI 2016

10.1.3. Journal

10.1.3.1. Member of the Editorial Boards

- PY. Oudeyer has been editor of IEEE CIS Newsletter on Cognitive and Developmental Systems: <https://openlab-flowers.inria.fr/t/ieee-cis-newsletter-on-cognitive-and-developmental-systems/129>
- PY. Oudeyer has been associate editor of IEEE Transactions on Cognitive and Developmental Systems
- PY Oudeyer has been associate editor of Robotics and Automation Letters (RA-L).
- PY. Oudeyer has been associate editor of Frontiers in Neurorobotics and Frontiers in Humanoid Robotics.
- PY. Oudeyer has been Associate editor of International Journal of Social Robotics (Springer).

10.1.3.2. Reviewer - Reviewing Activities

- David Filliat was reviewer for Journal of Intelligent Service Robotics.
- Alexander Gepperth was reviewer IEEE Transactions on Intelligent Transportation Systems
- Anna-Lisa Vollmer was reviewer for Frontiers in Robotics and AI and IEEE Transactions on Cognitive and Developmental Systems.
- PY. Oudeyer has been a reviewer for the Robotics and Automation Magazine, the Journal of Language Evolution.

10.1.4. Invited Talks

- David Filliat gave an invited presentation “Apprentissage pour les vehicules intelligents et la robotique developpementale” during the workshop “Intelligence Artificielle et Véhicule à Conduite Deleguee” organized by VEDECOM on september 28th.
- PY. Oudeyer, "Open-source art/science with Poppy Project", 15th january, Journée ECARTS, Univ. Bordeaux.
- PY. Oudeyer, "Mondes Mosaïques", Librairie Mollat, 2 février, Bordeaux.
- PY. Oudeyer, "Self-organization and active learning of language", 21 mars, Lattice, ENS Paris.
- PY. Oudeyer, "Intelligence artificielle et robotique", 21 mars, Grand Palais, Paris.
- PY. Oudeyer, "Intelligence artificielle et philosophie", 20 mai, Bordeaux.
- PY Oudeyer, "How robotic modelling can help us understand complex dynamics in development", 22 may, Views by Two keynote, International Conference on Infant Studies, New-Orleans.
- PY. Oudeyer, "Robotique éducative: les projets de l'équipe Flowers", Colloque Robotique et Education, Bordeaux.
- PY. Oudeyer, "Curiosity, exploration and learning in humans and machines", 9 july, ISSAS Summer School, Geneva, Switzerland.
- PY. Oudeyer, "How robotic modelling can help us understand complex dynamics in language and sensorimotor development", 9th september, Creativity and Evolution Summer School, Como, Italy.
- PY Oudeyer, "Comment la modélisation robotique aide à comprendre la dynamique du développement de l'enfant", 18 septembre, Colloque Biologie et Information, Cerisy, France.
- PY. Oudeyer, "Active exploration for lifelong developmental learning in humans and machines: intrinsic motivation, maturation and social guidance", 5th october, Google Deepmind seminar, London, UK.
- PY. Oudeyer, "Diversity of forms and developmental functions of curiosity-driven exploration", 8th october, London UK.
- PY. Oudeyer, "Intelligence artificielle et humain", Entretiens de la Cité, 5th november, Lyon, France.
- PY. Oudeyer, "Artificial intelligence and robotics: scientific, technological and societal challenges", 8th november, Académie des Technologies, Paris, France.
- PY. Oudeyer, "From fundamental research in models of human learning to educational applications", 16th november, Journée Learning Lab, Paris, France.
- PY. Oudeyer, "Diversity of forms and developmental functions of curiosity-driven exploration", 17th november, Journée GdR Robotique et Neuroscience, Bordeaux.
- PY. Oudeyer, "Machine learning and robotics", 5th december, Technion ConnectedWorld conference, Paris.

10.1.5. Leadership within the Scientific Community

PY. Oudeyer has been chair of IEEE Computational Intelligence Society technical committee on cognitive and developmental systems (10 task forces, 65 members); The activities of the TC are described at: <https://openlab-flowers.inria.fr/t/ieee-cis-tc-on-cognitive-and-developmental-systems/41>

10.1.6. Scientific Expertise

- M Lopes was expert for the EU Commission scientific programme.
- PY. Oudeyer has been an expert for the European Commission, the Polish National Research Agency, and the Swedish National Research Agency.
- PY. Oudeyer has been expert for Main à la Pâte for the textbook project “1, 2, 3: Codez!” to teach computer science in primary schools.
- PY. Oudeyer has been expert for Académie des Technologies and OPECST on artificial intelligence and its interaction with society.

10.1.7. Research Administration

PY. Oudeyer has been scientific responsible of Inria-Ensta-ParisTech EPC.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

- Master: Robotique Developmental et Cognitive, 35 heures, Nantes, (Manuel Lopes et PY Oudeyer)
- Master: Robotique Developmental et Cognitive, 35 heures, Universite de Bordeaux, (Manuel Lopes et PY Oudeyer)
- License: Inteligencia Artificial, 90 heures, Instituto Superior Tecnico, Lisboa, (Manuel Lopes)
- License: Introduction to Matlab, 21 heures. L3, ENSTA - ParisTech (David Filliat).
- Master: Robotique Mobile, 21 heures. M2, ENSTA - ParisTech (David Filliat).
- Master: Perception pour la Robotique, 6 heures. M2, ENSTA - ParisTech (David Filliat).
- Master: Perception pour la robotique, 12 heures. M2 Systemes Avances et Robotique, University Pierre et Marie Curie (David Filliat)
- Master: Perception pour la Robotique Développementale, 3 hours, CogMaster (David Filliat)
- Licence Informatique, 64h Bordeaux University (Sébastien Forestier)
- PY. Oudeyer taught a course on "Robotic modelling of cognitive development" at ENS Rennes, 12 h
- PY. Oudeyer taught a course on "Robotic modelling of cognitive development" at Enseirb, 2 h
- PY. Oudeyer taught a course on "Robotic modelling of cognitive development" at CogMaster, Paris, 3 h
- PY. Oudeyer taught a course on "Developmental and cognitive robotics" at Univ. Mons, Belgium, 3h
- PY. Oudeyer coordinated the project Poppy Education, which has developed several educational robotics kits for computer science education in high-schools
- Continuing education: Robotics for education, 30 h, EPFL (Didier Roy)

10.2.2. Supervision

- PhD in progress: Sébastien Forestier, Models of curiosity-driven learning of tool use and speech development, started in sept. 2015 (superv. P-Y. Oudeyer)
- PhD in progress: William Schueller, Study of the impact of active learning and teaching in naming games dynamics, started in sept. 2015 (superv. P-Y. Oudeyer)
- PhD in progress: Alvaro Ovalle-Castaneda, Computational models of intrinsically motivated learning and exploration, started in oct. 2016 (superv. P-Y. Oudeyer)
- PhD in progress: Thibault Desprez, Design and study of the impact of educational robotic kits in computer science education, started in dec. 2016 (superv. P-Y. Oudeyer)
- PY. Oudeyer supervised three master thesis internship: Thibault Desprez (M2, educational robotics), Marie Demangeat (M2, educational robotics), Sébastien Mick (M2, design and study of robotic prosthesis)
- PY. Oudeyer supervised a team of computer and pedagogical engineers and researchers for the project Poppy Education (Didier Roy, Stéphanie Noirpoudre, Théo Segonds, Damien Caselli, Nicolas Rabault, Matthieu Lapeure)
- PhD in progress: Thomas Hecht, Bio-inspired sensor fusion, started November 2013 (superv. Alexander Gepperth).
- PhD : Egor Sattarov, Multimodal vehicle perception architecture, Université Paris-Saclay, 9/12/2016 (co-superv. Alexander Gepperth).
- PhD : Thomas Kopinski, Machine Learning for human-machine interaction, Université Paris-Saclay, ENSTA ParisTech, 12/02/2016 (superv. Alexander Gepperth).

PhD in progress: Benjamin Clement, Intelligent Tutoring Systems, started oct 2015 (superv. Manuel Lopes and Pierre-Yves Oudeyer).

PhD in progress: Thibaut Munzer, Learning from Instruction, started oct 2013 (superv. Manuel Lopes).

PhD in progress: Baptiste Busch, Interactive Learning, started oct 2014 (superv. Manuel Lopes).

PhD in progress: Alexandra Delmas, Auto-Apprentissage Auto-Adaptable pour la compliance au traitement, started oct 2014 (superv. Manuel Lopes).

PhD : Alexandre Armand, Situation Understanding and Risk Assessment Framework for Preventive Driver Assistance, Université Paris-Saclay, ENSTA ParisTech, 31/05/2016, superv. David Filliat, Javier Ibanez-Guzmann

PhD in progress: Yuxin Chen, Interactive learning of objects and names on a humanoid robot, started oct. 2013 (superv. David Filliat).

PhD in progress: Celine Craye, Curiosity and visual attention for the guidance of an exploration robot, started apr. 2014 (superv. David Filliat).

PhD in progress: Adrien Matricon : Task dependent visual feature selection for optimising and generalizing robotics skills (superv. David Filliat, Pierre-Yves Oudeyer).

PhD in progress: José Magno Mendes Filho, Planning and control of an autonomous AGV in environment shared with humans, started Oct. 2015 (superv. David Filliat and Eric Lucet (CEA))

PhD in progress: Joris Guery, Domain adaptation for visual object recognition, started Oct. 2014 (superv. David Filliat and Bertrand Le Saulx (ONERA))

HdR :Alexander Gepperth, New learning paradigms for real-world environment perception, université Pierre et Marie Curie, 27/6/2016

10.2.3. Juries

Manuel Lopes was in the jury of Ben-Manson Toussaint (2016), Modeling Perceptual-Gestural Knowledge for Intelligent Tutoring Systems, supervised by Vanda Luengo, University of Grenoble, France

David Filliat was in the jury of Isabelle Leang (15/12/2016, Rapporteur) : Fusion en ligne d'algorithmes de suivi visuel d'objet

David Filliat was in the jury of Egor Sattarov (09/12/2016, Examineur) : Etude et quantification de la contribution des systèmes de perception multimodale assistés par des informations de contexte pour la détection et le suivi d'objets dynamiques

Alexander Gepperth was in the jury of Egor Sattarov (09/12/2016, Examineur) : Etude et quantification de la contribution des systèmes de perception multimodale assistés par des informations de contexte pour la détection et le suivi d'objets dynamiques

Alexander Gepperth was in the jury of Thomas Kopinski (12/2/2016, Examineur) : Machine learning method for human-machine interaction

David Filliat was in the jury of Fabrice Mayran de Chamiso (18/11/2016, Examineur) : Navigation exploratoire au long de la vie une approche intégrant planification, navigation, cartographie et localisation pour des robots mobiles disposant de ressources finies

David Filliat was in the jury of Chunlei Yu (15/09/2016, Examineur) : Contribution to evidential models for perception grids Application to intelligent vehicle navigation

David Filliat was in the jury of Hendry Ferreira Chame (10/01/2016, Rapporteur) : Egocentric Representations for Autonomous Navigation of Humanoid Robots

PY. Oudeyer was a member of the PhD juries of Maxime Carrere (Combiner les apprentissages motivés et associatifs, Univ. Bordeaux), Remi Fresnoy (Modélisation de l'activité gestuelle et sélection automatique de feedback pour des environnements interactifs d'apprentissage : application à la calligraphie, UTC Compiègne), Raphaël Rose-Andrieux (Modèle probabiliste hiérarchique de la locomotion bipède).

PY. Oudeyer was a member of the HdR of Alexander Gepperth, "New learning paradigms for real-world environment perception", Ensta ParisTech, Paris.

PY. Oudeyer was a member of the jury for selecting ENS Rennes (France) PhD grants.

10.3. Popularization

10.3.1. Poppy Education

10.3.1.1. Events participation

January 2016, Observation Sequence for students from middle-school (Inria Bordeaux Sud-Ouest): S. Noirpoudre, T. Desprez, M. Demangeat, T. Laine) - We welcomed 5 students from middle-school (14 years old) during a week to discover the working environment and to introduce them to robotics

January 2016, Robot makers' day (Talence): S. Noirpoudre, D. Caselli, T. Desprez - Exhibition stand to show the projet Poppy Education and Poppy robots

January 2016, Training day at Espe de Bordeaux (Ecole supérieure du professorat et de l'éducation): D. Roy, S. Noirpoudre, T. Desprez, M. Demangeat) - Train a group of teachers initiate in programming with the language visual Snap! and to robotics with Poppy Ergo Jr)

January 2016, Robots day (Multimedia library of Talence): P. Rouanet, T. Segonds - Programming workshop with Poppy torso robot

January 2016, Robots day (Multimedia library of Talence): P. Rouanet - A talk to present the platform robotics Poppy through science, art and education.

January 2016, Symposium Didastic-Didapro (Namur): D. Roy - Talk to present Poppy Education

January 2016, Eidos 2016 event (Dax): S. Noirpoudre - A talk to present Poppy Education

March 2016, Education exhibition Educatice-Educatec (Paris) : S. Noirpoudre, D. Roy - Exhibition stand to present the robotics plateforme Poppy and the use in Education (Poppy Education)

March 2016, Training day at Espe de Bordeaux (Ecole supérieure du professorat et de l'éducation): T. Desprez - Train a group of teachers in Snap!

March 2016, SNCEEL (organisation professionnelle de chefs d'établissement d'enseignement libre), Journées Collèges event (Paris), T. Desprez - Talk to present Poppy project and the pedagogical activities

April 2016, Connect thouars event (Talence): T. Desprez, S. Noirpoudre, M. Demangeat - Exhibition stand to present the project Poppy Education and workshop animation for kids (programming of Ergo in Snap!)

April 2016, Rob'o d'Evian: D. Roy (Evian) - Talk to present Poppy Education

May 2016, Robotics and Education days (ENS Lyon): D. Roy, S. Noirpoudre - Talk to present Poppy project and the pedagogical activities

May 2016, Bordeaux Geek Festival (Bordeaux): M. Demangeat, T. Desprez - Exhibition stand to show/present the robotics platform Poppy

May 2016, Forum des Nouvelles Initiatives de Médiation Scientifique (Bordeaux): D. Roy - Talk to present the project Poppy Education

May 2016, Forum des Nouvelles Initiatives de Médiation Scientifique (Bordeaux): T. Desprez, S. Noirpoudre - Exhibition stand to present the project Poppy Education and show the robots (real demonstrations) and pedagogical activities

May 2016, Visit of teachers of Espe Aquitaine (Inria - Bordeaux Surd-Ouest): S. Noirpoudre, D. Roy - Visit of the research center and presentation of Poppy Education project and to the robotic kits (25 teachers)

June 2016, Symposium Education and Robotics (Talence): D. Roy, T. Desprez - Talk to present Poppy Education project (purpose, pedagogical activities and the results)

June 2016, Symposium Education and Robotics (Talence): S. Noirpoudre - Exhibition stand to show Poppy Education project (demonstrations)

August 2016, Université d'été Ludovia (Ax-les-Thermes): P. Rouanet, M. Demangeat - Exhibition stand Poppy Education during 3 days in partnership with l'Académie de Bordeaux

August 2016, Université d'été Ludovia (Ax-les-Thermes): D. Roy, P. Rouanet, M. Demangeat - Workshop / presentation / demonstration of Poppy Education as part of the ExplorCamps.

October 2016, Coding Pi Science Day (CERN close to Geneva): S. Noirpoudre, T. Segonds - Conference to present the pedagogical robotic kit Poppy Ergo Jr

October 2016, Coding Pi Science Day (CERN close to Geneva): S. Noirpoudre, T. Segonds - Robotics workshop, one day to build and program a robot (30 participants)

October 2016, Fête de la science (Inria Bordeaux Sud-Ouest): S. Noirpoudre - 8 programming workshop in 2 days (with middle school students) using Snap! and the robot Poppy Ergo Jr

November 2016, Erasmus project "ICT WORLD : Imaging, Coding, Transforming and Modeling the World" (Inria Bordeaux Sud-Ouest): S. Noirpoudre, programming workshop using Snap! and the robot Poppy Ergo Jr (35 students and 14 teachers)

Novembre 2016, Inria Learning Lab (Paris): D. Roy - Presentation of Poppy Education

December 2016, Observation Sequence for Grade 3 Students (Inria Bordeaux Sud-Ouest): S. Noirpoudre, T. Desprez) - We welcomed 2 students from middle-school during a week to discover the working environment and to introduce them to robotics

10.3.1.2. Training and meeting

- January 2016, Meeting with teachers partners of the Poppy Education: Poppy Education project team - Talking about pedagogical activities and robots availabilities
- March 2016, Meeting with teachers partners of Poppy Education, Poppy Education project Team - Feedback and presentations on pedagogical activities and the use of robots in the classroom
- May 2016, Meeting with teachers partners of Poppy Education, Poppy Education project team - Feedback on pedagogical activities and the use of robots in the classroom
- May 2016, Train Inria workers (from scientific mediation), S. Noirpoudre - Learn how to present the Poppy project
- June 2016, Train Canope 33 workers, S. Noirpoudre - Programming the robot Ergo Jr using Snap!
- October 2016, Meeting with teachers partners of the Poppy Education project: Poppy Education project team - Presentation of the progress of the year and presentations of pedagogical activities
- November 2016, Train new teachers partners of Poppy Education: S. Noirpoudre - Building and programming the robot Poppy Ergo Jr

10.3.2. Inirobot

10.3.2.1. Events participation

January 2016, Training day at Espe de Bordeaux (Ecole supérieure du professorat et de l'éducation): D. Roy, S. Noirpoudre, T. Desprez, M. Demangeat) - Train a group of teachers initiate in programmation with the Inirobot kit.

January 2016, Symposium Didastic-Didapro (Namur): D. Roy - Talk to present Inirobot kit.

March 2016, Education exhibition Educacice-Educatec (Paris) : S. Noirpoudre, D. Roy - Exhibition stand to present the robotics kit Inirobot.

March 2016, SNCEEL (organisation professionnelle de chefs d'établissement d'enseignement libre), Journées Collèges event (Paris), T. Desprez - Talk to present Inirobot kit.

April 2016, Rob'o d'Evian: D. Roy (Evian) - Talk to present Inirobot kit.

May 2016, Robotics and Education days (ENS Lyon): D. Roy, S. Noirpoudre - Talk to present Inirobot kit.

May 2016, Forum des Nouvelles Initiatives de Médiation Scientifique (Bordeaux): D. Roy - Talk to present inirobot kit.

June 2016, Symposium Education and Robotics (Talence): D. Roy - Talk to present Inirobot kit.

August 2016, Université d'été Ludovia (Ax-les-Thermes): P. Rouanet, M. Demangeat - Exhibition stand Inirobot during 3 days in partnership with l'Académie de Bordeaux

August 2016, Université d'été Ludovia (Ax-les-Thermes): D. Roy, P. Rouanet - Workshop / presentation / demonstration of Inirobot kit as part of the ExplorCamps.

August 2016, Université d'été Ludovia (Ax-les-Thermes): D. Roy wins Ludovia Prize. <http://ludovia.org/2016/coups-de-coeur-de-ludovia/>

September 2016, Colloque sur les contenus périscolaires (Artigues-près-Bordeaux): D. Roy - inirobot (organized by Senator Françoise Cartron)

October 2016, Journées APMEP (Lyon): J. Rivet, G. Lassus, members of Poppy Education teachers team - workshops on Inirobot and Poppy Education, organized by D. Roy

October 2016, Journées APMEP (Lyon): D. Roy wins Hoquenghem Prize. <https://www.inria.fr/centre/bordeaux/actualites/didier-roy-recoit-le-prix-serge-hocquenghem>

Novembre 2016, Inria Learning Lab (Paris): D. Roy - Presentation of Inirobot kit.

10.3.2.2. Training and meeting

- Février 2016, French Senat (Paris), audition by Senator Françoise Cartron for educational activities : D. Roy - presentation / demonstration of Inirobot kit .
- October 2016, Robotics for education Training week "Graines de sciences": D. Roy (Fondation "La Main à la Pâte", Marseille CIRM)

10.3.3. KidBreath

February 11th 2016, 2nd Meeting for Aquitaine and Euskadi companies in Biology and Health: A. Delmas - Poster presentation of KidBreath project.

September 16th to 18th 2016, Hackathon of innovation in pulmonary diseases Respirhacktion: A. Delmas - Oral presentation and project development in hackathon.

October 5th to 7th 2016, 5th Conference in Health Ergonomics and Patient Safety: A. Delmas - Poster presentation of KidBreath project [102],

November 16th 2016, Learning Lab day: A. Delmas, B. Clément, P-Y. Oudeyer, D. Roy - Oral presentation of Flowers projects linked to Education.

December 2nd to 3rd 2016, 5th edition of Serious Games in Medicine Conference: A. Delmas - Oral presentation of KidBreath project

10.3.4. Other

PY Oudeyer wrote popular science articles about computer science, artificial intelligence and robotics, and gave several interviews in the general press and at radio and TV programs: see <http://www.pyoudeyer.com/popular-science/> and <http://www.pyoudeyer.com/press/> and has been maintaining a youtube channel showing popular science videos https://www.youtube.com/channel/UC7QuDF8AaE6mqEM9W_S30RA/featured

D. Roy is co-organiser of R2T2 International Mission with EPFL and ESPE Martinique: Remote Robotics programming with children. <https://www.thymio.org/en:thymio-r2t2>

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Major publications by the team in recent years

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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

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- 3.4.7. - Kernel methods
- 3.4.8. - Deep learning
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 - 5.3.2. - Sparse modeling and image representation
 - 5.3.3. - Pattern recognition
 - 5.3.5. - Computational photography
- 5.7. - Audio modeling and processing
 - 5.7.3. - Speech
 - 5.7.4. - Analysis
- 5.9. - Signal processing
 - 5.9.2. - Estimation, modeling
 - 5.9.3. - Reconstruction, enhancement
 - 5.9.5. - Sparsity-aware processing

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- 2. - Health
 - 2.2. - Physiology and diseases
 - 2.2.1. - Cardiovascular and respiratory diseases
 - 2.2.6. - Neurodegenerative diseases
- 3. - Environment and planet
 - 3.3. - Geosciences
 - 3.3.2. - Water: sea & ocean, lake & river
 - 3.3.4. - Atmosphere

1. Members

Research Scientists

- Hussein Yahia [Team leader, Inria, Researcher, HDR]
- Nicolas Brodu [Inria, Researcher]
- Khalid Daoudi [Inria, Researcher]

PhD Students

- Camila Artana [Univ. Paris VI]
- Anass El Aouni [co-supervision, Rabat & Bordeaux University]
- Gopal Phartiyal [IIT Roorkee, from Aug 2016 until Oct 2016]
- Hicham Badri [co-supervision, Rabat & Bordeaux University, with *EyeEm* company until Aug 2016]

Post-Doctoral Fellows

- Guillaume Attuel [Inria, until Aug 2016]
- Oriol Pont [INP Toulouse, until Nov 2016]

Binbin Xu [Bâle University from Aug 2016]

Visiting Scientist

Dharmendra Singh [IIT Roorkee, until Jul 2016]

Administrative Assistant

Cecile Boutros [Inria]

2. Overall Objectives

2.1. Overall Objectives

Singularity exponent A measure of the unpredictability around a point in a complex signal. Based on local reconstruction around a point, singularity exponents can be evaluated in different ways and in different contexts (e.g. non-localized, through the consideration of moments and structure functions, through the computation of singularity spectra). In GEOSTAT we study approaches corresponding to *far from equilibrium* hypothesis (e.g. microcanonical) leading to geometrically localized singularity exponents.

Singularity spectrum The mapping from scaling exponents to Hausdorff dimensions. The singularity spectrum quantifies the degree of nonlinearity in a signal or process, and is used to characterize globally the complexity of a signal.

Most Singular Manifold The set of most unpredictable points in a signal, identified to the set of strongest transitions as defined by the singularity exponents. From that set the whole signal can be reconstructed.

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.

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 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 determination of the changes a physical system undergoes under different distance scales. As a consequence, different macroscopic phenomena displaying a multiscale structure (and their acquisition in the form of complex signals) can be grouped into different sets of universality classes.

Every signal conveys, as a measure experiment, information on the physical system whose signal is an acquisition. As a consequence, it seems therefore natural that signal analysis or compression makes 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 problems.

Physics of turbulence also introduces phenomenological approaches based on singularity exponents. Energy cascades are indeed closely related to singular geometrical sets defined randomly. At these structures' scales, information of the process is lost by dissipation. However, all the cascade is encoded in the singular sets. How do these structures organize in space and time, in other words, how do the entropy cascade itself? To unify these two notions, a description in term of free energy of a generic physical model is possible, such as an elastic interface model in a random nonlinear energy landscape: this is for instance the correspondance between compressible stochastic Burgers equation and directed polymers in a disordered medium. Typical of such systems, degrading transition indicates that each singularity can be understood as a transition between two metastable states. Each of these transitions marks large fluctuations of the system which visits randomly the minima of the free energy. A signal which is an acquisition of such systems displays statistical properties characteristic of different classes, and the nature of noise is determinant. In particular, the dynamics enters a so-called Griffiths phase if for example noise gets structured like a hierarchical network, connected on long range distances, locally recursive, and randomly sparse. In such a context, phenomenologies related to cascades and multi-affine intermittence are present. As a typical example, in the study of cardiac dynamics (a subject that gets interest among statistical physicists) an effective model belonging to a similar category can be contemplated. In such model, an explicitly broken symmetry is restored spontaneously. This is a consequence from the existence of an abelian symmetry of topological solutions, where these topological solutions are fronts excited by limiting conditions. A statistical gauge is the signature of a nonlinear intrinsic disorder which emerges for certain regions of parameter space. Such areas have a *vitrous* nature (Griffiths). The gauge is responsible for jumps between different metastable states and allows to recover singularity exponents of acquired signals. Conversely, the exploration of the phase space in such models can lead to a possible "testing" of the measured system through the computation of singularity exponents and the determination of the nature of intrinsic noise. From these considerations and in a heuristical framework, one sees that the recovering of a *semantics* in a measured signal can be contemplated.

GEOSTAT is a research project in **nonlinear signal processing** which develops on these considerations: it considers the signals as the realizations of complex dynamic systems. The driving approach is to understand 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 is related to the effective presence of a multiscale hierarchy, 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 understanding their dynamical properties and, as a consequence, their analysis. We use this approach to derive novel solution methods for **super-resolution** and data fusion in Universe Sciences acquisitions [10]. Another example can be found heartbeat signal analysis, where singularity exponents help understand the distribution of activation points in a signal during episodes of atrial fibrillation. 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. Research in GEOSTAT is structured in two parts:

- Theoretical and methodological aspects.
- Applicative aspects which encompass biomedical data (heartbeat signal analysis, biomedical applications in speech signal analysis) and the study of universe science datasets.

The theoretical objectives are:

- multiscale description in terms of multiplicative cascade (essential in the characterization of turbulent systems).
- Excitable systems (cardiac electrophysiology): study of intermittency phenomena.

The methodological tools used in reaching these objectives place GEOSTAT at the forefront of nonlinear signal processing and complex systems. We cite: singularity exponents [48], [7] [11], how these exponents can be related to *sparse representations* with reconstruction formulae [13] [49], [5] and super-resolution in Oceanography and Earth Observation [10], [2], comparison with embedding techniques, such as the one provided by the classical theorem of Takens [46], [38], the use of Lyapunov exponents [34], how they are related to intermittency, large deviations and singularity exponents, various forms of entropies, persistence along the scales, *optimal wavelets* [6], comparison with other approaches such as sparse representations and compressive sensing [<https://hal.inria.fr/tel-01239958>], and, above all, **the ways that lead to effective numerical and high precision determination of nonlinear characteristics in real signals**. Presently GEOSTAT explores new methods for analyzing and understanding complex signals in different applicative domains [47]. Derived from ideas in Statistical Physics, the methods developed in GEOSTAT provide new ways to relate and evaluate quantitatively the *local irregularity* in complex signals and systems, the statistical concepts of *information content* and *most informative subset*. As a result, GEOSTAT is aimed at providing *radically new approaches* to the study of signals acquired from different complex systems (their analysis, their classification, the study of their dynamical properties etc.). A common characteristic of these signals, which is related to *universality classes* [41] [42] [39], being the existence of a *multiscale organization* of the systems. For instance, the classical notion of *edge* or *border*, which is of multiscale nature, and whose importance is well known in Computer Vision and Image Processing, receives profound and rigorous new definitions, in relation with the more physical notion of *transition* and fits adequately to the case of chaotic data. The description is analogous to the modeling of states far from equilibrium, that is to say, there is no stationarity assumption. From this formalism we derive methods able to determine geometrically the most informative part in a signal, which also defines its global properties and allows for *compact representation* in the wake of known problematics addressed, for instance, in *time-frequency analysis*. It appears that the notion of *transition front* in a signal is much more complex than previously expected and, most importantly, related to multiscale notions encountered in the study of nonlinearity [44]. For instance, we give new insights to the computation of dynamical properties in complex signals, in particular in signals for which the classical tools for analyzing dynamics give poor results (such as, for example, correlation methods or optical flow for determining motion in turbulent datasets).

3. Research Program

3.1. Multiscale description in terms of multiplicative cascade

GEOSTAT is studying complex signals under the point of view of methods developed in *statistical physics* to study complex systems, with a strong emphasis on multiresolution analysis. Linear methods in signal processing refer to the standard point of view under which operators are expressed by simple convolutions with impulse responses. Linear methods in signal processing are widely used, from least-square deconvolution methods in adaptive optics to source-filter models in speech processing. 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 (Detrended Fluctuation Analysis), Time-frequency analysis, variations on curvelets [45] 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. One 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 [36], [33], [50], [40]. Some quantities related to nonlinearity, such as Lyapunov exponents, Kolmogorov-Sinai entropy etc. can be computed at least in the phase space [34]. 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 [46] about strange attractors in turbulence has motivated the determination of discrete dynamical systems associated to time series [38], and consequently 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. Time-frequency analysis [35] and multiscale/multiresolution are the subjects of intense research and are profoundly reshaping the analysis of complex signals by nonlinear approaches [32], [37]. 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 and deduce from that singularity exponents [11] [7]. We are working on:

- the determination of quantities related to universality classes,
- the geometric localization of multiscale properties in complex signals,
- cascading characteristics of physical variables.

The alternative approach taken in GEOSTAT is microscopical, or geometrical: the multiscale structures which have their "fingerprint" in complex signals are being isolated in a single realization of the complex system, i.e. using the data of the signal itself, as opposed to the consideration of grand ensembles or a wide set of realizations. This is much harder than the ergodic approaches, but it is possible because a reconstruction formula such as the one derived in [47] is local and reconstruction in the signal's domain is related to predictability. This approach is analogous to the consideration of "microcanonical ensembles" in statistical mechanics.

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, 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. In GEOSTAT, the approach to singularity exponents is done within a microcanonical setting, which can interestingly be compared with other approaches such that wavelet leaders, WTMM or DFA. During the past decades, classical approaches (here called "canonical" because they use the analogy taken from the consideration of "canonical ensembles" in statistical mechanics) 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 $\hat{\beta} = 1/\mathcal{T}$, then the scaling exponents

associated to moments of intensive variables $p \rightarrow \tau_p$ 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.

The singularity exponents belong to a universality class, independently of microscopic properties in the phase space of various complex systems, and beyond the particular case of turbulent data (where the existence of a multiscale hierarchy, of multifractal nature, can be inferred directly from physical considerations). They describe common multiscale statistical organizations in different complex systems [44], and this is why GEOSTAT is working on nonlinear signal processing tools that are applied to very different types of signals.

For example we give some insight about the collaboration with LEGOS Dynbio team⁰ about high-resolution ocean dynamics from microcanonical formulations in nonlinear complex signal analysis. Indeed, synoptic determination of ocean circulation using data acquired from space, with a coherent depiction of its turbulent characteristics remains a fundamental challenge in oceanography. This determination has the potential of revealing all aspects of the ocean dynamic variability on a wide range of spatio-temporal scales and will enhance our understanding of ocean-atmosphere exchanges at super resolution, as required in the present context of climate change. We show that the determination of a multiresolution analysis associated to the multiplicative cascade of a typical physical variable like the Sea Surface Temperature permits an *optimal inference* of oceanic motion field across the scales, resulting in a new method for deriving super resolution oceanic motion from lower resolution altimetry data; the resulting oceanic motion field is validated at super resolution with the use of Lagrangian buoy data available from the Global Drifter Program⁰. In FDT, singularity exponents range in a bounded interval: $]h_\infty, h_{\max}[$ with $h_\infty < 0$ being the most singular exponent. Points \mathbf{r} for which $h(\mathbf{r}) < 0$ localize the stongest transitions in the turbulent fluid, where an intensive physical variable like sea surface temperature behaves like $1/|\mathbf{r}|^{h(\mathbf{r})}$. The links between the geometrically localized singularity exponents, the scaling exponents of structure functions, the multiplicative cascade and the multiscale hierarchy \mathcal{F}_h is the following:

$$\left\{ \begin{array}{l} \mathcal{F}_h = \{\mathbf{r} \mid h(\mathbf{r}) = h\} \\ D(h) = \dim \mathcal{F}_h \\ \tau_p = \inf_h \{ph + 3 - D(h)\} \\ D(h) = \inf_p \{ph + 3 - \tau_p\} \end{array} \right. \quad (2)$$

Let $\mathfrak{S}(\mathbf{x})$ be the bidimensionnal signal recording, for each sample point \mathbf{x} representing a pixel on the surface of the ocean of given resolution, the sea surface temperature (sst). To this signal we associate a measure μ whose density w.r.t Lebesgue measure is the signal's gradient norm, and from which the singularity exponents are computed [6]. It is fundamental to notice here that, contrary to other types of exponents computed in Oceanography, such as Finite Size Lyapunov exponents, singularity exponents are computed at instantaneous time, and do not need time series.

Having computed the singularity exponents at each point of a SST signal, a microcanonical version of the multiplicative cascade associated to the scaling properties of the sst become available. The idea of the existence of a geometrically localized multiplicative cascade goes back to [43]. The multiplicative cascade, written pointwise, introduces random variables $\eta_{l'/l}(\mathbf{x})$ for $0 < l' < l$ such that

$$\mathcal{T}_\psi \mu(\mathbf{x}, l') = \eta_{l'/l}(\mathbf{x}) \mathcal{T}_\psi \mu(\mathbf{x}, l) \quad (3)$$

in which the equality is valid pointwise and not only in distribution. Any mother wavelet ψ such that the process $\eta_{l'/l}(\mathbf{x})$ is independant of $\mathcal{T}_\psi \mu(\mathbf{x}, l')$ is called an optimal wavelet: it optimizes inference of physical variables across the scales and consequently describes the multiplicative cascade at each point \mathbf{x} in the signal domain. The injection variables $\eta_{l'/l}(\mathbf{x})$ are indefinitely divisible: $\eta_k(\mathbf{x})\eta_{k'}(\mathbf{x}) \doteq \eta_{kk'}(\mathbf{x})$. It is possible to optimize cross-scale inference of physical variables by considering a *multiresolution analysis*

⁰<http://www.legos.obs-mip.fr/recherches/equipements/dynbio>.

⁰<http://www.aoml.noaa.gov/phod/dac/index.php>.

associated to a discrete covering of the "space-frequency" domain. Denoting as usual $(V_j)_{j \in \mathbb{Z}}$ and $(W_j)_{j \in \mathbb{Z}}$ the discrete sequence of approximation and detail spaces associated to a given scaling function, and denoting by $\psi \in L^2(\mathbb{R}^2)$ a wavelet which generates an Hilbertian basis on each detail space W_j , it is known that the detail spaces encode borders and transition information, which is ideally described in the case of turbulent signals by the singularity exponents $\mathbf{h}(\mathbf{x})$. Consequently, a novel idea for super-resolution consists in computing a multiresolution analysis on the signal of singularity exponents $\mathbf{h}(\mathbf{x})$, and to consider that the detail information coming from spaces W_j is given the signal $\mathbf{h}(\mathbf{x})$. The associated orthogonal projection $\pi_j : L^2(\mathbb{R}^2) \rightarrow W_j$ defined by $\pi_j(\mathbf{h}) = \sum_{n \in \mathbb{Z}} \langle \mathbf{h} | \psi_{j,n} \rangle \psi_{j,n}$ is then used in the reconstruction formula for retrieving a physical variable at higher resolution from its low resolution counterpart. If $\mathfrak{S}(\mathbf{x})$ is such a variable, we use a reconstruction formula: $A_{j-1}\mathfrak{S} = A_j\mathfrak{S} + \pi_j(\mathbf{h})$ with $A_j : L^2(\mathbb{R}^2) \rightarrow V_j$ is the orthogonal projection on the space V_j (approximation operator) and π_j is the orthogonal projection on the detail spaces W_j associated to the signal of singularity exponents $\mathbf{h}(\mathbf{x})$. Validation is performed using Lagrangian buoy data with very good results [10]. We have realized a demonstration movie showing the turbulent ocean dynamics at an SST resolution of 4 km computed from the SST microcanonical cascade and the low-resolution GEKCO product for the year 2006 over the southwestern part of the Indian Ocean. We replace the missing data in the SST MODIS product (clouds and satellite swath) by the corresponding data available from the Operational SST and Sea Ice Analysis (OSTIA) provided by the Group for High-Resolution SST Project [11], which, however, is of lower quality. Two images per day are generated for the whole year of 2006. The resulting images show the norm of the vector field in the background rendered using the line integral convolution algorithm. In the foreground, we show the resulting vector field in a linear gray-scale color map. See [link to movie \(size: 800 Mo\)](#).

3.2. Excitable systems and heartbeat signal analysis

We are developing novel approaches to heartbeat signal analysis for understanding chronic atrial fibrillation. The noisy aspect of data recorded by electrodes, on the inner surface of human atria during episodes of atrial fibrillation, exhibit intriguing features for excitable media. Instead of phase chaos as typically expected, it shares many common traits of non-equilibrium fluctuations in disordered systems or strong turbulence. To assess those peculiar observations we investigate a *synaptic plasticity* that affects conduction properties. Electrical synapses comprise many different kinds of connexins, which may be affected by diverse factors, so we use a generic approach. Slight detuning of their linear response leads to an instability of the modulating agents, here an excess charge. Acting on slow time scales of repolarisation, it is understood as *collective modes* propagating through and retroacting on each synapse: the medium is *desynchronised*. It is not a syncytium. We propose to associate transient states with a phenomenon called *electrical remodelling*, which has not received any accepted description thus far. Moreover, from the properties of the model it is possible to start exploring phase space. Transitions between different regimes could help decipher stages in the evolution of the disease from acute to chronic, one main goal of cardiovascular research.

Theoretically, a myocardium is an excitable tissue acting under normal circumstances as a functional syncytium of myocardial cells. Models of excitability for the heart are reaction-diffusion systems describing the propagation of electric pulses called action potentials similarly to models for axons. Reaction results from ionic exchange cycles between the cytoplasm of excitable cells and their extra-cellular medium, when initiated by a stimulus above some threshold. Pulses are robust topological structures.

Considering the stable fixed point as a phase resetting state, chaos may arise in spatio-temporal sequences. This is the paradigm for cardiac fibrillation. But, it is incompatible with the following observations: the distributions of amplitudes all collapse on a scaling function G . We map exponents on data patients provided by IHU LIRYC showing non-universal properties. Singular exponents are observed with consistent Hausdorff dimension of sets $D(h)$. Negative contribution is high, suggesting an underlying multiplicative process.

Excess charge in cells like of Ca may perturb the dynamics of synapses. We consider a physiologically plausible linear response of synapses to the electro-chemical potential. This response is unknown as of today. The new dynamics may interact with excitability. It has the specific form of a Rayleigh instability.

Cycles become retarded or advanced. Hopf bifurcation and chaos are allowed creating EADs (Early After Depolarization). Regarding propagation, pulses are pinned and released on a chaotic background. Cycle modulations create defects via facilitation through the third dimension. Defects proliferate creating a glassy phase, which back-scatter fronts in 1D and roughens them in 2D. Further effective inhibitor diffusion splits them. Electrical remodelling is here the abnormal modification of the cell dynamics without any membrane alteration.

There are features of Self Organized Criticality (SOC) in large regions of phase space. Pulses have a phase and propagate on a random medium. For instance one paradigm we investigate would be:

$$\partial_t \theta + \sin(\theta + \tilde{\phi}) = \Omega + \partial_{xx} \theta \quad (4)$$

(θ : phase of activation front, Ω : tachycardia frequency, $\tilde{\phi}$: phase perturbation). Randomness reactualises non-linearly, which tells that the noise is quenched and reset. For instance in 1 + 1D, spatio-temporal maps look very much like optimal directed paths along diagonals. In 1 + 2D, we are guessing that pulses do propagate in the (q)KPZ universality class, just as the remodelling front does. This class is only fractal, but together with large deviations of the fluctuations, it may be consistent with a multi-affine process. Physiologically, one interesting bonus is the interpretation of non-reentrant Tachycardia as dislocation patterns slowly evolving.

3.3. Speech analysis

Our research in speech processing focus on the development of novel nonlinear analysis methods for the characterization and classification of pathological and affective speech. For the latter, classical linear methods do not generally capture the nonlinearity, aperiodicity, turbulence and noise that can be present in pathological voices. We thus aim to design and extract new features that allow better characterization/classification of such voices, while being easy to interpret by clinicians. For the former, recent research have shown that the voice source signal information allow significant improvement of speech emotion detection systems. Our goal is to develop novel nonlinear techniques to extract relevant voice source features and to design efficient machine learning algorithms for robust emotion classification.

4. Highlights of the Year

4.1. Highlights of the Year

- N. Brodu is joining GEOSTAT as a research associate (2016).
- K. Daoudi has been invited to the Senate on June 20th 2016 to accompany BatVoice which was finalist of the 2016 edition of “Tremplin Entreprises”.

4.1.1. Award

Hicham Badri is winning the AFRIF PhD price 2015 for his PhD *Sparse and Scale-Invariant Methods in Image Processing* [<https://hal.inria.fr/tel-01239958>].

5. New Software and Platforms

5.1. Flux

KEYWORDS: Signal - Signal processing

SCIENTIFIC DESCRIPTION

Flux is a package consisting of the Microcanonical Multiscale Formalism for 1D, 2D 3D and 3D+t general signals.

FUNCTIONAL DESCRIPTION Flutex is a C++ library developed under Gforge. Flutex is a library in nonlinear signal processing. Flutex is able to analyze turbulent and natural complex signals, Flutex is able to determine low level features in these signals that cannot be determined using standard linear techniques.

- Participants: Rémi Paties and Hussein Yahia
- Contact: Hussein Yahia
- URL: <https://geostat.bordeaux.inria.fr/index.php/downloads.html>
- URL: <https://bil.inria.fr/fr/software/view/2113/tab>

5.2. FluidExponents

- Participants: Hussein Yahia and Antonio Turiel
- Contact: Hussein Yahia
- URL: <https://bil.inria.fr/fr/software/view/336/tab>

6. New Results

6.1. Automatic segmentation of activation periods in an electrogram during atrial fibrillation

Participants: G. Attuel, H. Yahia.

Experiments show that the multiscale properties displayed in signals recording the electrical activity of the heart during (atrial) fibrillation are of the type *out of equilibrium dynamics*. These dynamics have common features, possibly shared by "subclasses": " $1/f$ power spectrum", large probability laws for the distributions of the amplitude increments, multifractal spectra. Theoretically these dynamics are at least the result of a competition between elastic energies and disorder, which leads to the emergence of collective behaviours. Mathematically, the universality classes involved are not those corresponding to the central limit theorem, but generalize it in its more elaborated forms (Levy & Gnedenko). A class has recently been described completely: directed polymers on a random medium. Scaling exponents are known, together with the fluctuations' statistics. Large deviation theory plays a central role. The fixed point of the associated dynamics is that of KPZ (Kardar-Parisi-Zhang). We have indications that heartbeat dynamics in episodes of atrial fibrillation belongs to that class. In such a context, the questions raised relate to finite size effects when asymptotic convergence is slow. From an experimental point of view, the problem of determining universality classes is very hard. However, it is possible to formulate hypothesis on the universality class so as to extract important information from acquisition signals. A good *modus operandi* consists in using key properties of a model stated *a priori*, to combine them with experimental signal analysis in order to produce *a posteriori* characteristics of interest. Last year, we developed the first model of cardiac dynamics compatible with observed data. The model allows us to test the efficiency of a combined methodology using singularity exponents and Bayesian analysis. This has led us to a first automatic method able to identify periods of cardiac activity and make the distinction with measure noise. From this, the fine automatic determination of activity periods become tractable. This will lead to an automatic quantitative determination of fragmentation, hence opening the way for a determination of universality classes. We illustrate some steps in the figures below.

Publications: [24], [23], [25]

6.2. Pathological voice classification

Participants: K. Daoudi, N. Brodu.

We propose a fully reproducible speech-based technique for objective differential diagnosis between progressive supranuclear palsy (PSP) and multiple system atrophy (MSA). Our technique yields a classification mean accuracy of 86.1% which is a significant improvement as compared to a recent pioneer study on this task. We also show that information extracted through a variety of speech tasks can be used to estimate the degree of Parkinson's disease severity.

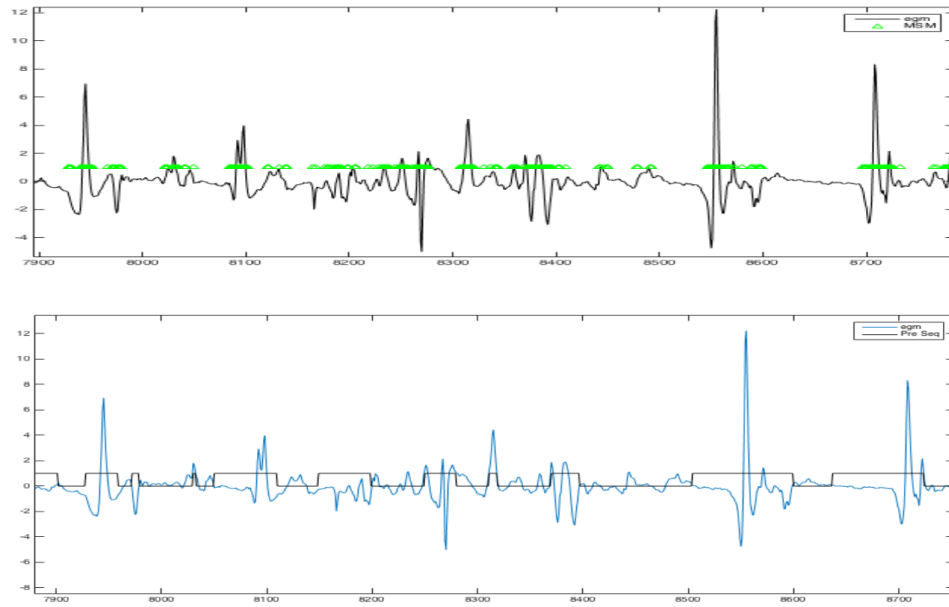


Figure 1. Egm during fibrillation (in black). Density of the most singular manifold (in green). Result of a 2-state HMM (in blue).

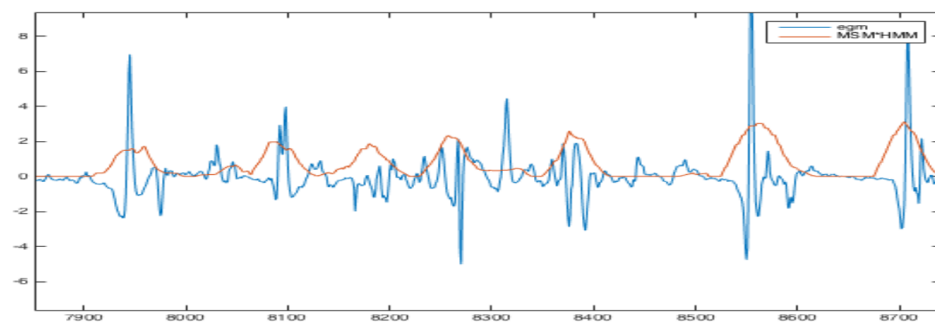


Figure 2. Egm during fibrillation (in blue). Signal of activation probability computed with the result of an HMM and the singularity density (in red).

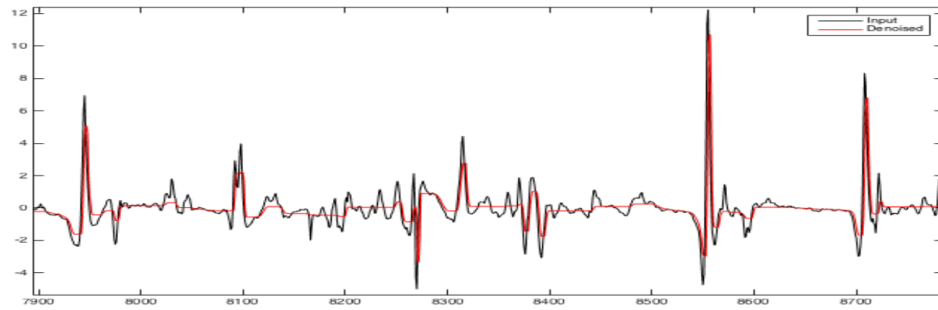


Figure 3. Egm during fibrillation (in black). Signal denoised (norm L^p) (in red).

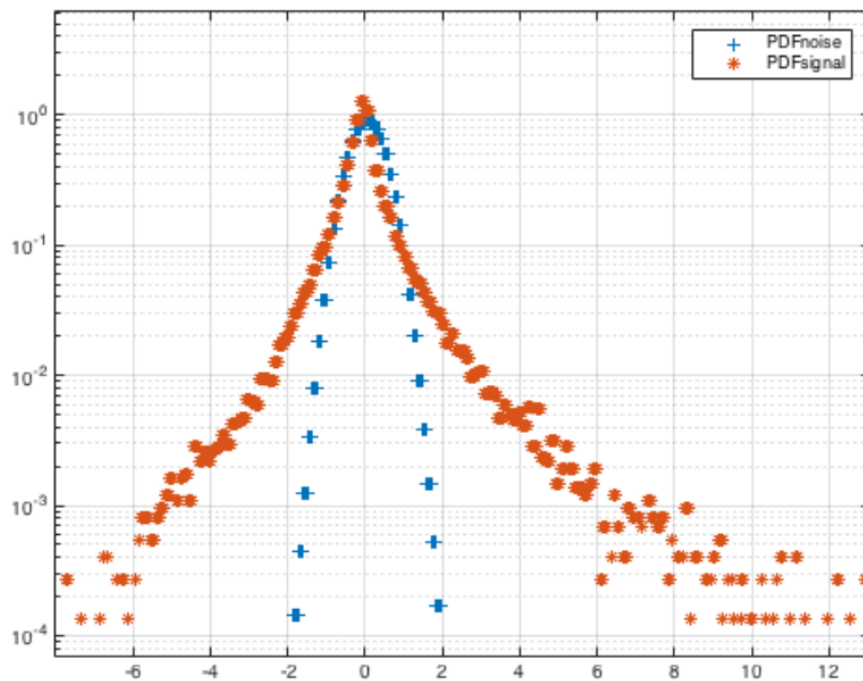


Figure 4. Probability distribution of estimated noise (in blue). Distribution of estimated active dynamics (in red).

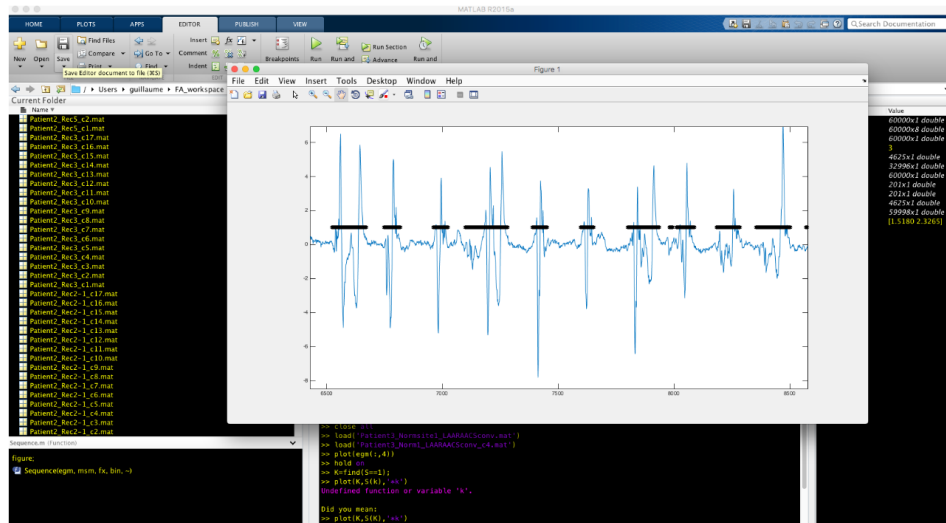


Figure 5. Snapshot of the software (written partially in Matlab and which makes use of FluidExponents). The image shows the result of sequencing, with average confidence level, of a real egm

Publications: [18], [20], [<https://hal.inria.fr/hal-01360038>].

6.3. Temporal evolution of coastal upwelling

Participants: A. El Aouni, K. Minaoui, A. Tamim, K. Daoudi, H. Yahia, A. Atillah, D. Aboutajdine.

We present a new methodology to derive rigorous SST-based coastal upwelling index for the purpose of conducting a seasonal variability of upwelling area along the Moroccan Atlantic coast. The method is based on the scientific knowledge of upwelling area and its spatial distribution provided by expert oceanographers. The latter consists in automatically identify and extract the region covered by the upwelling waters in the coastal ocean of Morocco using the Fuzzy c-means algorithm and finding regions of homogeneous pixels. Then Region Growing process is used to filter out the remaining noisy structures in the offshore waters. The methodology is used to provide a statistical view of the spatial and temporal variability of the Moroccan upwelling activity. The relevance of the proposed Coastal Upwelling Index (CUI) is evaluated by an oceanographer using 86 8-days sea surface temperature images and it is shown to be superior to that of the standard upwelling index.

Publication: [<https://hal.inria.fr/hal-01424036>].

6.4. Non-local and low rank approach for integrability

Participants: H. Badri, H. Yahia.

A formulation is proposed which consists in a sparse gradient data-fitting term to handle outliers together with a gradient-domain non-local low-rank prior.

Publication: [15].

6.5. Low-Rankness transfer for realistic denoising

Participants: H. Badri, H. Yahia, D. Aboutajdine.

Current state-of-the-art denoising methods such as non-local low-rank approaches are mainly tuned to work with uniform Gaussian noise corruption and known variance, which is far from the real noise scenario. Noise level estimation is already a challenging problem and denoising methods are quite sensitive to this parameter. Moreover, these methods are based on shrinkage models that are too simple to reflect reality, which results in over-smoothing of important structures such as small-scale text and textures. We propose a new approach for more realistic image restoration based on the concept of low-rankness transfer (LRT).

Publication: [14].

6.6. Multiscale methods for Earth Observation data

Participants: H. Yahia, N. Brodu, V. Garçon, J. Sudre, S. Kumar Maji, D. Singh, K. Daoudi, D. Aboutajdine. Earth observation data of different kinds are tested for super-resolution or analysis using the multiscale approaches developed in the team. This paragraph is mainly concerned with the publications of last year results.

Publications: [<https://hal.inria.fr/hal-01254482>], [<https://hal.archives-ouvertes.fr/hal-01425021>], [<https://hal.inria.fr/hal-01287182>], [<https://hal.inria.fr/hal-01287181>], [<https://hal.inria.fr/hal-01426666>], [16], [27], [30], [28], [31], [21].

6.7. Signal analysis of ultrasonic dental response

Participants: H. Yahia, G. Rosi, S. Jaffard, S. Seuret.

The long-term success of a dental implant is related to the properties of the bone-implant interface. It is important to follow the evolution of bone remodeling phenomena around the implant. Methods based on ultrasound wave propagation were already successfully used by collaborators, in the qualitative and quantitative evaluation of primary and secondary stability of dental implants. Results, numerical and experimental, are analysed with signal processing tools based on multifractal methods. Analysis of the first results shows that these methods are potentially efficient in this case because they can explore and exploit the multi-scale structure of the signal.

Publication: [22].

6.8. Complexity in Electrophysiological Dynamics

Participants: O. Pont, H. Yahia, B. Xu.

Action potentials play an important role in the dynamics of cell-cell communication and they are thus of key relevance in neural tissues. We show that typical real-world electrophysiological signals, with smooth deviations from harmonicity, are typically well described with just the first few terms and result in a rather compact, sparse representation. In particular, we have done an analysis of FitzHugh-Nagumo impulse trains; we have found that 3 anharmonic terms reconstruct better than an equivalent 8-term Fourier representation, with less than half the PSNR and no artifacts from Gibbs phenomenon.

Publication: [17].

6.9. Nonlinear trend removal and heart rate variability analysis

Participants: B. Xu, R. Dubois, O. Pont, H. Yahia.

Publication: [29].

7. Bilateral Contracts and Grants with Industry

7.1. Carnot-Inria

GeoStat has been granted in 2015 a Carnot-Inria project to fund a 1 year engineer to develop a prototype of a speech emotion detection system. This contact, led by K. Daoudi, is in collaboration with the start-up BatVoice which targets the commercialization of affect-interactive digital systems. The prototype was developed and transferred to BatVoice for 48000 euros. The phase 2 of the collaboration is under discussion. Engineer: N. Brodu.

7.2. Bilateral Grants with Industry

- With Batvoice company: *Détection des émotions à partir de la voix*. Startup Batvoice: M. Sendrek & G. Maluréanu.
- With CARDIOLOGS company, headed by Y. Fleureau. Contacts and first collaborations started in 2016.

Patent in the process of being first deposited in January 2017 *Dispositif analyseur de rythme cardiaque*, Inria-185.

8. Partnerships and Cooperations

8.1. Regional Initiatives

GEOSTAT is working with the following regional partners:

- GEOSTAT has a decade-long close scientific collaboration with team SYSCO2 (LEGOS Laboratory UMR 5566): V. Garçon, B. Dewitte, J. Sudre.
- Laboratoire d'Astrophysique de Bordeaux (S. Bontemps, N. Schneider).
- Flood monitoring in Equator : Luc Bourrel (GET Toulouse / IRD) and Frédéric Frappart (GET / UMR EPOC). Co-supervision of Christophe Fatras (post-doc).
- With Bruno Castelle (EPOC).
- With LOMA (Laboratoire Ondes & Matière d'Aquitaine): A. Arneodo & F. Argoul.
- With Dominique Gibert (OSUR) on signal and image processing.
- CHU Bordeaux : Prof. Wassilios Meissner (IMN), Dr. Solange Milhé de Saint Victor (service ORL).
- CHU Toulouse : Dr. Anne Pavy Le traon (service Neurologie), Prof. Virginie Woisard (service ORL)
- IRIT : Prof. Régine André-Obrecht, Dr. Julie Mauclair
- IMT (Institut de Mathématique de Toulouse) : Dr. Sébastien Déjean, Dr. Laurent Risser.
- Mercator Océan: Dr. Abdelali El Moussaoui.

8.2. National Initiatives

- ANR project *Voice4PD-MSA*, led by K. Daoudi, which targets the differential diagnosis between Parkinson's disease and Multiple System Atrophy, has been accepted. 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).
- ICARODE [2013-2016]. Participants : Hussein Yahia, Oriol Pont, Véronique Garçon, Joel Sudre, Antonio Turiel, Christine Provost [LOCEAN]. 4-year contract, CNES-NASA funding, started 2013. Title: *ICARODE: Integration and cascading for high resolution ocean dynamics*. Project leader: H. Yahia.
- PhD grant for C. Artnana from UPMC University, under co-supervision with H. Yahia and C. Provost (LOCEAN, Paris).
- PhD grant for G. Singh from IIT Roorkee, under co-supervision with D. Singh (IIT Roorkee).
- PhD grant for A. El Aouni from PHC Toubkal and Moroccan government, under co-supervision with K. Minaoui and D. Aboutajdine (LRIT).

8.3. International Initiatives

8.3.1. OPTIC

Title: Optimal inference in Complex and Turbulent data

International Partner (Institution - Laboratory - Researcher):

IITR (India) - Dept. Of Electrical Engineering - Dharmendra Singh

Start year: 2014

See also: <https://optic.bordeaux.inria.fr/>

The OptIC associated team targets the extension and development of a strong collaboration between Inria GEOSTAT team and INDIAN INSTITUTE OF TECHNOLOGY ROORKEE Dept of Electronics and Computer Engineering (Prof. D. Singh's group) on non-linear Signal Processing for Universe Sciences, with a strong emphasis on data fusion in Earth Observation and monitoring. Non-linear Physics puts strong evidence of the fundamental role played by multiscale hierarchies in complex and turbulent data: in these data, the information content is statistically localized in geometrical arrangements in the signal's domain, while such geometrical organization is not attainable by classical methods in linear signal processing. This is one of the major drawbacks in the classical analysis of complex and turbulent signals. The goal of this associated team is to show that inference of physical variables along the scales of complex and turbulent signals can be performed through optimal multiresolution analysis performed on non-linear features and data extracted from the signals, resulting in novel and powerful approaches for data fusion between different acquisitions (in temporal/spatial/spectral resolutions). This program needs both strong expertise in the physical processes beyond the acquisitions and the application of non-linear physics ideas on the behavior of the acquired physical phenomena. The proposal will focus on specific applications in Earth Observation and monitoring for which the Indian partner has developed a very strong expertise, notably in its knowledge and use of the physical processes in remote sensing acquisitions. This partnership is an extremely interesting and high potential collaboration between two teams which focus separately either on the acquisition of the physical processes or their analysis by Complex Systems and non-linear physics methodologies. The recent results obtained in super-resolution by GEOSTAT promises strong applications to a much wider range of Universe Sciences problems, notably with a strong emphasis on data fusion between the physical variables acquired on related but different acquisitions. OptiC builds on a collaboration between Inria and IIT ROORKEE teams, added with partners in Universe Sciences and earth observation (ONERA, CNRS) already involved in research actions with GEOSTAT.

8.3.2. Inria International Partners

8.3.2.1. Informal International Partners

- Laboratory LRIT from Rabat University (K. Minaoui, D. Aboutajdine).
- Czech Technical University in Prague (Jan Ruzs).
- Brno University of Technology (Jiri Mekyska).
- University of Heidelberg (C. Garbe).

8.3.3. Participation in Other International Programs

8.3.3.1. Indo-French Center of Applied Mathematics

OPTIC

Title: Optimal Inference in complex and turbulent data

International Partner (Institution - Laboratory - Researcher):

Institutions: Inria and IIT Roorkee

Duration: 2013 - 2016

Start year: 2013

See above.

8.3.3.2. PHC-Toubkal

PHC-Toubkal

Title: Caractérisation multi-capteurs et suivi spatio-temporel de l'Upwelling sur la côte atlantique marocaine par imagerie satellitaire

International Partner (Institution - Laboratory - Researcher):

- GEOSTAT.
- CRTS (Centre Royal de Télédétection Spatiale), Rabat.
- Faculté des sciences de Rabat.
- Mercator-Océan.

Duration: from January 1st 2016 to 31 December 2018.

Start year: 2016.

8.4. International Research Visitors

8.4.1. Visits of International Scientists

- Prof. D. Singh (IIT roorkee, OPTIC Associated Team). Duration: 1 month.
- G. Singh (phd student in co-supervision, IIT roorkee, OPTIC Associated Team).
- A. El Aouni (PhD student in co-supervision, PHC Toubkal).
- Dr. Nicola Schneider (Koln University): nonlinear signal processing for astronomical data.

9. Dissemination

9.1. Promoting Scientific Activities

9.1.1. Scientific Events Organisation

9.1.1.1. General Chair, Scientific Chair

H. Yahia: organization of the conference *Signals & Physics* in October 2016, Inria Paris.

9.1.1.2. Member of the Organizing Committees

H. Yahia: organization of the conference *Signals & Physics* in October 2016, Inria Paris.

9.1.2. Scientific Events Selection

9.1.2.1. Chair of Conference Program Committees

H. Yahia, N. Brodu and K. Daoudi are members of the advisory board committee of the IEEE *11th International Conference on Industrial and Information Systems* (ICIIS 2016), 3-4 December 2016, IIT Roorkee, India, <http://www.iciis2016.org/commitee.html>.

9.1.2.2. Member of the Conference Program Committees

N. Brodu is co-organizing an EGU session (European Geophysical Union) and has presented 2 papers in the session.

9.1.2.3. Reviewer

H. Yahia and N. Brodu have reviewed papers for the ICIIS 2016 conference.

9.1.3. Journal

9.1.3.1. Member of the Editorial Boards

- G. Attuel is a member of the editorial board of CMSIM journal (from CHAOS Conference), sections plasma and biophysics.
- H. Yahia: *Frontiers in Fractal Physiology*.

9.1.3.2. Reviewer - Reviewing Activities

- N. Brodu: PRL (physical review letters), PRE, Remote Sensing.
- K. Doudi: reviewer for IEEE Transactions on Audio, Speech and Language Processing.
- H. Badri: ICIP Conference.

9.1.4. Invited Talks

- H. Badri is invited to give an oral presentation at the conference RFIA 2016 for the reception of his AFRIF 2015 Best PhD award. Title of the presentation: *Sparse and Scale-invariant methods in image processing*.
- H. Yahia was an invited keynote speaker at the 11th International Conference on Industrial and Information Systems (ICIIS 2016), 3-4 December 2016, IIT Roorkee, India. Title: *Non-convex sparsity. Applications in Image processing*.
- N. Brodu was an invited keynote speaker on the subject of super-resolution at the 11th International Conference on Industrial and Information Systems (ICIIS 2016), 3-4 December 2016, IIT Roorkee, India. Title: *Super-resolving multiresolution images with band-independent geometry of multispectral pixels*.

9.1.5. Leadership within the Scientific Community

- N. Brodu has given a presentation at the RISC-E school held at Rennes in October 2016. The presentation corresponds to 2 master UE.
- N. Brodu has given a presentation in February 2016 at the LaBRI/IMS/IMB lab: *Super-resolution of multispectral images* (part 1) and *Stochastic image analysis* (part 2).

9.1.6. Scientific Expertise

- H. Yahia and K. Daoudi have proposed scientific expertise for the I2S company, with an industrial collaboration prepared and submitted for 2017.
- H. Yahia and N. Brodu have proposed scientific expertise for the LECTRA company.

9.2. Teaching - Supervision - Juries

9.2.1. Teaching

Doctorat: H. Yahia, *Advancement in Signal Processing, Application to Earth Observation*, 30 hours, IIT Roorkee, GIAN courses, India.

Master : K. Daoudi, *financial mathematics*, 20 hours, Master2 MIAGE, University of Lorraine.

Master: N. Brodu, *Analyse de données massives par apprentissage automatique*, 2 days, EDMI Bordeaux.

Licence : A. El Aouni, *Programmation web (PHP, javascript, CSS)*, 24 hours, L3, Rabat University, Morocco.

9.2.2. Juries

- H. Yahia: member of the HDR jury of S. Jacquir (Bourgogne University, Laboratoire LE2I UMR CNRS 6306).
- N. Brodu: 1st year PhD jury.

9.3. Popularization

N. Brodu has given a presentation at Inria's *Unithé ou café* : (April 1st): Title: « Des images satellites aux messages sur les sites »

10. Bibliography

Major publications by the team in recent years

- [1] H. BADRI, H. YAHIA, K. DAOUDI. *Fast and Accurate Texture Recognition with Multilayer Convolution and Multifractal Analysis*, in "European Conference on Computer Vision", Zürich, Switzerland, ECCV 2014, September 2014, <https://hal.inria.fr/hal-01064793>.
- [2] I. HERNÁNDEZ-CARRASCO, J. SUDRE, V. GARÇON, H. YAHIA, C. GARBE, A. PAULMIER, B. DEWITTE, S. ILLIG, I. DADOU, M. GONZÁLEZ-DÁVILA, J. SANTANA CASIANO. *Reconstruction of super-resolution ocean pCO₂ and air-sea fluxes of CO₂ from satellite imagery in the Southeastern Atlantic*, in "Biogeosciences", September 2015, 20, This work is a contribution to ESA Support To Science Element Grant N 400014715/11/I-NB OceanFlux- Upwelling Theme. The Surface Ocean CO₂ Atlas (SOCAT) is an international effort, supported by the International Ocean Carbon Coordination Project (IOCCP), the Surface Ocean Lower Atmosphere Study (SOLAS), and the Integrated Marine Biogeochemistry and Ecosystem Research program (IMBER), to deliver a uniformly quality-controlled surface ocean CO₂ database. The many researchers and funding agencies responsible for the collection of data and quality control are thanked for their contributions to SOCAT, <https://hal.inria.fr/hal-01193339>.
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- [5] S. K. MAJI, H. YAHIA. *Edges, Transitions and Criticality*, in "Pattern Recognition", January 2014, <http://hal.inria.fr/hal-00924137>.
- [6] O. PONT, A. TURIEL, C. PEREZ-VICENTE. *On optimal wavelet bases for the realization of microcanonical cascade processes*, in "International Journal of Wavelets Multiresolution and Information Processing", 2011, vol. 9, p. 35-61.
- [7] O. PONT, A. TURIEL, H. YAHIA. *Singularity analysis in digital signals through the evaluation of their Unpredictable Point Manifold*, in "International Journal of Computer Mathematics", 2012, <http://hal.inria.fr/hal-00688715>.
- [8] O. PONT, H. YAHIA, R. DUBOIS, M. HAÏSSAGUERRE. *A Singularity-analysis Approach to characterize Epicardial Electric Potential*, in "Computing in Cardiology", 2012, <http://hal.inria.fr/hal-00750003>.
- [9] O. PONT, H. YAHIA, B. XU. *Arrhythmic dynamics from singularity analysis of electrocardiographic maps*, in "EBMC'13-The 35th Annual International Conference of the IEEE Engineering in Medicine and Biology Society", Osaka, Japan, IEEE, July 2013 [DOI : 10.1109/EMBC.2013.6610955], <http://hal.inria.fr/hal-00823856>.
- [10] J. SUDRE, H. YAHIA, O. PONT, V. GARÇON. *Ocean Turbulent Dynamics at Superresolution From Optimal Multiresolution Analysis and Multiplicative Cascade*, in "IEEE Transactions on Geoscience and Remote Sensing", June 2015, vol. 53, n^o 11, 12 [DOI : 10.1109/TGRS.2015.2436431], <https://hal.inria.fr/hal-01166170>.
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Publications of the year

Articles in International Peer-Reviewed Journal

- [14] H. BADRI, H. YAHIA, D. ABOUTAJDINE. *Low-Rankness Transfer for Realistic Denoising*, in "IEEE Transactions on Image Processing", November 2016, <https://hal.inria.fr/hal-01361246>.
- [15] H. BADRI, H. YAHIA. *A Non-Local Low-Rank Approach to Enforce Integrability*, in "IEEE Transactions on Image Processing", June 2016, <https://hal.inria.fr/hal-01317151>.

Invited Conferences

- [16] N. BRODU, D. SINGH, A. GARG. *A sub-pixel resolution enhancement model for multiple-resolution multispectral images*, in "European Geophysical Union General Assembly 2016", Vienne, Austria, April 2016,

Présentation orale ayant pour titre "Super-Resolution of Sentinel-2 multispectral images", <https://hal.inria.fr/hal-01287184>.

- [17] O. PONT, H. YAHIA, B. XU. *Complexity in Electrophysiological Dynamics. Emergence and measures of organization*, in "2nd BCAM Workshop on Nonlinear Dynamics in Biological System", Bilbao, Spain, Basque Center for Applied Mathematics Bilbao, Spain, September 2016, <https://hal.inria.fr/hal-01392644>.

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- [18] K. DAOUDI, N. BRODU, J. RUSZ, J. KLEMPER. *Objective discrimination between Progressive Supranuclear Palsy and Multiple System Atrophy using speech analysis*, in "38th Annual International Conference of the IEEE Engineering in Medicine and Biology Society (IEEE-EMBC'16)", Orlando, United States, August 2016, <https://hal.inria.fr/hal-01328206>.
- [19] A. EL AOUNI, K. MINAOU, A. TAMIM, K. DAOUDI, H. YAHIA, D. ABOUTAJDINE. *An improved method for accurate computation of coastal upwelling index using Sea Surface Temperature Images*, in "13th ACS/IEEE International Conference on Computer Systems and Applications", Agadir, Morocco, 13th ACS/IEEE International Conference on Computer Systems and Applications, ACS/IEEE, November 2016, <https://hal.inria.fr/hal-01424036>.
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- [21] A. GARG, S. VARDHAN NAIDU, S. GUPTA, D. SINGH, N. BRODU, H. YAHIA. *A novel approach for optimal weight factor of DT-CWT coefficients for land cover classification using MODIS data*, in "Geoscience and Remote Sensing Symposium (IGARSS), 2016 IEEE International", Beijing, China, IEEE, July 2016 [DOI : 10.1109/IGARSS.2016.7730181], <https://hal.inria.fr/hal-01400795>.
- [22] G. ROSI, I. SCALA, V. NGUYEN, S. NAILI, R. VAYRON, G. HAIAT, H. YAHIA, S. SEURET, S. JAF-FARD. *Caractérisation de la Réponse Ultrasonore d'Implant Dentaire : Simulation Numérique et Analyse des Signaux*, in "Congrès Français d'Acoustique 2016", Le Mans, France, Actes en ligne du Congrès Français d'Acoustique, April 2016, <https://hal.inria.fr/hal-01356146>.

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- [23] G. ATTUEL. *Surprising "quantum statistical" treatment of Landau damping: discussion on simple models*, in "The 9th Chaotic Modeling and Simulation International Conference, CHAOS 2016", London, United Kingdom, CMSIM Journal, May 2016, <https://hal.inria.fr/hal-01322853>.

Scientific Books (or Scientific Book chapters)

- [24] G. ATTUEL, O. PONT, B. XU, H. YAHIA. *Sudden cardiac death and turbulence*, in "The Foundations of Chaos Revisited: From Poincaré to Recent Advancements", C. SKIADAS (editor), Understanding Complex Systems, Springer Verlag, May 2016, X, 224 [DOI : 10.1007/978-3-319-29701-9], <https://hal.inria.fr/hal-01279000>.

Other Publications

- [25] G. ATTUEL, H. YAHIA. *The role of abnormal inhibitory transmission at the gap junctions of cardiac cells in fibrillation*, January 2016, Physical Principles of Biological and Active Systems - IOP Topical Meeting, Poster, <https://hal.inria.fr/hal-01253790>.
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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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Project-Team HIEPACS

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- 7.2. - Discrete mathematics, combinatorics

Other Research Topics and Application Domains:

- 3.3.1. - Earth and subsoil
- 3.4.2. - Industrial risks and waste
- 4.1. - Fossile energy production (oil, gas)
- 4.2.2. - Fusion
- 5.5. - Materials
- 9.4.1. - Computer science
- 9.4.2. - Mathematics
- 9.4.4. - Chemistry

1. Members

Research Scientists

- Emmanuel Agullo [Inria, Researcher]
- Olivier Coulaud [Inria, Senior Researcher, HDR]
- Luc Giraud [Team leader, Inria, Senior Researcher, HDR]
- Jean Roman [Inria, Senior Researcher, Direction for Science and half-time in **HIEPACS**, Professor at Bordeaux INP on secondment, HDR]

Faculty Members

- Aurélien Esnard [Univ. Bordeaux, Associate Professor]
- Mathieu Faverge [Bordeaux INP, Associate Professor]
- Abdou Guermouche [Univ. Bordeaux, Associate Professor]
- Pierre Ramet [Univ. Bordeaux, Associate Professor]

Technical Staff

- Patrick Dos Santos [Univ. Bordeaux, until Apr 2016]
- Matias Hastaran [Inria, granted by FP7 PRACE-4IP project]
- Quentin Khan [Inria]
- Florent Pruvost [Inria, SED]
- Julien Pedron [Inria, until Sep 2016, granted by Labex CPI]
- Cyrille Piacibello [Inria, granted by Hi-Box DGA project]
- Gilles Marait [Inria, granted by H2020 **EoCoE**, from Sep 2016]

PhD Students

- Pierre Blanchard [French Ministry through ENS Cachan]
- Nicolas Bouzat [Inria, co-supervised with **TONUS** project-team]

Astrid Casadei [Inria, until Mar 2016]
Jean-Marie Couteyen [Airbus Safran Launchers, granted by ANRT-CIFRE, until Jan 2016]
Arnaud Durocher [CEA, granted by ANRT-CIFRE]
Aurélien Falco [Inria, granted by Conseil Régional Aquitaine - Airbus Group Innovations]
Cyril Fournier [CERFACS]
Grégoire Pichon [Inria, granted by DGA-Inria]
Louis Poirel [Inria, granted by ANR **DEDALES** project]
Maria Predari [Inria, granted by Conseil Régional Aquitaine - Inria]

Post-Doctoral Fellows

Matthieu Kuhn [Inria, granted by **TECSER** project]
Ian Masliah [Inria, from Nov 2016]
Yuval Harness [Inria, granted by Conseil Régional Aquitaine - Inria]
Emrullah Fatih Yetkin [Inria, granted by FP7 **EXA2CT** project, until Aug 2016]

Administrative Assistant

Chrystel Plumejeau [Inria]

Others

Alban Bellot [Inria, Internship, from Jun 2016 until Jul 2016]
Pierre Brenner [Airbus Safran Launchers, Engineer Expert]
Mathieu Deschamps [Inria, Internship, from Jun 2016 until Sep 2016]
Martin Khannouz [Inria, Internship, from Feb 2016 until Aug 2016]
Guillaume Latu [CEA Cadarache, IRFM, Research Scientist]
Alexandre Moreau [Inria, Internship, Feb-Aug 2016]
Mathis Rade Morzadec [Inria, Internship, from May 2016 until Aug 2016]
Hugues Rauwel [Inria, Internship, from Jul 2016 until Aug 2016]
Guillaume Sylvand [Airbus Group Innovations, Engineer expert]
Nathan Thomasset [Inria, Internship, from May 2016 until Jul 2016]
Hugo Vikstrom [Inria, Internship, from Jun 2016 until Aug 2016]

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 conducted on close collaboration in particular with European and US initiatives and likely in the framework of H2020 European 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 perspectives in scalable parallel linear algebra techniques are addressed, ranging from dense direct, sparse direct, iterative and hybrid approaches for large linear systems. Then we consider research plans for 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 multidisciplinary context with colleagues in other academic or industrial groups where our contribution is related to our expertises. Not only these collaborations enable our knowledges 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 Group/Conseil Régional 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 two ongoing associated teams, namely **MORSE** and **FASTLA** we contribute with world leading groups 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, which are involved in the IPL **C2S@EXA**, 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, some of them being involved in the IPL **C2S@EXA**. 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 Coulaud, Mathieu Faverge, Luc Giraud, Abdou Guermouche, Matias Hastaran, Guillaume Latu, Grégoire Pichon, Florent Pruvost, Pierre Ramet, Jean Roman, Emrullah Fatih Yetkin.

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. Of course, this work requires the use/design of scheduling algorithms and models specifically to tackle our target problems. This has to be done in collaboration with our colleagues from the

scheduling community like for example O. Beaumont (Inria **REALOPT** Project-Team). It is important to note that this topic is strongly linked to the underlying programming model. Indeed, considering multicore 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 behaviour 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 that framework, the **SOLHAR** 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. 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. **SOLHAR** proposes an innovative approach which relies on the efficiency and portability of runtime systems, such as the **StarPU** tool developed in the **STORM** team. 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. Our final goal would be to have high performance solvers and tools which can efficiently run on all these types of complex architectures by exploiting all the resources of the platform (even if they are heterogeneous).

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. The framework that hosts all these research activities is the associate team **MORSE**. 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. In that respect, we are involved in the **EXA2CT** FP7 project.

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, Mathieu Faverge, Aurélien Falco, Luc Giraud, Abdou Guermouche, Yuval Harness, Matias Hastaran, Matthieu Kuhn, Gilles Marait, Julien Pedron, Cyrille Piacibello, Grégoire Pichon, Louis Poirel, Pierre Ramet, Jean Roman.

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 solver

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 hierarchical matrices algebra.

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 associate team **MORSE** and the ANR **SOLHAR** 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 (**REALOPT** 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 Group Innovations.

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 intend to 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 preconditioned 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 libraries **HIPS** and **MaPHYs**. This activity will be developed in the context of the ANR **DEDALES** 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 library will be developed in the context of the DGA HiBOX project.
- 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 through 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.

3.4. High performance Fast Multipole Method for N-body problems

Participants: Emmanuel Agullo, Olivier Coulaud, Quentin Khan, Cyrille Piacibello, 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 conducted 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 conducted on close connection with the activity described

in Section 3.3. Following our earlier experience, we plan to first consider approximate inverse preconditioners that can efficiently exploit these data structures.

3.5. Load balancing algorithms for complex simulations

Participants: Astrid Casadei, Olivier Coulaud, Aurélien Esnard, Maria Predari, Pierre Ramet, Jean Roman.

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 use 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 **HIPS** or **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: Pierre Blanchard, Olivier Coulaud.

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 achieve 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 for scalable numerical algorithms in scientific applications

Participants: Nicolas Bouzat, Pierre Brenner, Jean-Marie Couteyen, Mathieu Faverge, Guillaume Latu, Pierre Ramet, Jean Roman.

The research activities concerning the ITER challenge are involved in the Inria Project Lab (IPL) **C2S@EXA**.

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 were involved in the Inria Project Lab **C2S@EXA** in collaboration with **CEA-IRFM** and are 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 **JOKE** code).

Currently, **GYSELA** is parallelized in an hybrid MPI+OpenMP way and can exploit the power of the current greatest supercomputers. To simulate faithfully the plasma physic, **GYSELA** handles a huge amount of data and today, the memory consumption is a bottleneck on very large simulations. In this context, mastering the memory consumption of the code becomes critical to consolidate its scalability and to enable the implementation of new numerical and physical features to fully benefit from the extreme scale architectures.

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.

4.2.2. SN Cartesian solver for nuclear core simulation

As part of its activity, EDF R&D is developing a new nuclear core simulation code named COCAGNE that relies on a Simplified PN (SPN) method to compute the neutron flux inside the core for eigenvalue calculations. In order to assess the accuracy of SPN results, a 3D Cartesian model of PWR nuclear cores has been designed and a reference neutron flux inside this core has been computed with a Monte Carlo transport code from Oak Ridge National Lab. This kind of 3D whole core probabilistic evaluation of the flux is computationally very demanding. An efficient deterministic approach is therefore required to reduce the computation effort dedicated to reference simulations.

In this collaboration, we work on the parallelization (for shared and distributed memories) of the DOMINO code, a parallel 3D Cartesian SN solver specialized for PWR core reactivity computations which is fully integrated in the COCAGNE system.

4.2.3. 3D aerodynamics for unsteady problems with bodies in relative motion

Airbus Defence and Space has developed for 20 years the FLUSEPA code which focuses on unsteady phenomenon with changing topology like stage separation or rocket launch. The code is based on a finite volume formulation with temporal adaptive time integration and supports bodies in relative motion. The temporal adaptive integration classifies cells in several temporal levels and this repartition can evolve during the computation, leading to load-balancing issues in a parallel computation context. Bodies in relative motion are managed through a CHIMERA-like technique which allows building a composite mesh by merging multiple meshes. The meshes with the highest priorities recover the least ones, and at the boundaries of the covered mesh, an intersection is computed. Unlike classical CHIMERA technique, no interpolation is performed, allowing a conservative flow integration. The main objective of this collaboration is to design a new scalable version of FLUSEPA from a task-based parallelization over a runtime system (**StarPU**) in order to run efficiently on modern heterogeneous multicore parallel architectures very large 3D simulations (for example ARIANE 5 and 6 booster separation).

5. Highlights of the Year

5.1. Highlights of the Year

5.1.1. Conference organization

We organized the 9th International workshop on Parallel Matrix Algorithms and Application (PMAA'16 - July 6-8) in collaboration with Bordeaux INP, CNRS and Université de Bordeaux. The conference that was composed of 4 invited plenary presentations and 76 regular talks. Around 120 people attended the conference, 70 % were from Europe, 20 % from North America, 7 % from Asia; among them more than 25 % were students. We succeeded to offer free registration to the students thanks to the sponsorship we arose from Airbus DS, CEA, CERFACS, Clustervision, Labex CPU, DELL, EDF, IBM and Total that contributed to balance our budget.

More details can be found on <http://pmaa16.inria.fr>

6. New Software and Platforms

6.1. Spack-morse

The radical change we have adopted in terms of methodology (task-based programming strongly) changes the software design. In particular, our codes become more and more modular and the complexity of their inter-dependencies is subsequently very high.

In order to address this complexity we have chosen to rely on the **Spack** flexible package manager designed to support multiple versions, configurations, platforms, and compilers (<http://software.llnl.gov/spack> developed and maintained at LLNL). We have integrated all our libraries above this package manager in the **Spack-Morse** extension that we maintain in **HIEPACS**.

- Audience: A-4 (large audience, used by people outside the team).
- Software originality: SO-3 (original software reusing known ideas and introducing new ideas).
- Software maturity: SM-3 (well-developed software, good documentation, reasonable software engineering).
- Evolution and maintenance: EM-3 (good quality middle-term maintenance).
- Software distribution and licensing: SDL-4 (public source or binary distribution on the Web). source distribution or a commercially-distributed product).
- Contact: Florent Pruvost
- URL: <http://morse.gforge.inria.fr/spack/spack.html>

6.2. Chameleon

Chameleon is a dense linear algebra software relying on the STF sequential task-based programming paradigm. It implements the tile algorithms originally designed for multicore architectures in the **PLASMA** package and extends them so that they can be processed on by a runtime system to exploit any type of hardware architecture (multicore, GPU, heterogeneous, supercomputer). This software is central for the team as it allows to investigate in a relatively simple context (regular dense linear algebra algorithms) new types of designs before implementing them for the more irregular algorithms implemented in the software packages described below.

- Audience: A-4 (large audience, used by people outside the team).
- Software originality: SO-4 (original software implementing a fair number of original ideas).
- Software maturity: SM-3 (well-developed software, good documentation, reasonable software engineering).
- Evolution and maintenance: EM-3 (good quality middle-term maintenance).
- Software distribution and licensing: SDL-4 (public source or binary distribution on the Web). source distribution or a commercially-distributed product).
- Contact: Emmanuel Agullo
- URL: <https://project.inria.fr/chameleon>

6.3. HIPS

HIPS (Hierarchical Iterative Parallel Solver) is a scientific library that provides an efficient parallel iterative solver for very large sparse linear systems.

The key point of the methods implemented in **HIPS** is to define an ordering and a partition of the unknowns that relies on a form of nested dissection ordering in which cross points in the separators play a special role (Hierarchical Interface Decomposition ordering). The subgraphs obtained by nested dissection correspond to the unknowns that are eliminated using a direct method and the Schur complement system on the remaining of the unknowns (that correspond to the interface between the sub-graphs viewed as sub-domains) is solved using an iterative method (GMRES or Conjugate Gradient at the time being).

Thus, **HIPS** is a software library that provides several methods to build an efficient preconditioner in almost all situations.

- Audience: A-4 (large audience, used by people outside the team).
- Software originality: SO-4 (original software implementing a fair number of original ideas).
- Software maturity: SM-3 (well-developed software, good documentation, reasonable software engineering).
- Evolution and maintenance: EM-2 (basic maintenance to keep the software alive).
- Software distribution and licensing: SDL-4 (public source or binary distribution on the Web).
- Contact: Pierre Ramet
- URL: <http://hips.gforge.inria.fr>

6.4. MaPHYs

MaPHYs (Massively Parallel Hybrid Solver) is an hybrid iterative/direct parallel (MPI-threads) sparse linear solver based on algebraic domain decomposition technique for real/complex symmetric positive definite/unsym/-metric matrices. For a given number of MPI processes/domains, **MaPHYs** solves the Schur complement computed from the adjacency graph of the sparse matrix using a preconditioned Krylov subspace method (CG or GMRES). The provided preconditioners are variants of an algebraic Additive Schwarz methods. A prototype version of a two level preconditionner using an algebraic coarse space is available but not yet publicly distributed (provided upon request for beta testers).

- Audience: A-4 (large audience, used by people outside the team).
- Software originality: SO-4 (original software implementing a fair number of original ideas).
- Software maturity: SM-3 (well-developed software, good documentation, reasonable software engineering).
- Evolution and maintenance: EM-4 (well-defined and implemented plans for future maintenance and evolution).
- Software distribution and licensing: SDL-4 (public source or binary distribution on the Web).
- Contact: Emmanuel Agullo
- URL: <https://project.inria.fr/maphys/fr>

6.5. MetaPart

MetaPart is a library that addresses the challenge of (dynamic) load balancing for emerging complex parallel simulations, such as multi-physics or multi-scale coupling applications. First, it offers a uniform API over state-of-the-art (hyper-) graph partitioning & ordering software packages such as **Scotch**, PaToH, METIS, Zoltan, Mondriaan, etc. Based upon this API, it provides a framework that facilitates the development and the evaluation of high-level partitioning methods, such as MxN repartitioning or coupling-aware partitioning (co-partitioning).

- Audience: A-1 (internal prototype).
- Software originality: SO-3 (original software reusing known ideas and introducing new ideas).
- Software maturity: SM-2 (basic usage works, terse documentation).
- Evolution and maintenance: EM-3 (good quality middle-term maintenance).
- Software distribution and licensing: SDL-4 (public source or binary distribution on the Web).
- Contact: Aurélien Esnard
- URL: <http://metapart.gforge.inria.fr>

6.6. PaStiX

PaStiX (Parallel Sparse matriX package) 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) iterative methods. Numerical algorithms are implemented in single or double precision (real or complex): LLt (Cholesky), LDLt (Crout) and LU with static pivoting (for non symmetric matrices having a symmetric pattern).

The **PaStiX** solver is suitable for any heterogeneous parallel/distributed architecture when its performance is predictable, such as clusters of multicore nodes. In particular, we now offer 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.

- Audience: A-5 (wide audience, large user's community).
- Software originality: SO-4 (original software implementing a fair number of original ideas).
- Software maturity: SM-4 (major software project, strong software engineering).
- Evolution and maintenance: EM-4 (well-defined and implemented plans for future maintenance and evolution).
- Software distribution and licensing: SDL-5 (external packaging and distribution, as part of a popular open source distribution or a commercially-distributed product).
- Contact: Pierre Ramet
- URL: <http://pastix.gforge.inria.fr>

6.7. QR_Mumps

qr_mumps is a software package for the solution of sparse, linear systems on multicore computers. It implements a direct solution method based on the QR factorization of the input matrix. Therefore, it is suited to solving sparse least-squares problems and to computing the minimum-norm solution of sparse, under-determined problems. It can obviously be used for solving square problems in which case the stability provided by the use of orthogonal transformations comes at the cost of a higher operation count with respect to solvers based on, e.g., the LU factorization. **qr_mumps** supports real and complex, single or double precision arithmetic.

qr_mumps is mainly developed and maintained by the APO team of the IRIT laboratory of Toulouse. **HIEPACS** is an active contributor to this project.

- Audience: A-4 (large audience, used by people outside the team).
- Software originality: SO-4 (original software implementing a fair number of original ideas).
- Software maturity: SM-3 (well-developed software, good documentation, reasonable software engineering).
- Evolution and maintenance: EM-3 (good quality middle-term maintenance).
- Software distribution and licensing: SDL-4 (public source or binary distribution on the Web).
- Contact: Emmanuel Agullo
- URL: http://buttari.perso.enseeiht.fr/qr_mumps/

6.8. ScalFMM

ScalFMM is a library to compute N-body interactions using the Fast Multipole Method. This is a parallel kernel independent fast multipole method based on interpolation (Chebyshev or equispaced grid points).

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 (fork-join and tasks models), MPI and runtime system (**StarPU**). 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 tree structure (hierarchical octree and Group-Tree) and the parallel algorithms ;
- the kernels (scalar, tensorial and multi-rhs). Classical kernels are available (Coulombic, Leonard-Jones, Gaussian, Stokes, ...)

This modular architecture allows us to easily add new FMM algorithms or kernels and new paradigm of parallelization. Today, we also proposed the FMM based on spherical harmonic expansion with Blas or rotation optimization for Coulombic potential) and all algorithms are designed to treat more complex kernels by adding multiple right-hand sides, tensorial structures, ...

- Audience: A-4 (large audience, used by people outside the team).
- Software originality: SO-4 (original software implementing a fair number of original ideas).
- Software maturity: SM-3 (well-developed software, good documentation, reasonable software engineering).
- Evolution and maintenance: EM-3 (good quality middle-term maintenance).
- Software distribution and licensing: SDL-4 (public source or binary distribution on the Web).
- Contact: Olivier Coulaud
- URL: <http://scalfmm-public.gforge.inria.fr/doc/>

6.9. ViTE

ViTE is a trace explorer. It is a tool to visualize execution traces in Pajé or OTF format for debugging and profiling parallel or distributed applications. It is developed with C++ programming language with OpenGL and Qt technologies.

- Audience: A-4 (large audience, used by people outside the team).
- Software originality: SO-3 (original software reusing known ideas and introducing new ideas).
- Software maturity: SM-3 (well-developed software, good documentation, reasonable software engineering).
- Evolution and maintenance: EM-2 (basic maintenance to keep the software alive).
- Software distribution and licensing: SDL-4 (public source or binary distribution on the Web).
- Contact: Mathieu Faverge
- URL: <http://vite.gforge.inria.fr>

6.10. Platforms

6.10.1. PlaFRIM: Plateforme Fédérative pour la Recherche en Informatique et Mathématiques

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. Numerical recovery strategies for parallel resilient Krylov linear solvers

As the computational power of high performance computing (HPC) systems continues to increase by using a huge number of cores or specialized processing units, HPC applications are increasingly prone to faults. In this paper, we present a new class of numerical fault tolerance algorithms to cope with node crashes in parallel distributed environments. This new resilient scheme is designed at application level and does not require extra resources, i.e., computational unit or computing time, when no fault occurs. In the framework of iterative methods for the solution of sparse linear systems, we present numerical algorithms to extract relevant information from available data after a fault, assuming a separate mechanism ensures the fault detection. After data extraction, a well chosen part of missing data is regenerated through interpolation strategies to constitute meaningful inputs to restart the iterative scheme. We have developed these methods, referred to as Interpolation-Restart techniques, for Krylov subspace linear solvers. After a fault, lost entries of the current iterate computed by the solver are interpolated to define a new initial guess to restart the Krylov method. A well suited initial guess is computed by using the entries of the faulty iterate available on surviving nodes. We present two interpolation policies that preserve key numerical properties of well-known linear solvers, namely the monotonic decrease of the A-norm of the error of the conjugate gradient or the residual norm decrease of GMRES. The qualitative numerical behavior of the resulting scheme have been validated with sequential simulations, when the number of faults and the amount of data losses are varied. Finally, the computational costs associated with the recovery mechanism have been evaluated through parallel experiments.

More details on this work can be found in [7].

7.1.2. Interpolation-restart strategies for resilient eigensolvers

The solution of large eigenproblems is involved in many scientific and engineering applications when for instance, stability analysis is a concern. For large simulation in material physics or thermo-acoustics, the calculation can last for many hours on large parallel platforms. On future large-scale systems, the mean time between failures (MTBF) of the system is expected to decrease so that many faults could occur during the solution of large eigenproblems. Consequently, it becomes critical to design parallel eigensolvers that can survive faults. In that framework, we investigate the relevance of approaches relying on numerical techniques, which might be combined with more classical techniques for real large-scale parallel implementations. Because we focus on numerical remedies we do not consider parallel implementations nor parallel experiments but only numerical experiments. We assume that a separate mechanism ensures the fault detection and that a system layer provides support for setting back the environment (processes, . . .) in a running state. Once the system is in a running state, after a fault, our main objective is to provide robust resilient schemes so that the eigensolver may keep converging in the presence of the fault without restarting the calculation from scratch. For this purpose, we extend the interpolation-restart (IR) strategies initially introduced for the solution of linear systems in a previous work to the solution of eigenproblems in this paper. For a given numerical scheme, the IR strategies consist of extracting relevant spectral information from available data after a fault. After data extraction, a well-selected part of the missing data is regenerated through interpolation strategies

to constitute a meaningful input to restart the numerical algorithm. One of the main features of this numerical remedy is that it does not require extra resources, i.e., computational unit or computing time, when no fault occurs. In this paper, we revisit a few state-of-the-art methods for solving large sparse eigenvalue problems namely the Arnoldi methods, subspace iteration methods and the Jacobi-Davidson method, in the light of our IR strategies. For each considered eigensolver, we adapt the IR strategies to regenerate as much spectral information as possible. Through extensive numerical experiments, we study the respective robustness of the resulting resilient schemes with respect to the MTBF and to the amount of data loss via qualitative and quantitative illustrations.

More details on this work can be found in [8].

7.2. High performance solvers for large linear algebra problems

7.2.1. Exploiting Kepler architecture in sparse direct solver with runtime systems

Many works have addressed heterogeneous architectures to exploit accelerators such as GPUs or Intel Xeon Phi with interesting speedup. Despite researches towards generic solutions to efficiently exploit those accelerators, their hardware evolution requires continual adaptation of the kernels running on those architectures. The recent Nvidia architectures, as Kepler, present a larger number of parallel units thus requiring more data to feed every computational units. A solution considered to supply enough computation has been to study problems with large number of small computations. The batched BLAS libraries proposed by Intel, Nvidia, or the University of Tennessee are examples of this solution. We have investigated the use of the variable size batched matrix-matrix multiply to improve the performance of a the PaStiX sparse direct solver. Indeed, this kernel suits the super-nodal method of the solver, and the multiple updates of variable sizes that occur during the numerical factorization.

These contributions have been presented at the PMAA'16 conference [28].

7.2.2. Blocking strategy optimizations for sparse direct linear solver on heterogeneous architectures

The preprocessing steps of sparse direct solvers, ordering and block-symbolic factorization, are two major steps that lead to a reduced amount of computation and memory and to a better task granularity to reach a good level of performance when using BLAS kernels. With the advent of GPUs, the granularity of the block computations became more important than ever. In this paper, we present a reordering strategy that increases this block granularity. This strategy relies on the block-symbolic factorization to refine the ordering produced by tools such as METIS or Scotch, but it does not impact the number of operations required to solve the problem. We integrate this algorithm in the PaStiX solver and show an important reduction of the number of off-diagonal blocks on a large spectrum of matrices. This improvement leads to an increase in efficiency of up to 10% on CPUs and up to 40% on GPUs.

These contributions have been presented at the SIAM PP'16 conference [35] and an extended paper has been submitted to SIAM Journal on Matrix Analysis and Applications [49].

7.2.3. Sparse supernodal solver using hierarchical compression

In the context of FASTLA associate team, during the last 3 years, we are collaborating with Eric Darve, professor in the Institute for Computational and Mathematical Engineering and the Mechanical Engineering Department at Stanford, on the design of a new efficient sparse direct solvers.

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 hierarchical matrices algebra. In the first step, we are targeting an $O(N^{4/3})$ solver. Preliminary benchmarks indicate that a speed up of 2x to 10x is possible (on the largest test cases).

In the context of the **FASTLA** team, we have been working on applying fast direct solvers for dense matrices to the solution of sparse direct systems. We observed that the extend-add operation (during the sparse factorization) is the most time-consuming step. We have therefore developed a series of algorithms to reduce this computational cost. We presented a new implementation of the **PaStiX** solver using hierarchical compression to reduce the burden on large blocks appearing during the nested dissection process. To improve the efficiency of our sparse update kernel for both BLR (block low-rank) and HODLR (hierarchically off-diagonal low-rank), we are now investigating to BDLR (boundary distance low-rank) approximation scheme to preselect rows and columns in the low-rank approximation algorithm. We also have to improve our ordering strategies to enhance data locality and compressibility. The implementation is based on runtime systems to exploit parallelism.

Some contributions have already been presented at the workshops on Fast Solvers [32], [31], [30]. This work is a joint effort between Professor Darve's group at Stanford and the Inria HiePACS team within **FASTLA**.

7.2.4. Hierarchical hybrid sparse linear solver for multicore platforms

The solution of large sparse linear systems is a critical operation for many numerical simulations. To cope with the hierarchical design of modern supercomputers, hybrid solvers based on Domain Decomposition Methods (DDM) have been proposed. Among them, approaches consisting of solving the problem on the interior of the domains with a sparse direct method and the problem on their interface with a preconditioned iterative method applied to the related Schur Complement have shown an attractive potential as they can combine the robustness of direct methods and the low memory footprint of iterative methods. In this report, we consider an additive Schwarz preconditioner for the Schur Complement, which represents a scalable candidate but whose numerical robustness may decrease when the number of domains becomes too large. We thus propose a two-level MPI/thread parallel approach to control the number of domains and hence the numerical behaviour. We illustrate our discussion with large-scale matrices arising from real-life applications and processed on both a modern cluster and a supercomputer. We show that the resulting method can process matrices such as `tdr455k` for which we previously either ran out of memory on few nodes or failed to converge on a larger number of nodes. Matrices such as `Nachos_4M` that could not be correctly processed in the past can now be efficiently processed up to a very large number of CPU cores (24 576 cores). The corresponding code has been incorporated into the **MaPHyS** package.

More details on this work can be found in [44]

7.2.5. Task-based conjugate gradient: from multi-GPU towards heterogeneous architectures

Whereas most parallel High Performance Computing (HPC) numerical libraries have been written as highly tuned and mostly monolithic codes, the increased complexity of modern architectures led the computational science and engineering community to consider more modular programming paradigms such as task-based paradigms to design new generation of parallel simulation code; this enables to delegate part of the work to a third party software such as a runtime system. That latter approach has been shown to be very productive and efficient with compute-intensive algorithms, such as dense linear algebra and sparse direct solvers. In this study, we consider a much more irregular, and synchronizing algorithm, namely the Conjugate Gradient (CG) algorithm. We propose a task-based formulation of the algorithm together with a very fine instrumentation of the runtime system. We show that almost optimum speed up may be reached on a multi-GPU platform (relatively to the mono-GPU case) and, as a very preliminary but promising result, that the approach can be effectively used to handle heterogeneous architectures composed of a multicore chip and multiple GPUs. We expect that these results will pave the way for investigating the design of new advanced, irregular numerical algorithms on top of runtime systems.

More details on this work can be found in [42]

7.2.6. Analysis of rounding error accumulation in conjugate gradients to improve the maximal attainable accuracy of pipelined CG

Pipelined Krylov solvers typically offer better scalability in the strong scaling limit compared to standard Krylov methods. The synchronization bottleneck is mitigated by overlapping time-consuming global communications with useful computations in the algorithm. However, to achieve this communication hiding strategy, pipelined methods feature multiple recurrence relations on additional auxiliary variables to update the guess for the solution. This paper aims at studying the influence of rounding errors on the convergence of the pipelined Conjugate Gradient method. It is analyzed why rounding effects have a significantly larger impact on the maximal attainable accuracy of the pipelined CG algorithm compared to the traditional CG method. Furthermore, an algebraic model for the accumulation of rounding errors throughout the (pipelined) CG algorithm is derived. Based on this rounding error model, we then propose an automated residual replacement strategy to reduce the effect of rounding errors on the final iterative solution. The resulting pipelined CG method with automated residual replacement improves the maximal attainable accuracy of pipelined CG to a precision comparable to that of standard CG, while maintaining the efficient parallel performance of the pipelined method.

More details on this work can be found in [46].

7.2.7. *Nearly optimal fast preconditioning of symmetric positive definite matrices*

We consider the hierarchical off-diagonal low-rank preconditioning of symmetric positive definite matrices arising from second order elliptic boundary value problems. When the scale of such problems becomes large combined with possibly complex geometry or unstable of boundary conditions, the representing matrix is large and typically ill-conditioned. Multilevel methods such as the hierarchical matrix approximation are often a necessity to obtain an efficient solution. We propose a novel hierarchical preconditioner that attempts to minimize the condition number of the preconditioned system. The method is based on approximating the low-rank off-diagonal blocks in a norm adapted to the hierarchical structure. Our analysis shows that the new preconditioner effectively maps both small and large eigenvalues of the system approximately to 1. Finally through numerical experiments, we illustrate the effectiveness of the new designed scheme which outperforms more classical techniques based on regular SVD to approximate the off-diagonal blocks and SVD with filtering.

This work is a joint effort between Professor Darve's group at Stanford and the Inria HiePACS team within **FASTLA**. More details on this work can be found in [41].

7.2.8. *Robust coarse spaces for abstract Schwarz preconditioners via generalized eigenproblems*

The solution of large sparse linear systems is one of the most important kernels in many numerical simulations. The domain decomposition methods (DDM) community has developed many efficient and robust solvers in the last decades. While many of these solvers fall in Abstract Schwarz (AS) framework, their robustness has often been demonstrated on a case-by-case basis. In this paper, 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 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, leading to a new powerful and versatile substructuring method. Numerical experiments illustrate these statements.

More details on this work can be found in [45]

7.3. High performance fast multipole method for N-body problems

7.3.1. Task-based fast multipole method

With the advent of complex modern architectures, the low-level paradigms long considered sufficient to build High Performance Computing (HPC) numerical codes have met their limits. Achieving efficiency, ensuring portability, while preserving programming tractability on such hardware prompted the HPC community to design new, higher level paradigms. The successful ports of fully-featured numerical libraries on several recent runtime system proposals have shown, indeed, the benefit of task-based parallelism models in terms of performance portability on complex platforms. However, the common weakness of these projects is to deeply tie applications to specific expert-only runtime system APIs. The OPENMP specification, which aims at providing a common parallel programming means for shared-memory platforms, appears as a good candidate to address this issue thanks to the latest task-based constructs introduced as part of its revision 4.0. The goal of this paper is to assess the effectiveness and limits of this support for designing a high-performance numerical library. We illustrate our discussion with the **ScalFMM** library, which implements state-of-the-art fast multipole method (FMM) algorithms, that we have deeply re-designed with respect to the most advanced features provided by OPENMP 4. We show that OPENMP 4 allows for significant performance improvements over previous OPENMP revisions on recent multicore processors. We furthermore propose extensions to the OPENMP 4 standard and show how they can enhance FMM performance. To assess our statement, we have implemented this support within the **KLANG-OMP** source-to-source compiler that translates OPENMP directives into calls to the **StarPU** task-based runtime system. This study, [38] shows that we can take advantage of the advanced capabilities of a fully-featured runtime system without resorting to a specific, native runtime port, hence bridging the gap between the OPENMP standard and the very high performance that was so far reserved to expert-only runtime system APIs.

7.3.2. Task-based fast multipole method for clusters of multicore processors

Most high-performance, scientific libraries have adopted hybrid parallelization schemes - such as the popular MPI+OpenMP hybridization - to benefit from the capacities of modern distributed-memory machines. While these approaches have shown to achieve high performance, they require a lot of effort to design and maintain sophisticated synchronization/communication strategies. On the other hand, task-based programming paradigms aim at delegating this burden to a runtime system for maximizing productivity. In this article, we assess the potential of task-based fast multipole methods (FMM) on clusters of multicore processors. We propose both a hybrid MPI+task FMM parallelization and a pure task-based parallelization where the MPI communications are implicitly handled by the runtime system. The latter approach yields a very compact code following a sequential task-based programming model. We show that task-based approaches can compete with a hybrid MPI+OpenMP highly optimized code and that furthermore the compact task-based scheme fully matches the performance of the sophisticated, hybrid MPI+task version, ensuring performance while maximizing productivity. In [40] we illustrate our discussion with the ScalFMM FMM library and the StarPU runtime system.

7.4. Efficient algorithmic for load balancing and code coupling in complex simulations

7.4.1. Load Balancing for Coupled Simulations

In the field of scientific computing, the load balancing is an important step conditioning the performance of parallel programs. The goal is to distribute the computational load across multiple processors in order to minimize the execution time. This is a well-known problem that is unfortunately NP-hard. The most common approach to solve it is based on graph or hypergraph partitioning method, using mature and efficient software tools such as Metis, Zoltan or Scotch. Nowadays, numerical simulation are becoming more and more complex, mixing several models and codes to represent different physics or scales. Here, the key idea

is to reuse available legacy codes through a coupling framework instead of merging them into a standalone application. For instance, the simulation of the earth's climate system typically involves at least 4 codes for atmosphere, ocean, land surface and sea-ice. Combining such different codes are still a challenge to reach high performance and scalability. 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 codes and not only for each standalone code, as it is 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, that can dramatically decrease the overall performance. Therefore, one argues that it is required to model the coupling itself in order to ensure a good scalability, especially when running on tens of thousands of processors. In this work, we develop new algorithms to perform a coupling-aware partitioning of the whole application.

Surprisingly, we observe in our experiments that our proposed algorithms do not highly degrade the global edgcut for either component and thus the internal communication among processors of the same component is still minimized. This is not the case for the *Multiconst* method especially as the number of processors increases. Regarding the coupled simulation for the real application AVTP-AVBP (provided by Cerfacs), we noticed that one may carefully decide the parameters of the co-partitioning algorithms in order not to increase the global edgcut. More precisely, the number of processors assigned in the coupling interface is an important factor that needs to be determined based on the geometry of the problem and the ratio of the coupling interface compared to the entire domain. Again, we remark that our work on co-partitioning is still theoretical and further investigation should be conducted with different geometries and more coupled simulations that are more or less coupling-intensive.

This work corresponds to the PhD of Maria Predari, defended on December 9th 2016.

7.5. Application Domains

7.5.1. Material physics

7.5.1.1. Molecular vibrational spectroscopy

Quantum chemistry eigenvalue problem is a big challenge in recent research. Here we are interested in solving eigenvalue problems coming from the molecular vibrational analysis. These problems are challenging because the size of the vibrational Hamiltonian matrix to be diagonalized is exponentially increasing with the size of the molecule we are studying. So, for molecules bigger than 10 atoms the actual existent algorithms suffer from a curse of dimensionality or computational time.

A new variational algorithm called adaptive vibrational configuration interaction (A-VCI) intended for the resolution of the vibrational Schrödinger equation was developed. The main advantage of this approach is to efficiently reduce the dimension of the active space generated into the configuration interaction (CI) process. Here, we assume that the Hamiltonian writes as a sum of products of operators. This adaptive algorithm was developed with the use of three correlated conditions i.e. a suitable starting space; a criterion for convergence, and a procedure to expand the approximate space. The velocity of the algorithm was increased with the use of a posteriori error estimator (residue) to select the most relevant direction to increase the space. Two examples have been selected for benchmark. In the case of H₂CO, we mainly study the performance of A-VCI algorithm: comparison with the variation-perturbation method, choice of the initial space, residual contributions. For CH₃CN, we compare the A-VCI results with a computed reference spectrum using the same potential energy surface and for an active space reduced by about 90%. This work was published in [9].

7.5.1.2. Dislocations

We have focused on the improvements in collision detection in the Optidis Code. Junction formation mechanisms are essential to characterize material behavior such as strain hardening and irradiation effects. Dislocations junctions appear when dislocation segments collide with each other, therefore, reliable collision detection algorithms must be used to detect and handle junction formations. Collision detection is also a very costly operation in dislocation dynamics simulations, and performance must be carefully optimized to allow massive simulations.

During the first year of this PhD thesis, new collision algorithms have been implemented for the Dislocation Dynamics code OptiDis. The aim was to allow fast and accurate collision detection between dislocation segments using hierarchical methods. The complexity to solve the N-body collision problem can be reduced to $O(N)$ using spatial partitioning; computation can be accelerated using fast-reject techniques, and OpenMP parallelism. Finally, new collision handling algorithms for dislocations have been implemented to increase the reliability of the simulation.

7.5.2. Co-design for scalable numerical algorithms in scientific applications

7.5.2.1. Interior penalty discontinuous Galerkin method for coupled elasto-acoustic media

We introduce a high order interior penalty discontinuous Galerkin scheme for the numerical solution of wave propagation in coupled elasto-acoustic media. A displacement formulation is used, which allows for the solution of the acoustic and elastic wave equations within the same framework. Weakly imposing the correct transmission condition is achieved by the derivation of adapted numerical fluxes. This generalization does not weaken the discontinuous Galerkin method, thus *hp*-non-conforming meshes are supported. Interior penalty discontinuous Galerkin methods were originally developed for scalar equations. Therefore, we propose an optimized formulation for vectorial equations more suited than the straightforward standard transposition. We prove consistency and stability of the proposed schemes. To study the numerical accuracy and convergence, we achieve a classic plane wave analysis. Finally, we show the relevance of our method on numerical experiments.

More details on this work can be found in [47].

7.5.2.2. High performance simulation for ITER tokamak

Concerning the **GYSELA** global non-linear electrostatic code, the efforts during the period have concentrated on the design of a more efficient parallel gyro-average operator for the deployment of very large (future) **GYSELA** runs. The main unknown of the computation is a distribution function that represents either the density of the guiding centers, either the density of the particles in a tokamak. The switch between these two representations is done thanks to the gyro-average operator. In the previous version of **GYSELA**, the computation of this operator was achieved thanks to a Padé approximation. In order to improve the precision of the gyro-averaging, a new parallel version based on an Hermite interpolation has been done (in collaboration with the Inria **TONUS** project-team and IPP Garching). The integration of this new implementation of the gyro-average operator has been done in **GYSELA** and the parallel benchmarks have been successful. This work had been carried on in the framework of Fabien Rozar's PhD in collaboration with **CEA-IRFM** (defended in November 2015) and is continued in the PhD of Nicolas Bouzat funded by IPL **C2S@Exa**. The scientific objectives of this new work will be first to consolidate the parallel version of the gyro-average operator, in particular by designing a scalable MPI+OpenMP parallel version and using a new communication scheme, and second to design new numerical methods for the gyro-average, source and collision operators to deal with new physics in **GYSELA**. The objective is to tackle kinetic electron configurations for more realistic complex large simulations.

7.5.2.3. 3D aerodynamics for unsteady problems with bodies in relative motion

The first part of our research work concerning the parallel aerodynamic code FLUSEPA has been to design an operational MPI+OpenMP version based on a domain decomposition. We achieved an efficient parallel version up to 400 cores and the temporal adaptive method used without bodies in relative motion has been tested successfully for complex 3D take-off blast wave computations. Moreover, an asynchronous strategy for computing bodies in relative motion and mesh intersections has been developed and has been used for 3D stage separation cases. This first version is the current industrial production version of FLUSEPA for Airbus Safran Launchers.

However, this intermediate version shows synchronization problems for the aerodynamic solver due to the time integration used. To tackle this issue, a task-based version over the runtime system **StarPU** has been developed and evaluated. Task generation functions have been designed in order to maximize asynchronism during execution while respecting the data pattern access of the code. This led to the re-factorization of the FLUSEPA computation kernels. It's clearly a successful proof of concept as a task-based version is now

available for the aerodynamic solver and for both shared and distributed memory. It uses three parallelism levels : MPI processes between sub-domains, **StarPU** workers in shared memory (for each sub-domain) themselves running OpenMP parallel tasks. This version has been validated for large 3D take-off blast wave computations (80 millions of cells) and is much more efficient than the previous MPI+OpenMP version: we achieve a gain in computation time equal to 70 % for 320 cores and to 50 % for 560 cores. The next step will consist in extending the task-based version to the motion and intersection operations. This work has been carried on in the framework of Jean-Marie Couteyen's PhD (defended in September 2016) in collaboration with Airbus Safran Launchers ([2], [17]).

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Grants with Industry

Airbus Safran Launchers research and development contract:

- Design of a parallel version of the FLUSEPA software (Jean-Marie Couteyen (PhD); Pierre Brenner, Jean Roman).

Airbus Group Innovations research and development contract:

- Design and implementation of linear algebra kernel for FEM-BEM coupling (A. Falco (PhD); Emmanuel Agullo, Luc Giraud, Guillaume Sylvand).
- Design and implementation of FMM and block Krylov solver for BEM applications. The HiBOX project is led by the SME IMACS and funded by the DGA Rapid programme (C. Piacibello (Engineer), Olivier Coulaud, Luc Giraud).

9. Partnerships and Cooperations

9.1. National Initiatives

9.1.1. Inria Project Lab

9.1.1.1. C2S@Exa - Computer and Computational Sciences at Exascale

Since January 2013, the team is participating to the **C2S@Exa** Inria Project Lab (IPL). This national initiative aims at the development of numerical modeling methodologies that fully exploit the processing capabilities of modern massively parallel architectures in the context of a number of selected applications related to important scientific and technological challenges for the quality and the security of life in our society. At the current state of the art in technologies and methodologies, a multidisciplinary approach is required to overcome the challenges raised by the development of highly scalable numerical simulation software that can exploit computing platforms offering several hundreds of thousands of cores. Hence, the main objective of **C2S@Exa** is the establishment of a continuum of expertise in the computer science and numerical mathematics domains, by gathering researchers from Inria project-teams whose research and development activities are tightly linked to high performance computing issues in these domains. More precisely, this collaborative effort involves computer scientists that are experts of programming models, environments and tools for harnessing massively parallel systems, algorithmists that propose algorithms and contribute to generic libraries and core solvers in order to take benefit from all the parallelism levels with the main goal of optimal scaling on very large numbers of computing entities and, numerical mathematicians that are studying numerical schemes and scalable solvers for systems of partial differential equations in view of the simulation of very large-scale problems.

9.1.2. ANR

9.1.2.1. SOLHAR: SOLvers for Heterogeneous Architectures over Runtime systems

Participants: Emmanuel Agullo, Mathieu Faverge, Abdou Guermouche, Pierre Ramet, Jean Roman, Guillaume Sylvand.

Grant: ANR-MONU

Dates: 2013 – 2017

Partners: Inria (**REALOPT**, **STORM** Bordeaux Sud-Ouest et **ROMA** Rhone-Alpes), IRIT/INPT, CEA-CESTA et Airbus Group Innovations.

Overview:

During the last five years, the interest of the scientific computing community towards accelerating devices has been rapidly growing. The reason for this interest lies in the massive computational power delivered by these devices. Several software libraries for dense linear algebra have been produced; the related algorithms are extremely rich in computation and exhibit a very regular pattern of access to data which makes them extremely good candidates for GPU execution. On the contrary, methods for the direct solution of sparse linear systems have irregular, indirect memory access patterns that adversely interact with typical GPU throughput optimizations.

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 computer 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. To date, the approaches proposed to achieve this objective are mostly based on a simple offloading of some computational tasks 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. The development of a production-quality, sparse direct solver requires a considerable research effort along three distinct axes:

- linear algebra: algorithms have to be adapted or redesigned in order to exhibit properties that make their implementation and execution on heterogeneous computing platforms efficient and reliable. This may require the development of novel methods for defining data access patterns that are more suitable for the dynamic scheduling of computational tasks on processing units with considerably different capabilities as well as techniques for guaranteeing a reliable and robust behavior and accurate solutions. In addition, it will be necessary to develop novel and efficient accelerator implementations of the specific dense linear algebra kernels that are used within sparse, direct solvers;
- runtime systems: tools such as the **StarPU** runtime system proved to be extremely efficient and robust for the implementation of dense linear algebra algorithms. Sparse linear algebra algorithms, however, are commonly characterized by complicated data access patterns, computational tasks with extremely variable granularity and complex dependencies. Therefore, a substantial research effort is necessary to design and implement features as well as interfaces to comply with the needs formalized by the research activity on direct methods;
- scheduling: executing a heterogeneous workload with complex dependencies on a heterogeneous architecture is a very challenging problem that demands the development of effective scheduling algorithms. These will be confronted with possibly limited views of dependencies among tasks and multiple, and potentially conflicting objectives, such as minimizing the makespan, maximizing the locality of data or, where it applies, minimizing the memory consumption.

Given the wide availability of computing platforms equipped with accelerators and the numerical robustness of direct solution methods for sparse linear systems, it is reasonable to expect that the outcome of this project will have a considerable impact on both academic and industrial scientific computing. This project will moreover provide a substantial contribution to the computational science and high-performance computing communities, as it will deliver an unprecedented example of a complex numerical code whose parallelization completely relies on runtime scheduling systems and which is, therefore, extremely portable, maintainable and evolvable towards future computing architectures.

9.1.2.2. ANEMOS: Advanced Numeric for ELMs : Modeling and Optimized Schemes

Participants: Guillaume Latu, Pierre Ramet.

Grant: ANR-MN

Dates: 2012 – 2016

Partners: Univ. Nice, CEA/IRFM, CNRS/MDS.

Overview: The main goal of the project is to make a significant progress in understanding of active control methods of plasma edge MHD instabilities Edge Localized Modes (ELMs) which represent particular danger with respect to heat and particle loads for Plasma Facing Components (PFC) in ITER. The project is focused in particular on the numerical modelling study of such ELM control methods as Resonant Magnetic Perturbations (RMPs) and pellet ELM pacing both foreseen in ITER. The goals of the project are to improve understanding of the related physics and propose possible new strategies to improve effectiveness of ELM control techniques. The tool for the non-linear MHD modeling is the **JOREK** code which was essentially developed within previous ANR **ASTER**. **JOREK** will be largely developed within the present project to include corresponding new physical models in conjunction with new developments in mathematics and computer science strategy. The present project will put the non-linear MHD modeling of ELMs and ELM control on the solid ground theoretically, computationally, and applications-wise in order to progress in urgently needed solutions for ITER.

Regarding our contributions, the **JOREK** code is mainly composed of numerical computations on 3D data. The toroidal dimension of the tokamak is treated in Fourier space, while the poloidal plane is decomposed in Bezier patches. The numerical scheme used involves a direct solver on a large sparse matrix as a main computation of one time step. Two main costs are clearly identified: the assembly of the sparse matrix, and the direct factorization and solve of the system that includes communications between all processors. The efficient parallelization of **JOREK** is one of our main goals, to do so we will reconsider: data distribution, computation distribution or GMRES implementation. The quality of the sparse solver is also crucial, both in term of performance and accuracy. In the current release of **JOREK**, the memory scaling is not satisfactory to solve problems listed above, since at present as one increases the number of processes for a given problem size, the memory footprint on each process does not reduce as much as one can expect. In order to access finer meshes on available supercomputers, memory savings have to be done in the whole code. Another key point for improving parallelization is to carefully profile the application to understand the regions of the code that do not scale well. Depending on the timings obtained, strategies to diminish communication overheads will be evaluated and schemes that improve load balancing will be initiated. **JOREK** uses **PaStiX** sparse matrix library for matrix inversion. However, large number of toroidal harmonics and particular thin structures to resolve for realistic plasma parameters and ITER machine size still require more aggressive optimisation in numeric dealing with numerical stability, adaptive meshes etc. However many possible applications of **JOREK** code we proposed here which represent urgent ITER relevant issues related to ELM control by RMPs and pellets remain to be solved.

9.1.2.3. *DEDALES: Algebraic and geometric domain decomposition for subsurface/groundwater flows*

Participants: Emmanuel Agullo, Mathieu Faverge, Luc Giraud, Louis Poirel.

Grant: ANR-14-CE23-0005

Dates: 2014 – 2018

Partners: Inria EPI POMDAPI (leader); Université Paris 13 - Laboratoire Analyse, Géométrie et Applications; Maison de la Simulation; Andra.

Overview: Project **DEDALES** aims at developing high performance software for the simulation of two phase flow in porous media. The project will specifically target parallel computers where each node is itself composed of a large number of processing cores, such as are found in new generation many-core architectures. The project will be driven by an application to radioactive waste deep geological disposal. Its main feature is phenomenological complexity: water-gas flow in highly heterogeneous medium, with widely varying space and time scales. The assessment of large scale model is of major importance and issue for this application, and realistic geological models have several million grid cells. Few, if at all, software codes provide the necessary physical features with massively parallel simulation capabilities. The aim of the **DEDALES** project is to study, and experiment with, new approaches to develop effective simulation tools with the capability to take advantage of modern computer architectures and their hierarchical structure. To achieve this goal, we will explore two complementary software approaches that both match the hierarchical hardware architecture: on the one hand, we will integrate a hybrid parallel linear solver into an existing flow and transport code, and on the other hand, we will explore a two level approach with the outer level using (space time) domain decomposition,

parallelized with a distributed memory approach, and the inner level as a subdomain solver that will exploit thread level parallelism. Linear solvers have always been, and will continue to be, at the center of simulation codes. However, parallelizing implicit methods on unstructured meshes, such as are required to accurately represent the fine geological details of the heterogeneous media considered, is notoriously difficult. It has also been suggested that time level parallelism could be a useful avenue to provide an extra degree of parallelism, so as to exploit the very large number of computing elements that will be part of these next generation computers. Project **DEDALES** will show that space-time DD methods can provide this extra level, and can usefully be combined with parallel linear solvers at the subdomain level. For all tasks, realistic test cases will be used to show the validity and the parallel scalability of the chosen approach. The most demanding models will be at the frontier of what is currently feasible for the size of models.

9.1.2.4. *TECSER: Novel high performance numerical solution techniques for RCS computations*

Participants: Emmanuel Agullo, Luc Giraud, Matthieu Kuhn.

Grant: ANR-14-ASTRID

Dates: 2014 – 2017

Partners: Inria EPI NACHOS (leader), Corida, HiePACS; Airbus Group Innovations, Nucléutudes.

Overview: the objective of the TECSER projet is to develop an innovative high performance numerical methodology for frequency-domain electromagnetics with applications to RCS (Radar Cross Section) calculation of complicated structures. This numerical methodology combines a high order hybridized DG method for the discretization of the frequency-domain Maxwell in heterogeneous media with a BEM (Boundary Element Method) discretization of an integral representation of Maxwell's equations in order to obtain the most accurate treatment of boundary truncation in the case of theoretically unbounded propagation domain. Beside, scalable hybrid iterative/direct domain decomposition based algorithms are used for the solution of the resulting algebraic system of equations.

9.2. European Initiatives

9.2.1. FP7 & H2020 Projects

9.2.1.1. *EoCoE*

Title: Energy oriented Centre of Excellence for computer applications

Programm: H2020

Duration: October 2015 - October 2018

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: Michel Kern

The aim of the present proposal is to establish an Energy Oriented Centre of Excellence for computing applications, (EoCoE). EoCoE (pronounce “Echo”) will use the prodigious potential offered by the ever-growing computing infrastructure to foster and accelerate the European transition to a reliable and low carbon energy supply. To achieve this goal, we believe that the present revolution in hardware technology calls for a similar paradigm change in the way application codes are designed. EoCoE will assist the energy transition via targeted support to four renewable energy pillars: Meteo, Materials, Water and Fusion, each with a heavy reliance on numerical modelling. These four pillars will be anchored within a strong transversal multidisciplinary basis providing high-end expertise in applied mathematics and HPC. EoCoE is structured around a central Franco-German hub coordinating a pan-European network, gathering a total of 8 countries and 23 teams. Its partners are strongly engaged in both the HPC and energy fields; a prerequisite for the long-term sustainability of EoCoE and also ensuring that it is deeply integrated in the overall European strategy for HPC. The primary goal of EoCoE is to create a new, long lasting and sustainable community around computational energy science. At the same time, EoCoE is committed to deliver high-impact results within the first three years. It will resolve current bottlenecks in application codes, leading to new modelling capabilities and scientific advances among the four user communities; it will develop cutting-edge mathematical and numerical methods, and tools to foster the usage of Exascale computing. Dedicated services for laboratories and industries will be established to leverage this expertise and to foster an ecosystem around HPC for energy. EoCoE will give birth to new collaborations and working methods and will encourage widely spread best practices.

9.2.1.2. HPC4E

Title: HPC for Energy

Programm: H2020

Duration: December 2015 - November 2017

Coordinator: Barcelona Supercomputing Center

Partners:

Centro de Investigaciones Energeticas, Medioambientales Y Tecnologicas-Ciemat (Spain)

Iberdrola Renovables Energia (Spain)

Repsol (Spain)

Total S.A. (France)

Lancaster University (United Kingdom)

Inria contact: Stéphane Lanteri

This project aims to apply the new exascale HPC techniques to energy industry simulations, customizing them, and going beyond the state-of-the-art in the required HPC exascale simulations for different energy sources: wind energy production and design, efficient combustion systems for biomass-derived fuels (biogas), and exploration geophysics for hydrocarbon reservoirs. For wind energy industry HPC is a must. The competitiveness of wind farms can be guaranteed only with accurate wind resource assessment, farm design and short-term micro-scale wind simulations to forecast the daily power production. The use of CFD LES models to analyse atmospheric flow in a wind farm capturing turbine wakes and array effects requires exascale HPC systems. Biogas, i.e. biomass-derived fuels by anaerobic digestion of organic wastes, is attractive because of its wide availability, renewability and reduction of CO₂ emissions, contribution to diversification of energy supply, rural development, and it does not compete with feed and food feedstock. However, its use in practical systems is still limited since the complex fuel composition might lead to unpredictable combustion performance and instabilities in industrial combustors. The next generation of exascale HPC systems will be able to run combustion simulations in parameter regimes relevant to industrial

applications using alternative fuels, which is required to design efficient furnaces, engines, clean burning vehicles and power plants. One of the main HPC consumers is the oil & gas (O&G) industry. The computational requirements arising from full wave-form modelling and inversion of seismic and electromagnetic data is ensuring that the O&G industry will be an early adopter of exascale computing technologies. By taking into account the complete physics of waves in the subsurface, imaging tools are able to reveal information about the Earth's interior with unprecedented quality.

9.2.1.3. EXA2CT

Title: EXascale Algorithms and Advanced Computational Techniques

Programm: FP7

Duration: September 2013 - August 2016

Coordinator: IMEC

Partners:

Fraunhofer-Gesellschaft Zur Foerderung Der Angewandten Forschung E.V (Germany)

Interuniversitair Micro-Electronica Centrum Vzw (Belgium)

Intel Corporations (France)

Numerical Algorithms Group Ltd (United Kingdom)

T-Systems Solutions for Research (Germany)

Universiteit Antwerpen (Belgium)

Universita della Svizzera italiana (Switzerland)

Universite de Versaillesint-Quentin-En-Yvelines. (France)

Vysoka Skola Banska - Technicka Univerzita Ostrava (Czech Republic)

Inria contact: Luc Giraud

Numerical simulation is a crucial part of science and industry in Europe. The advancement of simulation as a discipline relies on increasingly compute intensive models that require more computational resources to run. This is the driver for the evolution to exascale. Due to limits in the increase in single processor performance, exascale machines will rely on massive parallelism on and off chip, with a complex hierarchy of resources. The large number of components and the machine complexity introduce severe problems for reliability and programmability. The former of these will require novel fault-aware algorithms and support software. In addition, the scale of the numerical models exacerbates the difficulties by making the use of more complex simulation algorithms necessary, for numerical stability reasons. A key example of this is increased reliance on solvers. Such solvers require global communication, which impacts scalability, and are often used with preconditioners, increasing complexity again. Unless there is a major rethink of the design of solver algorithms, their components and software structure, a large class of important numerical simulations will not scale beyond petascale. This in turn will hold back the development of European science and industry which will fail to reap the benefits from exascale. The EXA2CT project brings together experts at the cutting edge of the development of solvers, related algorithmic techniques, and HPC software architects for programming models and communication. It will take a revolutionary approach to exascale solvers and programming models, rather than the incremental approach of other projects. We will produce modular open source proto-applications that demonstrate the algorithms and programming techniques developed in the project, to help boot-strap the creation of genuine exascale codes.

9.3. International Initiatives

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

9.3.1.1. MORSE

Title: Matrices Over Runtime Systems @ Exascale

International Partner (Institution - Laboratory - Researcher):

KAUST Supercomputing Laboratory (United States) - KSL - Hatem Ltaief

Start year: 2011

See also: <http://icl.cs.utk.edu/morse/index.html>

The goal of Matrices Over Runtime Systems at Exascale (MORSE) project is to design dense and sparse linear algebra methods that achieve the fastest possible time to an accurate solution on large-scale multicore systems with GPU accelerators, using all the processing power that future high end systems can make available. To develop software that will perform well on petascale and exascale systems with thousands of nodes and millions of cores, several daunting challenges have to be overcome, both by the numerical linear algebra and the runtime system communities. By designing a research framework for describing linear algebra algorithms at a high level of abstraction, the MORSE team will enable the strong collaboration between research groups in linear algebra, runtime systems and scheduling needed to develop methods and libraries that fully benefit from the potential of future large-scale machines. Our project will take a pioneering step in the effort to bridge the immense software gap that has opened up in front of the High-Performance Computing (HPC) community.

9.3.1.2. FASTLA

Title: Fast and Scalable Hierarchical Algorithms for Computational Linear Algebra

International Partner (Institution - Laboratory - Researcher):

Stanford University (USA) - Institute for Computational and Mathematical Engineering -
Eric Darve

Start year: 2015

See also: http://people.bordeaux.inria.fr/coulaud/projets/FastLA_Website/

In this project, we propose to study fast and scalable hierarchical numerical kernels and their implementations on heterogeneous manycore platforms for two major computational kernels in intensive challenging applications. Namely, fast multipole methods (FMM) and sparse linear solvers that appear in many intensive numerical simulations in computational sciences. For the solution of large linear systems, the ultimate goal is to design parallel scalable methods that rely on efficient sparse and dense direct methods using H-matrix arithmetic. Finally, the innovative algorithmic design will be essentially focused on heterogeneous manycore platforms by using task based runtime systems. The partners, Inria HiePACS, Lawrence Berkeley Nat. Lab and Stanford University, have strong, complementary and recognized experiences and backgrounds in these fields

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

10.1.1.1. General Chair, Scientific Chair

PMAA'16 The 9th International Workshop on Parallel Matrix Algorithms and Applications (PMAA16) was held in Bordeaux (France) and run from July 6 to 8, 2016.

10.1.1.2. Member of the Organizing Committees

The members of **HIEPACS** were involved in the **PMAA'16** organizing committees.

10.1.2. Scientific Events Selection

10.1.2.1. Member of the Conference Program Committees

IEEE PDP'16 (J. Roman), IPDPS'16 (L. Giraud), HiPC'16 (A. Guermouche), PDCN'16 (L. Giraud), PDSEC'16 (O. Coulaud, L. Giraud), SC'16 (E. Agullo, L. Giraud).

10.1.3. Journal

10.1.3.1. Member of the Editorial Boards

L. Giraud is member of the editorial board of the SIAM Journal on Matrix Analysis and Applications (SIMAX).

10.1.3.2. Reviewer - Reviewing Activities

ACM Trans. on Mathematical Software, Advances in Computational Mathematics, Computing and Fluid, IEEE Trans. on Parallel and Distributed Systems, International Journal of High Performance Computing Applications, Journal of Computational Physics, Journal of Scientific Computing, Linear algebra with applications, Mathematics and Computers in Simulation, Parallel Computing, SIAM J. Matrix Analysis and Applications, SIAM J. Scientific Computing, Theory of Computing Systems.

10.1.4. Invited Talks

L. Giraud, "Hard faults and soft-errors: possible numerical remedies in linear algebra solvers", VecPar'16, Porto.

10.1.5. Scientific Expertise

- E. Agullo: US Department of Energy's (DOE's) Exascale Computing Project (ECP) reviewing for research and development in Software Technology, specifically in the area of Math Libraries.
- P. Ramet is "Scientific Expert" at the CEA-DAM CESTA since oct. 2015.
- 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 Technical Group of GENCI and of the Scientific Advisory Board of the Maison de la Simulation.

10.1.6. Research Administration

Jean Roman is a member of the Direction for Science at Inria : he is the Deputy Scientific Director of the Inria research domain entitled *Applied Mathematics, Computation and Simulation* and is in charge at the national level of the Inria activities concerning High Performance Computing.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

We indicate below the number of hours spent in teaching activities on a yearly basis for each scientific staff member involved.

Undergraduate level/Licence

- A. Esnard: System programming 36h, Computer architecture 40h, Network 23h at Bordeaux University.
- M. Faverge: Programming environment 26h, Numerical algorithmic 30h, C projects 20h at Bordeaux INP (ENSEIRB-MatMeca).
- P. Ramet: System programming 24h, Databases 32h, Object programming 48h, Distributed programming 32h, Cryptography 32h 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 24h, Hierarchical methods 8h 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).
- M. Faverge: System programming 74h, Load balancing and scheduling 13h at Bordeaux INP (ENSEIRB-MatMeca).
He is also in charge of the second year of Embedded Electronic Systems option at Bordeaux INP (ENSEIRB-MatMeca).
- L. Giraud: Introduction to intensive computing and related programming tools 20h, INSA Toulouse; Introduction to high performance computing and applications 20h, ISAE; On mathematical tools for numerical simulations 10h, ENSEEIHT Toulouse; Parallel sparse linear algebra 11h at Bordeaux INP (ENSEIRB-MatMeca).
- A. Guermouche: Network management 92h, Network security 64h, Operating system 24h at Bordeaux University.
- P. Ramet: Load balancing and scheduling 13h, Numerical algorithms 30h at Bordeaux INP (ENSEIRB-MatMeca). He also gives classes on Cryptography 30h, Ho Chi Minh City in Vietnam.
- J. Roman: Parallel sparse linear algebra 10h, Algorithmic and parallel algorithms 22h at Bordeaux INP (ENSEIRB-MatMeca).
He is also in charge of the last year “Parallel and Distributed Computing” option at ENSEIRB-MatMeca which is specialized in HPC (methodologies and applications). This is a common training curriculum between Computer Science and MatMeca departments at Bordeaux INP and with Bordeaux University in the context of Computer Science Research Master. It provides a lot of well-trained internship students for Inria projects working on HPC and simulation.

Summer School: on an annual basis, we run a three day advanced training (lecture and hands on) on parallel linear algebra in the framework of the European PRACE PATC (PRACE Advanced Training Centres) initiative. This training has been organized in many places in France and will be held next year in Ostrava - Czech Republic.

10.2.2. Supervision

PhD in progress : Pierre Blanchard; Fast hierarchical algorithms for the low-rank approximation of dense matrices and applications ; O. Coulaud, E. Darve.

PhD in progress : Nicolas Bouzat; Fine grain algorithms and deployment methods for exascale plasma physic applications ; M.Mehrenberger, J.Roman, G. Latu (CEA Cadarache).

PhD : Jean-Marie Couteyen Carpaye; Contributions to the parallelization and the scalability of the FLUSEPA code; defended on September 19th; P. Brenner, J. Roman.

PhD in progress : Arnaud Durocher; High performance Dislocation Dynamics simulations on heterogeneous computing platforms for the study of creep deformation mechanisms for nuclear applications; O. Coulaud, L. Dupuy (CEA).

PhD in progress : Aurélien Falco; Data sparse calculation in FEM/BEM solution; E. Agullo, L. Giraud, G. Sylvand.

PhD in progress : Cyril Fournier; Task based programming for unstructured mesh calculations; L. Giraud, G. Stafelbach.

PhD in progress : Grégoire Pichon; Utilisation de techniques de compression \mathcal{H} -matrices pour solveur direct creux parallèle dans le cadre des applications FEM; L. Giraud, P. Ramet.

PhD in progress : Louis Poirel; Algebraic coarse space correction for parallel hybrid solvers; E. Agullo, L. Giraud.

PhD : Maria Predari; Load balancing for parallel coupled simulations; defended on December 9th; A. Esnard, J. Roman.

10.2.3. Juries

- Okba Hamitou, "Efficient preconditioning method for the CARP-CG iterative solver for the solution of the frequency- domain visco-elastic wave equation", referee: Jan S. Hesthaven, Luc Giraud; Université de Grenoble, spécialité: mathématiques appliquées, 22 Décembre 2016.
- Jean-Charles Papin, "A Scheduling and Partitioning Model for Stencil-based Applications on Many-Core Devices", referee Jean-François Méhaut, Olivier Coulaud; Université Paris-Saclay préparée à l'École Normale Supérieure de Cachan spécialité: mathématiques appliquées, 8 Septembre 2016.

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Publications of the year

Doctoral Dissertations and Habilitation Theses

- [1] B. BRAMAS. *Optimization and parallelization of the boundary element method for the wave equation in time domain*, Université de Bordeaux, February 2016, <https://tel.archives-ouvertes.fr/tel-01306571>.
- [2] J. M. COUTEYEN CARPAYE. *Contributions to the parallelization and the scalability of the FLUSEPA code*, Université de Bordeaux, September 2016, <https://tel.archives-ouvertes.fr/tel-01399952>.
- [3] P. MARIA. *Load Balancing for Parallel Coupled Simulations*, Université de Bordeaux, 2016.

Articles in International Peer-Reviewed Journal

- [4] E. AGULLO, P. R. AMESTOY, A. BUTTARI, A. GUERMOUCHE, J.-Y. L'EXCELLENT, F.-H. ROUET. *Robust memory-aware mappings for parallel multifrontal factorizations*, in "SIAM Journal on Scientific Computing", July 2016, vol. 38, n^o 3, 23, <https://hal.inria.fr/hal-01334113>.
- [5] E. AGULLO, B. BRAMAS, O. COULAUD, E. DARVE, M. MESSNER, T. TAKAHASHI. *Task-based FMM for heterogeneous architectures*, in "Concurrency and Computation: Practice and Experience", June 2016, vol. 28, n^o 9 [DOI : 10.1002/CPE.3723], <https://hal.inria.fr/hal-01359458>.
- [6] E. AGULLO, A. BUTTARI, A. GUERMOUCHE, F. LOPEZ. *Implementing multifrontal sparse solvers for multicore architectures with Sequential Task Flow runtime systems*, in "ACM Transactions on Mathematical Software", July 2016 [DOI : 10.1145/0000000.0000000], <https://hal.inria.fr/hal-01333645>.
- [7] E. AGULLO, L. GIRAUD, A. GUERMOUCHE, J. ROMAN, M. ZOUNON. *Numerical recovery strategies for parallel resilient Krylov linear solvers*, in "Numerical Linear Algebra with Applications", May 2016, <https://hal.inria.fr/hal-01323192>.
- [8] E. AGULLO, L. GIRAUD, P. SALAS, M. ZOUNON. *Interpolation-restart strategies for resilient eigensolvers*, in "SIAM Journal on Scientific Computing", 2016, vol. 38, n^o 5, p. C560-C583 [DOI : 10.1137/15M1042115], <https://hal.inria.fr/hal-01347793>.

- [9] R. GARNIER, M. ODUNLAMI, V. LE BRIS, D. BÉGUÉ, I. BARAILLE, O. COULAUD. *Adaptive vibrational configuration interaction (A-VCI): a posteriori error estimation to efficiently compute anharmonic IR spectra*, in "Journal of Chemical Physics", May 2016, vol. 144, n^o 20, <https://hal.inria.fr/hal-01310708>.

Invited Conferences

- [10] E. AGULLO, S. COOLS, L. GIRAUD, A. MOREAU, P. SALAS, W. VANROOSE, E. F. YETKIN, M. ZOUNON. *Hard faults and soft errors: possible numerical remedies in linear algebra solvers*, in "VecPar - International meeting on High Performance Computing for Computational science", Porto, Portugal, June 2016, <https://hal.inria.fr/hal-01334675>.

International Conferences with Proceedings

- [11] E. AGULLO, O. BEAUMONT, L. EYRAUD-DUBOIS, S. KUMAR. *Are Static Schedules so Bad ? A Case Study on Cholesky Factorization*, in "IEEE International Parallel & Distributed Processing Symposium (IPDPS 2016)", Chicago, IL, United States, IEEE, May 2016, <https://hal.inria.fr/hal-01223573>.
- [12] E. AGULLO, G. BOSILCA, A. BUTTARI, A. GUERMOUCHE, F. LOPEZ. *Exploiting a Parametrized Task Graph model for the parallelization of a sparse direct multifrontal solver*, in "Euro-Par 2016: Parallel Processing Workshops", Grenoble, France, August 2016, <https://hal.archives-ouvertes.fr/hal-01337748>.
- [13] E. AGULLO, L. GIRAUD, A. GUERMOUCHE, S. NAKOV, J. ROMAN. *Task-based Conjugate Gradient: from multi-GPU towards heterogeneous architectures*, in "HeteroPar'2016 workshop of Euro-Par", Grenoble, France, August 2016, <https://hal.inria.fr/hal-01334734>.
- [14] E. AGULLO, L. GIRAUD, S. NAKOV. *Task-based sparse hybrid linear solver for distributed memory heterogeneous architectures*, in "HeteroPar'2016 workshop of Euro-Par", Grenoble, France, August 2016, <https://hal.inria.fr/hal-01334738>.
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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

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- 9.4.2. - Mathematics

1. Members

Research Scientists

Andreas Enge [Team leader, Inria, Senior Researcher, HDR]
Fredrik Johansson [Inria, Researcher]
Damien Robert [Inria, Researcher]

Faculty Members

Karim Belabas [Univ. Bordeaux, Professor, HDR]
Guilhem Castagnos [Univ. Bordeaux, Associate Professor]
Jean-Paul Cerrri [Univ. Bordeaux, Associate Professor]
Jean-Marc Couveignes [Univ. Bordeaux I, Professor, HDR]

Technical Staff

Jared Guissmo Asuncion [Inria, from Oct 2016]
Bill Allombert [CNRS]

PhD Students

Pınar Kılıçer [Universities Leiden and Bordeaux]
Chloë Martindale [Universities Leiden and Bordeaux]
Iuliana Ciocanea-Teodorescu [Universities Leiden and Bordeaux]
Emmanouil Tzortzakos [Universities Leiden and Bordeaux]

Post-Doctoral Fellows

Cyril Bouvier [Univ. Bordeaux, until May 2016]
Enea Milio [Inria, until Mars 2016]

Visiting Scientists

Francisco Diaz Y Diaz [retraité]
Guillaume Hitsch [Univ. Blaise Pascal, Mar 2016]
Abdoulaye Maiga [Univ. Dakar, from Nov 2016]
Bernadette Perrin-Riou [Univ. Paris XI]

Administrative Assistants

Anne-Laure Gautier [Inria]
Joelle Rodrigues [Inria]

Other

Zhengying Liu [Inria, Master 1 Internship, from Mar 2016 until Jul 2016]

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 Schönhage–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, Karim Belabas, Cyril Bouvier, Jean-Paul Cerri, Iuliana Ciocanea-Teodorescu, Henri Cohen, Jean-Marc Couveignes, Andreas Enge, Fredrik Johansson, Pınar Kılıçer.

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 $n \geq 3$. For recent textbooks, see [5]. 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 $\sqrt[5]{3}$ 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 $\sqrt[5]{3}$ 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* $h_K = |\text{Cl}_K|$ 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 [28] 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 , $\zeta_K(s) := \prod_{\mathfrak{p} \text{ prime ideal of } \mathcal{O}_K} (1 - N\mathfrak{p}^{-s})^{-1}$, 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, Enea Milio, Damien Robert, Emmanouil Tzortzakis.

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 $g \geq 2$.

The cryptosystem is implemented in an associated finite abelian group, the *Jacobian* $\text{Jac}_{\mathcal{C}}$. 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 $\text{Jac}_{\mathcal{C}}$ 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 $(\sqrt{q} - 1)^{2g} \leq |\text{Jac}_{\mathcal{C}}| \leq (\sqrt{q} + 1)^{2g}$, or $|\text{Jac}_{\mathcal{C}}| \approx q^g$, 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 $\text{Jac}_{\mathcal{C}}$, it must be difficult to determine x . Computing x corresponds in fact to computing $\text{Jac}_{\mathcal{C}}$ 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 $\text{Jac}_{\mathcal{C}}$ 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: Karim Belabas, Henri Cohen, Jean-Marc Couveignes, Andreas Enge, Fredrik Johansson, Chloë Martindale, Enea Milio, Damien Robert.

Complex multiplication provides a link between number fields and algebraic curves; for a concise introduction in the elliptic curve case, see [30], for more background material, [29]. In fact, for most curves \mathcal{C} over a finite field, the endomorphism ring of $\text{Jac}_{\mathcal{C}}$, 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* $\text{Gal}_{H/K}$ 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 $\text{Gal}_{H/K}$ 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

Release of Pari 2.9 after two years of development. This stable releases includes three brand new modules (L -functions, Associative and Central Simple Algebras, and Modular Symbols), a major overhaul of the Elliptic Curves and Number Fields modules.

Iuliana Ciocanea-Teodorescu has defended her PhD thesis on *Algorithms for finite rings* in June 2016 <http://www.theses.fr/2016BORD0121>.

Pinar Kiliçer has defended her PhD thesis on *The class number one problem for genus-2 curves* in July 2016 [11].

5. New Software and Platforms

5.1. APIP

Another Pairing Implementation in PARI
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: Jérôme Milan
- URL: <http://www.lix.polytechnique.fr/~milanj/apip/apip.xhtml>

5.2. Arb

FUNCTIONAL DESCRIPTION

Arb is a C library for arbitrary-precision floating-point ball arithmetic. It supports real and complex numbers, polynomials, power series, matrices, and evaluation of many transcendental functions. All is done with automatic, rigorous error bounds. It has been accepted for inclusion in SageMath.

- Participant: Fredrik Johansson
- Contact: Fredrik Johansson
- URL: <http://fredrikj.net/arb/>

5.3. AVIsogenies

Abelian Varieties and Isogenies

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 (1,1)-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: Gaëtan Bisson, Romain Cosset and Damien Robert
- Contact: Damien Robert
- URL: <http://avisogenies.gforge.inria.fr/>

5.4. CM

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.

- Participant: Andreas Enge
- Contact: Andreas Enge
- URL: <http://www.multiprecision.org/index.php?prog=cm&page=home>

5.5. 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: Emmanuel Thomé, Andreas Enge and Regis Dupont
- Contact: Emmanuel Thomé
- URL: <http://cmh.gforge.inria.fr>

5.6. CUBIC

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-1.3.tgz>

5.7. Euclid

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: Pierre Lezowski and Jean-Paul Cerri
- Contact: Pierre Lezowski
- URL: <http://www.math.u-bordeaux1.fr/~plezowsk/euclid/index.php>

5.8. FLINT

FUNCTIONAL DESCRIPTION FLINT is a C library for number theory and basic computer algebra, maintained by William Hart with code by William Hart, Sebastian Pancratz, Andy Novocin, Fredrik Johansson, Tom Bachmann, Mike Hansen, Martin Lee, David Harvey, and a large number of other authors.

FLINT is used as a back end library for polynomial arithmetic and number theory functionality in a large number of applications, including SageMath and Singular.

- Participant: Fredrik Johansson
- Contact: William Hart
- URL: <http://flintlib.org/>

5.9. GNU MPC

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.

- Participants: Andreas Enge, Paul Zimmermann, Philippe Theveny and Mickaël Gastineau
- Contact: Andreas Enge
- URL: <http://www.multiprecision.org/>

5.10. KleinianGroups

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>

5.11. mpmath

FUNCTIONAL DESCRIPTION mpmath is a Python library for real and complex floating-point arithmetic with arbitrary precision. It has been developed by Fredrik Johansson since 2007, with help from many contributors.

As a dependency of the SymPy computer algebra system as well as SageMath, mpmath is a core component of the Python scientific software ecosystem.

- Participant: Fredrik Johansson
- Contact: Fredrik Johansson
- URL: <http://mpmath.org/>

5.12. MPFRCX

FUNCTIONAL DESCRIPTION

Mpfrx 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.

- Participant: Andreas Enge
- Contact: Andreas Enge
- URL: <http://www.multiprecision.org/index.php?prog=mpfrx>

5.13. Nemo

FUNCTIONAL DESCRIPTION Nemo is a computer algebra package for the Julia programming language maintained by William Hart with code by William Hart, Tommy Hofmann, Claus Fieker, Fredrik Johansson, Oleksandr Motsak).

The features of Nemo include multiprecision integers and rationals, integers modulo n , p -adic numbers, finite fields (prime and non-prime order), number field arithmetic, maximal orders of number fields, arithmetic of ideals in maximal orders, arbitrary precision real and complex balls, generic polynomials, power series, fraction fields, residue rings and matrices.

- Participant: Fredrik Johansson
- Contact: William Hart
- URL: <http://nemocas.org/>

5.14. PARI/GP

FUNCTIONAL DESCRIPTION

Pari/Gp is a widely used computer algebra system designed for fast computations in number theory (factorisation, algebraic number theory, elliptic curves, ...), 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: Karim Belabas, Bill Allombert, Henri Cohen and Andreas Enge
- Contact: Karim Belabas
- URL: <http://pari.math.u-bordeaux.fr/>

6. New Results

6.1. Class invariants in genus 2

Abelian surfaces, or equivalently, Jacobian varieties of genus 2 hyperelliptic curves, offer the same security as elliptic curves in a cryptographic setting and often better efficiency, and could thus be an attractive alternative. The theory of complex multiplication can be used to obtain cryptographically secure curves. Relying on Shimura reciprocity for Siegel modular forms, we have developed the necessary mathematical theory in [24]. It requires deeper algebraic reasoning than for elliptic curves: Ideals of the endomorphism rings of the abelian varieties are no more two-dimensional modules over the integers, but two-dimensional projective modules over quadratic number rings. We succeed in proving results adapted from the elliptic curve case by suitably normalising quadratic forms over number rings and using strong approximation. The result is an elegant theory that leads to clearly formulated and practical algorithms, which we illustrate by examples.

6.2. Elliptic curve and Abelian varieties cryptology

Participant: Damien Robert.

The paper [15] in which David Lubicz and Damien Robert explain how to improve the arithmetic of Abelian and Kummer varieties has been published in the journal *Finite Fields and Their Applications*. The speed of the arithmetic is a crucial factor in the performance of cryptosystems based on abelian varieties. Depending on the cryptographic application, the speed record holders are elliptic curves (in the Edwards model) or the Kummer surface of an hyperelliptic curves of genus 2 (in the level 2 theta model). One drawback of the Kummer surface is that only scalar multiplications are available, which may be a problem in certain cryptographic protocols. The previous known models to work on the Jacobian rather than the Kummer surface (Mumford coordinates or the theta model of level 4) are too slow and not competitive with elliptic curves. This paper explains how to use geometric properties (like projective normality) to speed up the arithmetic. In particular it introduces a novel addition algorithm on Kummer varieties (compatible addition), and uses it to speed up multi-exponentiations in Kummer varieties and to obtain new models of abelian surfaces in which the scalar multiplication is as fast as on the Kummer surface.

Theta functions, and in particular the Dedekind eta function, are at the heart of complex multiplication constructions of curves. They can be written as sparse power series with coefficients ± 1 . In [23] we devise optimised addition sequences for the occurring exponents, with a proof relying on classical number theory, which help us gain a factor of 2 compared to the standard approach and which is validated in practice by our two independent implementations. Using an approach from computer algebra and a proof relying on analytic number theory, we obtain another factor of 2.

6.3. Symbolic computation

The article [27], of which F. Johansson is a coauthor, was published. The article describes SymPy, an open source computer algebra system written in pure Python. It is built with a focus on extensibility and ease of use, through both interactive and programmatic applications. These characteristics have led SymPy to become a popular symbolic library for the scientific Python ecosystem. This paper presents the architecture of SymPy, a description of its features, and a discussion of select submodules. The supplementary material provide additional examples and further outline details of the architecture and features of SymPy.

Hypergeometric functions are among the most important mathematical functions, with a wide range of applications in everything from physics to number theory. The practical computation of such functions is a challenging problem. The preprint [26], presents an efficient implementation of hypergeometric functions in arbitrary-precision interval arithmetic. The functions ${}_0F_1$, ${}_1F_1$, ${}_2F_1$ and ${}_2F_0$ (or the Kummer U -function) are supported for unrestricted complex parameters and argument, and by extension, we cover exponential and trigonometric integrals, error functions, Fresnel integrals, incomplete gamma and beta functions, Bessel functions, Airy functions, Legendre functions, Jacobi polynomials, complete elliptic integrals, and other special functions. The output can be used directly for interval computations or to generate provably correct floating-point approximations in any format. Performance is competitive with earlier arbitrary-precision software, and sometimes orders of magnitude faster. We also partially cover the generalized hypergeometric function ${}_pF_q$ and computation of high-order parameter derivatives.

The preprint [25] is the corresponding paper for the software Arb developed by F. Johansson. Arb is a C library for arbitrary-precision interval arithmetic using the midpoint-radius representation, also known as ball arithmetic. It supports real and complex numbers, polynomials, power series, matrices, and evaluation of many special functions. The core number types are designed for versatility and speed in a range of scenarios, allowing performance that is competitive with non-interval arbitrary-precision types such as MPFR and MPC floating-point numbers. This paper discusses the low-level number representation, strategies for precision and error bounds, and the implementation of efficient polynomial arithmetic with interval coefficients.

6.4. Logarithmic Class Groups

Logarithmic class groups and units, introduced by Jaulent in 1994, are an intriguing ℓ -adic variation on the classical class and unit groups related to Iwasawa theory and the wild kernels of algebraic K -theory. These \mathbb{Z}_ℓ -modules of finite type provide direct access to invariants studied in standard conjectures about \mathbb{Z}_ℓ -extensions. In [12] we devised a new algorithm to explicitly compute them in subexponential time under standard conjectures (GRH and Gross-Kuz'min) and to validate unconditionally the computed results (now in exponential time). The algorithm has been implemented in the PARI/GP system.

6.5. Class groups and other invariants of number fields

The article by H. Cohen and F. Thorne on Dirichlet series associated to quartic fields with given cubic resolvent has been published. This article gives an explicit formula for the Dirichlet series $\sum_K |\Delta(K)|^{-s}$, where the sum is over isomorphism classes of all quartic fields whose resolvent field is isomorphic to a fixed cubic field k .

The article [22] by H. Cohen and F. Thorne generalizes the work of A. Morra and the authors, on giving explicit formulas for the Dirichlet series generating function of D_ℓ extensions of odd prime degree ℓ with given quadratic resolvent. Over the course of the proof, the authors explain connections between their formulas and the Ankeny-Artin-Chowla conjecture, the Ohno-Nakagawa relation for binary cubic forms, and other topics.

In her thesis, Iuliana Ciocanea-Teodorescu describes algorithms that answer questions arising in ring and module theory. The first main result of this thesis concerns the module isomorphism problem, how to compute a set of generators of minimal cardinality, and how to construct projective covers and injective hulls. The thesis also describe tests for module simplicity, projectivity, and injectivity, and constructive tests for existence of surjective module homomorphisms between two finite modules, one of which is projective. As a negative result, the problem of testing for existence of injective module homomorphisms between two finite modules, one of which is projective, is NP-complete. The last part of the thesis is concerned with finding a good working approximation of the Jacobson radical of a finite ring, that is, a two-sided nilpotent ideal such that the corresponding quotient ring is almost semisimple. The notion used to approximate semisimplicity is that of separability.

In her thesis [11], Pinar Kiliçer determines all CM curves of genus 2 defined over the reflex field. This extends the previous CM class number one problem for elliptic curves which asked to find all elliptic curves defined over the rationals with non-trivial endomorphism ring.

6.6. Number and function fields

The article [13] written by J. Brau and J. Nathan on "Elliptic curves with 2-torsion contained in the 3-torsion field" has been published. This article study the modular curve $X'(6)$ of level 6 defined over \mathbb{Q} whose \mathbb{Q} -rational points correspond to j -invariants of elliptic curves E over \mathbb{Q} for which $\mathbb{Q}(E[2])$ is a subfield of $\mathbb{Q}(E[3])$. The authors characterize the j -invariants of elliptic curves with this property by exhibiting an explicit model of $X'(6)$. $X'(6)(\mathbb{Q})$ then gives an infinite family of examples of elliptic curves with non-abelian "entanglement fields," which is relevant to the systematic study of correction factors of various conjectural constants for elliptic curves over \mathbb{Q} .

7. Partnerships and Cooperations

7.1. National Initiatives

7.1.1. ANR *Simpatic* – SIM and PAiring Theory for Information and Communications security

Participants: Guilhem Castagnos, Damien Robert.

<http://simpatic.orange-labs.fr>

The SIMPATIC project is an industrial research project, formed by academic research teams and industrial partners: Orange Labs, École Normale Supérieure, INVIA, Oberthur Technologies, ST-Ericsson France, Université de Bordeaux 1, Université de Caen Basse-Normandie, Université de Paris 8.

The aim of the SIMPATIC project is to provide the most efficient and secure hardware/software implementation of a bilinear pairing in a SIM card. This implementation will then be used to improve and develop new cryptographic algorithms and protocols in the context of mobile phones and SIM cards. The project will more precisely focus on e-ticketing and e-cash, on cloud storage and on the security of contactless and of remote payment systems.

D. Robert is a participant in the Task 2 whose role is to give state of the art algorithms for pairing computations, adapted to the specific hardware requirements of the Simpatic Project.

G. Castagnos is a participant in the Task 4 whose role is to design new cryptographic primitives adapted to the specific applications of the Simpatic Project.

The SIMPATIC project has ended in August 2016. The project has shown that pairings can now efficiently be integrated into smart cards publicly deployed, by obtaining performances that outperform the state of the art. Cryptographic tools designed by the project are moreover capable of combining complex functionalities and efficiency in many areas such as digital signatures, minimization of personal data in contactless services, pay TV, or protecting data stored in an untrusted cloud.

7.1.2. 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.

7.2. European Initiatives

7.2.1. FP7 & H2020 Projects

7.2.1.1. ANTICS

Title: Algorithmic Number Theory in Computer Science

Program: FP7

Duration: January 2012 - December 2016

Coordinator: Inria

Inria contact: Andreas Enge

'During the past twenty years, we have witnessed profound technological changes, summarised under the terms of digital revolution or entering the information age. It is evident that these technological changes will have a deep societal impact, and questions of privacy and security are primordial to ensure the survival of a free and open society. Cryptology is a main building block of any security solution, and at the heart of projects such as electronic identity and health cards, access control, digital content distribution or electronic voting, to mention only a few important applications. During the past decades, public-key cryptology has established itself as a research topic in computer science; tools of theoretical computer science are employed to "prove" the security of cryptographic primitives such as encryption or digital signatures and of more complex protocols. It is often forgotten, however, that all practically relevant public-key cryptosystems are rooted in pure mathematics, in particular, number theory and arithmetic geometry. In fact, the so-called security "proofs" are all conditional to the algorithmic untractability of certain number theoretic problems, such as factorisation of large integers or discrete logarithms in algebraic curves. Unfortunately, there is a large cultural gap between computer scientists using a black-box security reduction to a supposedly hard problem in algorithmic number theory and number theorists, who are often interested in solving small and easy instances of the same problem. The theoretical grounds on which current algorithmic number theory operates are actually rather shaky, and cryptologists are generally unaware of this fact. The central goal of ANTICS is to rebuild algorithmic number theory on the firm grounds of theoretical computer science.'

Title: OpenDreamKit

Program: H2020

Duration: January 2016 - December 2020

Inria contact: Karim Belabas

Description http://cordis.europa.eu/project/rcn/198334_en.html, <http://opendreamkit.org>

7.3. International Initiatives

7.3.1. Inria International Labs

7.3.1.1. International Laboratory for Research in Computer Science and Applied Mathematics

MACISA

Title: Mathematics Applied to Cryptology and Information Security in Africa

International Partner (Institution - Laboratory - Researcher):

Université des Sciences et Techniques de Masuku (Gabon) - Faculté des Sciences - Dpt de Mathématiques et Informatique - Tony Ezome

Duration: 2012 - 2016

The project aims at understanding the role played by algebraic maps in public key cryptography. Since this is a very broad topic, we will focus on objects of dimension zero (finite sets and rings) and one (algebraic curves, their differentials and jacobians). The proposed project-team consists of African and French researchers working in mathematical and statistical aspects of public-key cryptology. The French researchers work in the Inria project-team LFANT in Bordeaux, and the IRMAR (Institut de Recherche en Mathématiques et Applications de Rennes) in Rennes. The African researchers already cooperate in the project PRMAIS (Pole of Research in Mathematics and their Applications in Information Security in Sub-Saharan Africa) supported by the Simons' foundation.

The project is managed by a team of five permanent researchers: G. Nkiet, J.-M. Couveignes, T. Ezome, D. Robert and A. Enge. Since Sep. 2014 the coordinator is T. Ezome and the vice-coordinator is D. Robert. The managing team organises the cooperation, schedules meetings, prepares reports, controls expenses, reports to the LIRIMA managing team and administrative staff.

A non-exhaustive list of activities organised or sponsored by Macisa includes

- The Summer school (EMA) in Bamenda with the International Center for Pure and Applied Mathematics (ICPAM/CIMPA), June 2016;
- The visit of Abdoulaye Maiga in Bordeaux to work with D. Robert on canonical lifts of genus 2 curves.

2016 was the last year of Macisa. A new project FAST “(Harder Better) FAster STronger cryptography” has been proposed as an associated team between LFANT and the PREMA (Pole of Research in Mathematics and Applications in Africa) Simon’s foundation project.

7.3.2. Inria International Partners

7.3.2.1. Informal International Partners

The team is used to collaborate with Leiden University through the ALGANT program for PhD joint supervision.

Eduardo Friedman (U. of Chile), long term collaborator of K. Belabas and H. Cohen 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 Enea Milio (Inria Nancy Grand Est), Gregor Seiler (ETH Zurich), Aurélien Focqué (Industry) and Razvan Barbulescu (University Paris 6). Researchers visiting the team for collaboration include Bernadette Perrin-Riou (Paris-Sud).

7.4.2. Visits to International Teams

F. Johansson visited during 1 week the PolSys team at LIP6, Pierre et Marie Curie University.

F. Johansson visited during 1 week (two times) with the Computer Algebra group, TU Kaiserslautern.

8. Dissemination

8.1. Promoting Scientific Activities

8.1.1. Scientific Events Selection

8.1.1.1. Member of the Conference Program Committees

A. Enge: 20th Workshop on Elliptic Curve Cryptography ECC 2016, İzmir

D. Robert was a member of the scientific committee for the Ecole Mathématique Africaine organised by Emmanuel Fouotsa at Bamenda.

F. Johansson organized the session: High-precision arithmetic, effective analysis and special functions. ICMS 2016, The 5th International Congress on Mathematical Software, ZIB Berlin.

8.1.2. Journal

8.1.2.1. Member of the Editorial Boards

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 editorial board member of *Journal de Théorie des Nombres de Bordeaux*; he is an editor for the Springer book series *Algorithms and Computations in Mathematics (ACM)*.

J.-M. Couveignes is a member of the editorial board of the *Publications mathématiques de Besançon* since 2010.

A. Enge is an editor of *Designs, Codes and Cryptography* since 2004.

8.1.2.2. Reviewer - Reviewing Activities

F. Johansson reviewed for IEEE Transactions on Circuits and Systems I, IEEE Transactions on Computers, and ACM Transactions on Mathematical Software.

8.1.3. Invited Talks

- A. Enge: Mathematical Structures for Cryptography, Leiden: Short addition sequences for theta functions
- F. Johansson: talk at RAIM 2016, Banyuls-sur-mer on "Fast reversion of formal power series" and at FastRelax meeting, LAAS-CNRS, Toulouse on "Hypergeometric functions in Arb".

8.1.4. Scientific Expertise

J.-M. Couveignes is a member of the scientific council of the labex "Fondation Sciences Mathématiques de Paris", FSMP, Paris.

J.-M. Couveignes is a member of the 'conseil d'orientation' of the labex "Institut de Recherche en Mathématiques, Interactions et Applications", IRMIA, Strasbourg.

8.1.5. Research Administration

A. Enge: Head of COST-GTRI, responsible for the scientific evaluation of all international cooperations of Inria

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 is a member of the "Conseil National des Universités" (25th section, pure mathematics).

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.

Since January 2015, J.-M. Couveignes is the head of the Math Institute (IMB).

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*, 60h, M2, University of Bordeaux, France;

Master : D. Robert, *Courbes elliptiques*, 60h, M2, University of Bordeaux, France;

8.2.2. Supervision

Pinar Kiliçer: The class number one problem for genus-2 curves, Universities of Bordeaux and Leiden, supervised by A. Enge, M. Streng and P. Stevenhagen.

Iuliana Ciocanea-Teodorescu, Algorithms for finite rings, Universities of Bordeaux and Leiden, supervised by K. Belabas and H. Lenstra.

PhD in progress: Abdoulaye Maïga, *Computing canonical lift of genus 2 hyperelliptic curves*, University Dakar, supervised by Djiby Sow, Abdoul Aziz Ciss and D. Robert.

PhD in progress: Emmanouil Tzortzakis *Algorithms for \mathbb{Q} -curves*, supervised by K. Belabas and P. Bruin

PhD in progress: Pavel Solomatin *Topics on L-functions*, supervised by B. de Smit and K. Belabas

Liu Zhengying: Height of class polynomials. Ecole Polytechnique third year internship, supervised by D. Robert.

8.2.3. Juries

- PhD report by A. Enge on Loubna Ghammam: Utilisation des couplages en cryptographie asymétrique pour la micro-électronique, University of Rennes
- PhD report and jury by D. Robert on Alina Dudeanu: Computational Aspects of Jacobians of Hyperelliptic Curves, EPFL.
- D. Robert is a member of the jury of Agregations de Mathématiques. He is also the codirector with Alain Couvreur of the option “calcul formel” of the Modelisation part of the oral examination.

8.3. Popularization

D. Robert wrote with Sorina Ionica the chapter “Pairings” of the book Guide to Pairing-Based Cryptography [16] which will be published by CHAPMAN and HALL/CRC. This book aims to help Engineers understand and implement pairing based cryptography. In the Chapter Pairings D. Robert give a self contained definition and proof of the Weil and Tate pairing; including how to handle divisors with non disjoint support (this is often skipped in scientific papers but is important for practical implementations).

H. Cohen wrote a vulgarisation article [17] on Fermat’s last theorem. This article explain (through the example of congruent numbers) the role of elliptic curves and algebraic number theory in the solution of Fermat’s last theorem.

During the last PARIatelier four talks [19], [18], [20], [21] have been filmed and are available under a creative common licence. This will allow people from all the world to get started faster with PARI. The first two talks focus on setting up personal computers for the atelier and the new features of PARI. The next two are more technical and explain the new L-functions and modular forms features.

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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:

- 6. - Modeling, simulation and control
 - 6.1. - Mathematical Modeling
 - 6.1.1. - Continuous Modeling (PDE, ODE)
 - 6.1.4. - Multiscale modeling
 - 6.1.5. - Multiphysics modeling
 - 6.2. - Scientific Computing, Numerical Analysis & Optimization
 - 6.2.1. - Numerical analysis of PDE and ODE
 - 6.2.7. - High performance computing

Other Research Topics and Application Domains:

- 3. - Environment and planet
 - 3.3. - Geosciences
 - 3.3.1. - Earth and subsoil
- 4. - Energy
 - 4.1. - Fossile energy production (oil, gas)
- 5.5. - Materials

1. Members

Research Scientists

Hélène Barucq [Team leader, Inria, Senior Researcher, HDR]
Juliette Chabassier [Inria, Researcher]
Julien Diaz [Inria, Researcher, HDR]

Faculty Members

Marc Duruflé [Bordeaux INP, Associate Professor]
Victor Péron [Univ. Pau, Associate Professor]
Sébastien Tordeux [Univ. Pau, Associate Professor, HDR]

Technical Staff

Lionel Boillot [Inria, granted by Total E&p Recherche Développement]
Marie Bonnasse-Gahot [Inria, granted by Total E&p Recherche Développement]
Simon Ettouati [Inria, granted by Min. de L'Ens. Sup. et de la Rech., until Sep 2016]
Florian Faucher [Inria, granted by Total E&p Recherche Développement]

PhD Students

Izar Azpiroz Irigorri [Univ. Pau, granted by Min. de L'Ens. Sup. et de la Rech.]
Aurelien Citrain [Insa Rouen, granted by Min. de L'Ens. Sup. et de la Rech., from May 2016]
Vincent Darrigrand [Univ. Pau, Ikerbasque]
Aralar Erdozain [Inria, Cordi-S]
Hamza Hafidi Alaoui [Univ. Bordeaux, granted by Min. de L'Ens. Sup. et de la Rech.]
Justine Labat [Univ. Pau, from Mar 2016, granted by Min. de L'Ens. Sup. et de la Rech.]
Mamadou N'Diaye [Univ. Pau, granted by Total E&p Recherche Développement and by Conseil Général des Pyrénées Atlantiques]

Chengyi Shen [Univ. Pau, from Oct 2016, granted by Min. de L'Ens. Sup. et de la Rech.]

Elvira Shishenina [Inria, granted by Total E&p Recherche Developpement]

Post-Doctoral Fellow

Ha Pham [Inria]

Administrative Assistant

Sylvie Embolla [Inria]

Others

Mohamed Amara [Univ. Pau, Professor, HDR]

Anh-Tuan Ha [Inria, Internship, from May 2016 until Sep 2016]

Baptiste Olivier [Inria, Internship, from Jul 2016 until Aug 2016]

Remy Sourial [Inria, Internship, from Jun 2016 until Sep 2016]

2. Overall Objectives

2.1. General setting

MAGIQUE-3D is a joint project-team between Inria and the Department of Applied Mathematics (LMA) of the University of Pau, in partnership with CNRS. The 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.

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 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, and (c) the development of asymptotic models that are the primary candidate in the presence of heterogeneities that are small compared to the wave length. 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 at Bilbao, Spain; University of Novosibirsk, Russia).

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 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 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 can contribute to this task by improving the modeling and by deriving advanced numerical methods for solving wave problems.

Magique-3D proposes to organize its research around three main axes:

1. Mathematical modeling of multi-physics involving wave equations;
2. Supercomputing for Helmholtz problems;
3. Construction of high-order hybrid schemes.

These three research fields will be developed with the main objective of solving inverse problems dedicated to geophysical imaging.

3.2. Mathematical modeling of multi-physics involving wave equations

Wave propagation modeling is of great interest for many applications like oil and gas exploration, non destructive testing, medical imaging, etc. It involves equations which can be solved in time or frequency domain and their numerical approximation is not easy to handle, in particular when dealing with real-world problems. In both cases, the propagation domain is either infinite or its dimensions are much greater than the characteristic wavelength of the phenomenon of interest. But since wave problems are hyperbolic, the physical phenomenon can be accurately described by computing solutions in a bounded domain including the sources which have generated the waves. Until now, we have mainly worked on imaging techniques based on acoustic or elastic waves and we have developed advanced finite element software packages which are used by Total for oil exploration. Nevertheless, research on modeling must go on because there are simulations which can still not be performed because their computational cost is much too high. This is particularly true for complex tectonics involving coupled wave equations. We then propose to address the issue of coupling wave equations problems by working on the mathematical construction of reduced systems. By this way, we hope to improve simulations of elasto-acoustic and electro-seismic phenomena and then, to perform numerical imaging of strongly heterogeneous media. Even in the simplest situation where the wavelengths are similar (elasto-acoustic coupling), the dimension of the discrete coupled problem is huge and it is a genuine issue in the prospect of solving 3D inverse problems.

The accurate numerical simulation of full wave problems in heterogeneous media is computationally intensive since it needs numerical schemes based on grids. The size of the cells depends on the propagation velocity of waves. When coupling wave problems, conversion phenomena may occur and waves with very different propagation velocity coexist. The size of the cells is then defined from the smallest velocity and in most of the real-world cases, the computational cost is crippling. Regarding existing computing capabilities, we propose to derive intermediate models which require less computational burden and provide accurate solutions for a wide-ranging class of problems including Elasto-acoustics and Electro-seismology.

When it comes to mathematical analysis, we have identified two tasks which could help us simulate realistic 3D multi-physics wave problems and which are in the scope of our *savoir-faire*. They are construction of approximate and multiscale models which are different tasks. The construction of approximate problems aims at deriving systems of equations which discrete formulation involves middle-sized matrices and in general, they are based on high frequency hypothesis. Multiscale models are based on a rigorous analysis involving a small parameter which does not depend on the propagation velocity necessarily.

Recently, we have conducted research on the construction of approximate models for offshore imaging. Elastic and acoustic wave equations are coupled and we investigate the idea of eliminating the computations inside water by introducing equivalent interface conditions on the sea bottom. We apply an On-Surface-Radiation-Condition (OSRC) which is obtained from the approximation of the acoustic Dirichlet-to-Neumann (DtN) operator [74], [53]. To the best of our knowledge, OSRC method has never been used for solving reduced coupling wave problems and preliminary promising results are available at [56]. We would like to investigate this technique further because we could form a battery of problems which can be solved quickly. This would provide a set of solutions which we could use as initial guess for solving inverse problems. But we are concerned with the performance of the OSRC method when wave conversions with different wavelengths occur. Anyway, the approximation of the DtN operator is not obvious when the medium is strongly heterogeneous and multiscale analysis might be more adapted. For instance, according to existing results in Acoustics and Electromagnetism for the modeling of wire antennas [65], multiscale analysis should turn out to be very efficient when the propagation medium includes well logs, fractures and faults which are very thin structures when compared to the wavelength of seismic waves. Moreover, multiscale analysis should perform well when the medium is strongly oscillating like porous media. It could thus provide an alternative to homogenization techniques which can be applied only when the medium is periodic. We thus propose to develop reduced multi-scale models by performing rigorous mathematical procedure based on regular and singular multiscale analysis. Our approach distinguishes itself from others because it focuses on the numerical representation of small structures by time-dependent problems. This could give rise to the development of new finite element methods which would combine DG approximations with XFEM (Extended Finite Element Method) which has been created for the finite element treatment of thin structures like cracks.

But Earth imaging must be more than using elasto-acoustic wave propagation. Electromagnetic waves can also be used and in collaboration with Prof. D. Pardo (Iker Basque Foundation and University of Bilbao), we conduct researches on passive imaging to probe boreholes. Passive imaging is a recent technique of imaging which uses natural electromagnetic fields as sources. These fields are generated by hydromagnetic waves propagating in the magnetosphere which transform into electromagnetic waves when they reach the ionosphere. This is a mid-frequency imaging technique which applies also to mineral and geothermal exploration, to predict seismic hazard or for groundwater monitoring. We aim at developing software package for resistivity inversion, knowing that current numerical methods are not able to manage 3D inversion. We have obtained results based on a Petrov-Galerkin approximation [50], but they are limited to 2D cases. We have thus proposed to reduce the 3D problem by using 1D semi-analytic approximation of Maxwell equations [78]. This work has just started in the framework of a PhD thesis and we hope that it will give us the possibility of imaging 3D problems.

Magique-3D would like to expand its know-how by considering electro-seismic problems which are in the scope of coupling electromagnetic waves with seismic waves. Electro-seismic waves are involved in porous media imaging which is a tricky task because it is based on the coupling of waves with very different wavelengths described by Biot equations and Maxwell equations. Biot equations govern waves in saturated porous media and they represent a complex physical phenomenon involving a slow wave which is very difficult to simulate numerically. In [72], interesting results have been obtained for the simulation of piezoelectric sensors. They are based on a quasi-static approximation of the Maxwell model coupled with Elastodynamics. Now, we are concerned with the capability of using this model for Geophysical Imaging and we believe that the derivation and/or the analysis of suitable modelings is necessary. Collaborations with Geophysicists are thus mandatory in the prospect of using both experimental and numerical approaches. We would like to collaborate with Prof. C. Bordes and Prof. D. Brito (Laboratory of Complex Fluids and their Reservoirs, CNRS and University of Pau) who have efficient experimental devices for the propagation of electromagnetic waves inside saturated porous media [55]. This collaboration should be easy to organize since Magique-3D has a long-term experience in collaborating with geophysicists. We then believe that we will not need a lot of time to get joint results since we can use our advanced software packages Hou10ni and Montjoie and our colleagues have already obtained data. Electro-seismology is a very challenging research domain for us and we would like to enforce our collaborations with IsTerre (Institute of Earth Science, University of Grenoble) and for that topic with Prof. S. Garambois who is an expert in Electro-seismology [80], [81], [69], [70]. A joint research program could gather Geophysicists from the University of Pau and from IsTerre and Magique-3D.

In particular, it would be interesting to compare simulations performed with Hou10ni, Montjoie, with the code developed by Prof. S. Garambois and to use experimental simulations for validation.

3.3. Supercomputing for Helmholtz problems

Probing invisible with harmonic equations is a need for many scientists and it is also a topic offering a wealth of interesting problems for mathematicians. It is well-known that Helmholtz equations discretization is very sensitive to the frequency scale which can be wide-ranging for some applications. For example, depth imaging is searching for deeper layers which may contain hydrocarbons and frequencies must be of a few tens of Hertz with a very low resolution. If it is to detect hidden objects, the depth of the explored region does not exceed a few tens of meters and frequencies close to the kiloHertz are used. High performing numerical methods should thus be stable for a widest as possible frequency range. In particular, these methods should minimize phenomena of numerical pollution that generate errors which increase faster with frequency than with the inverse of space discretization step. As a consequence, there is a need of mesh refinement, in particular at high frequency.

During the period 2010-2014, the team has worked extensively on high order discontinuous Galerkin (DG) methods. Like standard Finite Element Methods, they are elaborated with polynomial basis functions and they are very popular because they are defined locally for each element. It is thus easy to use basis polynomial functions with different degrees and this shows the perfect flexibility of the approximation in case of heterogeneous media including homogeneous parts. Indeed, low degree basis functions can be used in heterogeneous regions where a fine grid is necessary while high degree polynomials can be used for coarse elements covering homogeneous parts. In particular, Magique-3D has developed Hou10ni that solves harmonic wave equations with DG methods and curved elements. We found that both the effects of pollution and dispersion, which are very significant when a conventional finite element method is used, are limited [57]. However, bad conditioning is persisting and reliability of the method is not guaranteed when the coefficients vary considerably. In addition, the number of unknowns of the linear system is too big to hope to solve a realistic 3D problem. So it is important to develop approximation methods that require fewer degrees of freedom. Magique-3D wishes to invest heavily in the development of new approximation methods for harmonic wave equations. It is a difficult subject for which we want to develop different tasks, in collaboration with academic researchers with whom we are already working or have established contacts. Research directions that we would like to follow are the following.

First, we will continue our long-term collaboration with Prof. Rabia Djellouli. We want to continue to work on hybrid finite element methods that rely on basis functions composed of plane waves and polynomials. These methods have demonstrated good resistance to the phenomenon of numerical pollution [51], [52], but their capability of solving industrial problems has not been illustrated. This is certainly due to the absence of guideline for choosing the plane waves. We are thus currently working on the implementation of a methodology that makes the choice of plane waves automatic for a given simulation (fixed propagation domain, data source, etc.). This is up-front investigation and there is certainly a lot of remaining work before being applied to geophysical imaging. But it gives the team the opportunity to test new ideas while remaining in contact with potential users of the methods.

Then we want to work with Prof. A. Bendali on developing methods of local integral equations which allow calculation of numerical fluxes on the edges of elements. One could then use these fluxes in a DG method for reconstructing the solution throughout the volume of calculation. This research is motivated by recent results which illustrate the difficulties of the existing methods which are not always able to approximate the propagating modes (plane waves) and the evanescent modes (polynomials) that may coexist, especially when one considers realistic applications. Integral equations are direct tools for computing fluxes and they are known for providing very good accuracy. They thus should help to improve the quality of approximation of DG methods which are fully flux-dependent. In addition, local integral equations would limit calculations at the interfaces, which would have the effect of limiting the number of unknowns generally high, especially for DG methods. Again, it is a matter of long-term research which success requires a significant amount of mathematical analysis, and also the development of non-trivial code.

To limit the effects of pollution and dispersion is not the only challenge that the team wants to tackle. Our experience alongside Total has made us aware of the difficulties in constructing meshes that are essential to achieve our simulations. There are several teams at Inria working on mesh generation and we are in contact with them, especially with Gamma3 (Paris-Rocquencourt Research Center). These teams develop meshes increasingly sophisticated to take account of the constraints imposed by realistic industrial benchmarks. But in our opinion, issues which are caused by the construction of meshes are not the only downside. Indeed, we have in mind to solve inverse problems and in this case it is necessary to mesh the domain at each iteration of Newton-type solver. It is therefore interesting to work on methods that either do not use mesh or rely on meshes which are very easy to construct. Regarding meshless methods, we have begun a collaboration with Prof. Djellouli which allowed us to propose a new approach called Mesh-based Frontier Free Formulation (MF3). The principle of this method is the use of fundamental solutions of Helmholtz equations as basic functions. One can then reduce the volumic variational formulation to a surfacic variational formulation which is close to an integral equation, but which does not require the calculation of singularities. The results are very promising and we hope to continue our study in the context of the application to geophysical imaging. An important step to validate this method will be particularly its extension to 3D because the results we have achieved so far are for 2D problems.

Keeping in mind the idea of limiting the difficulties of mesh, we want to study the method of virtual elements. This method attracts us because it relies on meshes that can be made of arbitrarily-shaped polygon and meshes should thus be fairly straightforward. Existing works on the subject have been mainly developed by the University of Pavia, in collaboration with Los Alamos National Laboratory [54], [61], [60], [58], [62]. None of them mentions the feasibility of the method for industrial applications and to our knowledge, there are no results on the method of virtual elements applied to the wave equations. First, we aim at applying the method described in [59] to the scalar Helmholtz equation and explore opportunities to use discontinuous elements within this framework. Then hp-adaptivity could be kept, which is particularly interesting for wave propagation in heterogeneous media.

DG methods are known to require a lot of unknowns that can exceed the limits accepted by the most advanced computers. This is particularly true for harmonic wave equations that require a large number of discretization points, even in the case of a conventional finite element method. We therefore wish to pursue a research activity that we have just started in collaboration with the project-team Nachos (Sophia-Antipolis Méditerranée Research Center). In order to reduce the number of degrees of freedom, we are interested in "hybrid mixed" Discontinuous Galerkin methods that provides a two-step procedure for solving the Helmholtz equations [73], [77], [76]. First, Lagrange multipliers are introduced to represent the flux of the numerical solution through the interface (edge or face) between two elements. The Lagrange multipliers are solution to a linear system which is constructed locally element by element. The number of degrees of freedom is then strongly reduced since for a standard DG method, there is a need of considering unknowns including volumetric values inside the element. And obviously, the gain is even more important when the order of the element is high. Next, the solution is reconstructed from the values of the multipliers and the cost of this step is negligible since it only requires inverting small-sized matrices. We have obtained promising results in the framework of the PhD thesis of Marie Bonnasse-Gahot and we want to apply it to the simulation of complex phenomena such as the 3D viscoelastic wave propagation.

Obviously, the success of all these works depends on our ability to consider realistic applications such as wave propagation in the Earth. And in these cases, it is quite possible that even if we manage to develop accurate less expensive numerical methods, the solution of inverse problems will still be computationally intensive. It is thus absolutely necessary that we conduct our research by taking advantage of the latest advances in high-performance computing. We have already initiated discussions with the project team HIEPACS (Bordeaux Sud-Ouest research Center) to test the performance of the latest features of Mumps <http://mumps.enseciht.fr/>, such as Low Rank Approximation or adaptation to hybrid CPU / GPU architectures and to Intel Xeon Phi, on realistic test cases. We are also in contact with the team Algorithm at Cerfacs (Toulouse) for the development of local integral equations solvers. These collaborations are essential for us and we believe that they will be decisive for the simulation of three-dimensional elasto-dynamic problems. However, our scientific contribution will be limited in this area because we are not experts in HPC.

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 [66], [63], [79], [75], [68] 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 [71].

Recently, Dolean *et al* [67] 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 [64]. 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 Hiepac 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.

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 5.3. 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. New Software and Platforms

5.1. Elasticus

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 DIVA and developed 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. Developed features should be easily transferred in the computing platform of Total. Contrary to DIVA which only computes approximate solutions with P1, P2 and P3 elements, Elasticus manages arbitrary orders for the spatial discretization with DG method.

- Participants: Simon Ettouati, Julien Diaz and Lionel Boillot
- Partner: TOTAL
- Contact: Julien Diaz

5.2. Hou10ni

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).

- Participants: Julien Diaz, Marie Bonnasse-Gahot and Lionel Boillot
- Contact: Julien Diaz

5.3. Montjoie

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, elasto-dynamic 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. For time-domain simulations, a wide range of ODE (Ordinary Differential Equation) solvers have been implemented : high-order explicit or implicit time schemes. Several applications are currently available : wave equation, elastodynamics, aero-acoustics, Maxwell's equations.

- Participants: Marc Duruflé, Juliette Chabassier, Mamadou N'Diaye and Michaël Leguèbe
- Contact: Marc Duruflé
- URL: <http://montjoie.gforge.inria.fr/>

5.4. TMBM-DG

Time-Marching Based Methods-Discontinuous Galerkin

SCIENTIFIC DESCRIPTION TMBM-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 TMBM-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.

- Participants: Julien Diaz, Lionel Boillot and Simon Ettouati
- Partner: TOTAL
- Contact: Julien Diaz

6. New Results

6.1. Seismic Imaging and Inverse Problems

6.1.1. Time-harmonic inverse problem

Participants: H el ene Barucq, Florian Faucher.

We study the seismic inverse problem for acoustic and elastic medium associated with the time-harmonic wave equation, and the underlying recovery of geophysical parameters. We employ Full Waveform Inversion (FWI) where the multi parameters reconstruction is based on iterative minimization techniques. This inverse problem shows a Lipschitz stability where the stability constant is related to the (conditional) lower bound of the Fr echet derivative, when assuming a piecewise constant representation of the parameters. We successively estimate the stability constant for different model partition in order to control the convergence of the scheme. Hence we define a multi-level (multi-scale, multi-frequency) algorithm where the natural progression of frequency is paired with the model partition. The method is implemented and numerical experiments are performed for elastic medium reconstruction, in particular for realistic geophysical situations.

6.1.2. *Shape-reconstruction and parameter identification of an elastic object immersed in a fluid*

Participants: Izar Azpiroz Irigorri, H el ene Barucq, Julien Diaz, Rabia Djellouli.

We investigate the inversion of a series of parameters in the context of a 2D elasto-acoustic scattering problem. The inverse problem is solved by using a Newton-like method, where the shape of the scatterer is assumed to be Lipschitz-continuous. Herein, we want to recover the shape and the material parameters in the case of isotropic and anisotropic materials. Based on the different influences of these parameters on the far field pattern, the final goal is to propose an iterative algorithm to retrieve the parameters separately, by devoting some iterations to the reconstruction of the shape and the others to the determination of the parameters. On the other hand, due to the difficulties to retrieve the material parameters, the penetrability of scatters have been studied. The conclusion has been that the recovery of material parameters can be feasible, provided that the scattered waves are not completely reflected. The results of this work have been presented to the conference Inverse Problems for PDE in Bremen, Germany [24].

6.2. Mathematical modeling of multi-physics involving wave equations

6.2.1. *A study of the numerical robustness of single-layer method with Fourier basis for multiple obstacle scattering in homogeneous media*

Participants: H el ene Barucq, Juliette Chabassier, Ha Pham, S ebastien Tordeux.

We investigate efficient methods to solve direct and inverse problems for the propagation of acoustic wave in strongly inhomogeneous media in low-frequency regime. We start our investigation with inhomogeneities created by compactly-supported and non-overlapping obstacles. With a large number of small obstacles, optimized softwares based on Finite Element Method (FEM) lose their robustness. As an alternative, we work with an integral equation method, which uses single-layer potentials and truncation of Fourier series to describe the scattered field. We limit our numerical experiments to disc-shaped obstacles. We first compare our method with Montjoie (a FEM-based software); secondly, we investigate the efficiency of different solver types (direct and iterative) in solving the dense linear system generated by the method. We observe that the optimal choice depends on the distance between obstacles, their size and number, and applications.

6.2.2. *Derivation and validation of impedance transmission conditions for the electric potential across a highly conductive casing*

Participants: H el ene Barucq, Aralar Erdozain, David Pardo, Victor P eron.

Borehole resistivity measurements are a common procedure when trying to obtain a better characterization of the Earth's subsurface. The possible risk of having borehole collapses makes the employment of a casing very suitable for this type of scenarios. Such casing protects the borehole but it also highly complicates the resistivity measurements due to the thinness of the casing and the large contrasts between the conductivities of the casing and the rock formations.

This work is motivated by realistic configurations where the resistivity of the casing is proportional to the cube of the thickness of the casing. In this framework, our aim is to derive Impedance Transmission Conditions (ITCs) for the electromagnetic field across such a casing. As a first approach we derive ITCs for the electric potential. We consider a transmission problem for the static case of the electric potential, set in an axisymmetric borehole shaped domain. This domain is composed of three different subdomains, the interior part of the borehole, the rock formations and the metallic casing.

In this framework, we address the issue of ITCs using two different approaches. The first one consists in deriving ITCs across the casing itself, whereas the second approach tackles the problem by deriving ITCs on an artificial interface located in the middle of the casing. We derive different models for the two considered approaches and we numerically assess them with a finite element method implementation. Then we perform a comparison on these models by showing the advantages and drawbacks of each model. Finally, we show an application to a borehole through-casing resistivity measurement scenario. This work delivers stability results and error estimates, leading to convergence of each approximate model. All the details regarding this work can be found in [43].and [10]. In addition it has been presented to the WONAPDE Conference [29].

6.2.3. *Semi-analytical solutions for asymptotic models for the electric potential across a highly conductive casing*

Participants: H el ene Barucq, Aralar Erdozain, Ignacio Muga, Victor P eron.

This work is performed in the framework of borehole through-casing resistivity measurements. A transmission problem for the electric potential is considered, where one part of the domain is a high-conductive casing. Numerical instabilities are created during the numerical simulations when such a casing is present in the configuration. Therefore, three different asymptotic models derived in [43] are considered, which are composed of impedance conditions specially designed to avoid the casing. These models correspond to approximations of orders one, two and four.

In this work, we employ analytical methods for the aforementioned asymptotic models, which provide a consistent solution to test and verify the numerical solutions (Finite Element Method). In addition, these methods are computationally cheaper than the purely numerical methods. The standard method we follow consists in employing cylindrical coordinates and assuming material homogeneity in the vertical and angular variables. The source term is represented as a Dirac distribution. Under these conditions, we represent the solution to our problem as an inverse Fourier integral in the vertical variable, and a Fourier series in the angular variable.

Numerical tests are carried out to compare with Finite Element solutions. Several difficulties have to be taken into account during the implementation of the semi-analytical solutions, like the treatment of the Dirac distribution and the presence of singularities when the Fourier variable tends to zero. These difficulties are also addressed in this work which is detailed in [10].

6.2.4. *Numerical investigation of instabilities of Perfectly Matched Layers coupled with DG-schemes in elastodynamic*

Participants: H el ene Barucq, Lionel Boillot, Henri Calandra, Julien Diaz, Simon Ettouati.

We observed long-term numerical instabilities when DG-schemes are coupled with PML in elastodynamic, even with isotropic media. To investigate the causes of this instabilities, we have led a series of numerical experiments with elasticus 5.1. The conclusion was that the instabilities only appear in truly elastodynamic media (i.e. when the velocities of S waves is positive) and that different factors impact the stability : the heterogeneities of the domain, the choice of the fluxes, the boundary conditions, the use of unstructured meshes... In the best scenario, using a cartesian grid with periodic boundary conditions for an homogeneous medium and centered fluxes, we did not observe instabilities. However, changing only one element of the configuration made the instabilities appear. Our conclusion is that we need a very particular flux in the PML that should be able to handle the heterogeneities of the domain and the structure of the mesh. This flux should also be adapted to discretize the boundary condition. We are now working on the design of this flux.

6.2.5. *Elasto-acoustic coupling*

Participants: H el ene Barucq, Lionel Boillot, Henri Calandra, Julien Diaz, Simon Ettouati.

Last year, we developed a Discontinuous Galerkin Method for the elastoacoustic coupling in time domain. The proposed solution methodology in general and can be applied to any kind of fluxes. The method had been implemented in Elasticus 5.1 and we have transferred it into the Total platform TMBM-DG 5.4.

In [23], we have considered elastoacoustic coupling with curved interfaces and we have proposed a solution methodology based on Finite Element techniques, which allows for a flexible coupling between the fluid and the solid domain by using non-conforming meshes and curved elements. Differently from other non-conforming approaches proposed so far, our technique is relatively simpler and requires only a geometrical adjustment at the coupling interface at a preprocessing stage, so that no extra computations are necessary during the time evolution of the simulation. This work, has been achieved in collaboration with Angel Rodriguez Rozas, former post-doc of the team.

6.2.6. *Atmospheric radiation boundary conditions for helioseismology*

Participants: Hélène Barucq, Juliette Chabassier, Marc Duruflé.

Modeling acoustic wave propagation inside a celestial body (as the Sun) prompts the question of imposing an adequate boundary condition. Classical atmosphere models suppose an exponential decay of the medium density and a constant wave celerity outside a given radius. This work proposes several radiation boundary conditions that mimic the presence of such an atmosphere and assesses their behavior numerically in radial and axisymmetric configurations.

6.2.7. *Hybrid discontinuous finite element approximation for the elasto-acoustics.*

Participants: Hélène Barucq, Henri Calandra, Julien Diaz, Elvira Shishenina.

Discontinuous finite element methods proved their accuracy and flexibility, but they are still criticized for the number of degrees of freedom which they use: it is much higher than the ones of the conventional methods based on continuous approximations.

Thus hybrid methods have been developed and their integration into the DIP is under way, both in the acoustic and elastic domains.

The global purpose of this work is to develop a new approach for solving wave equation in discontinuous function spaces. This will provide all propagators already developed in the CARBON platform. Possible directions in this research are for example the development of a Trefftz type approximation for elasto-acoustics, coupling with VEM, HDG.

Our current work is concentrated on using Trefftz method. The main idea of the method is that chosen basis functions of Trefftz approximation space are discrete local solutions of the initial equations to be solved.

The possible advantages of Trefftz type approximations compared to the standard ones are: 1) better orders of convergence; 2) flexibility in the choice of basis functions; 3) low dispersion; 4) incorporation of wave propagation directions in the discrete space; 5) adaptivity and local space-time mesh refinement.

The particularity of Trefftz methods is that in case of applying to time-dependent problems they require a space-time mesh.

We studied theory of application of the method to the coupled acoustic system, and implemented numerically Trefftz method to solve the first-order 1D acoustic wave propagation system. The obtained results were presented during annual workshop in Houston organized by Depth Imaging Partnership between Inria and Total.

6.3. Supercomputing for Helmholtz problems

6.3.1. *Extend task-based node parallelism to cluster level: applications to geophysics*

Participants: Emmanuel Agullo, Lionel Boillot, George Bosilca, Henri Calandra, Corentin Rossignon.

The context of this work is to replace static parallelism based on MPI + threads and/or CUDA by dynamic task-based parallelism on top of runtime systems. On a previous work, we demonstrated the speed-up of the new solution when applied to geophysics, at a node level. Moreover, this task paradigm proved its flexibility on several architectures such as ccNUMA big nodes or many-core Intel Xeon Phi co-processors.

We extended this principle to a set of nodes, eventually heterogeneous, in order to measure performance at a cluster level. Preliminary results on few homogeneous nodes were encouraging, ie still faster than pure MPI. Unfortunately, the geophysics algorithm being too repetitive, the load-balancing issue which can be removed within a node (i.e. between cores) comes back between nodes when they are numerous or few but heterogeneous. This is due to the work-stealing feature of the task paradigm which is by default enabled at the node level only.

To overcome this problem, we extended the work-stealing feature to cluster level. To do that we used the task identification by geometrical sub-meshes to detect candidates that can be exchanged between nodes. Then, we compared PAPI counters on these tasks to find the best choice. Finally, we use a separate task-based program to automatically do the main code task update. Preliminary results show clear improvement of load-balancing at cluster level.

This work has been presented to the conferences Rice Oil&Gas[34] and SIAM-PP (Parallel Processing) [35].

6.3.2. *Numerical libraries for hybrid meshes in a discontinuous Galerkin context*

Participants: H el ene Barucq, Lionel Boillot, Aurelien Citrain, Julien Diaz.

Elasticus team code 5.1 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). We are finalizing now the unstructured-goal.

The purpose is to use the h-adaptivity of discontinuous Galerkin method to easily encircle unstructured tetrahedra with hexahedra to form hybrid meshes (so in 3D). In addition, it would be interesting to couple numerical methods depending on the element types.

6.3.3. *Code transfer: TMBM-DG/THBM into Total R&D environment*

Participants: Lionel Boillot, Julien Diaz.

The goal of the DIP collaboration between Total and Inria is to transfer the validated research codes. At first, DIVA-DG has been created in conjunction with Total developers team. It concerns the time modeling of wave propagation. Then, we forked it into Elasticus code to focus on mathematical research at the Inria side. Finally, once validated, we managed its transfer into the recent Total R&D environment (so instead of DIVA template, we moved to TMBM template) to form the TMBM-DG 5.4 code. The entire code has been transferred now, including unit tests and full documentation.

In the meantime, another code emerged within the DIP collaboration, THBM, concerning the frequency modeling of wave propagation. The development is directly done since the beginning in the Total R&D environment. An important part is already validated while research still continues.

6.3.4. *Hybridizable Discontinuous Galerkin methods for solving the elastic Helmholtz equations*

Participants: Marie Bonnasse-Gahot, Henri Calandra, Julien Diaz, St ephane Lanteri.

The advantage of performing seismic imaging in frequency domain is that it is not necessary to store the solution at each time step of the forward simulation. Unfortunately, the drawback of the Helmholtz equations, when considering 3D realistic elastic cases, lies in solving large linear systems. This represents today a challenging task even with the use of High Performance Computing (HPC). To reduce the size of the global linear system, we developed a Hybridizable Discontinuous Galerkin method (HDGm). It consists in expressing the unknowns of the initial problem in function of the trace of the numerical solution on each face of the mesh cells. In this way the size of the matrix to be inverted only depends on the number of degrees of freedom on each face and on the number of the faces of the mesh, instead of the number of degrees of freedom on each cell and on the number of the cells of the mesh as we have for the classical Discontinuous Galerkin methods (DGm). The solution to the initial problem is then recovered thanks to independent elementwise calculation. This results were presented in a submitted paper.

Moreover, as the HDG global matrix is very sparse, we focus on a suitable solver for this kind of matrix. We tested two linear solvers: a parallel sparse direct solver MUMPS (Multifrontal Massively Parallel sparse direct Solver) and a hybrid solver MaPHyS (Massively Parallel Hybrid Solver) which combines direct and iterative methods. We compared the performances of the two solvers when solving 3D elastic waves propagation over HDGm. These comparisons were presented at the MATHIAS 2016 conference and at the DIP Workshop [36], [37]

6.3.5. A Symmetric Trefftz-DG Formulation based on a Local Boundary Element Method for the Solution of the Helmholtz Equation.

Participants: H el ene Barucq, Abderrahmane Bendali, M'barek Fares, Vanessa Mattesi, S ebastien Tordeux.

A general symmetric Trefftz Discontinuous Galerkin method is built in [12] for solving the Helmholtz equation with piecewise constant coefficients. The construction of the corresponding local solutions to the Helmholtz equation is based on a boundary element method. A series of numerical experiments displays an excellent stability of the method relatively to the penalty parameters, and more importantly its outstanding ability to reduce the instabilities known as the "pollution effect" in the literature on numerical simulations of long-range wave propagation.

6.4. Hybrid time discretizations of high-order

6.4.1. High order time discretization for dissipative wave equations.

Participants: Juliette Chabassier, Julien Diaz, Anh-Tuan Ha, S ebastien Imperiale.

Magique-3D team is interested in numerical methods for wave propagation in realistic media, which are naturally dissipative in many application cases. In this internship, we wish to investigate several dissipation models, that lead to Partial Differential Equations with different structures. The simplest model is the scalar wave equation with homogeneous and constant damping $\frac{\partial^2 u}{\partial t^2} + R \frac{\partial u}{\partial t} - \Delta u = f$. In order to approach the complexity of the propagating medium and its geometry, high order finite elements in space are used. Once the spatial discretization is fixed, we get a differential equation of the kind $\frac{d^2 u_h}{dt^2} + B_h \frac{du_h}{dt} + A_h u_h = f_h$, where the mass matrix is the identity thanks to the mass lumping technique followed by a renormalization, B_h is the dissipation matrix and A_h the stiffness matrix. Classically, this equation is discretized in time with a centered and second order finite difference scheme known as the θ -scheme ($\theta > 0$)

$$\frac{u_h^{n+1} - 2u_h^n + u_h^{n-1}}{\Delta t^2} + B_h \frac{u_h^{n+1} - u_h^{n-1}}{2\Delta t} + A_h (\theta u_h^{n+1} + (1 - 2\theta)u_h^n + \theta u_h^{n-1}) = f_h^n \quad (5)$$

In order to preserve the precision obtained with high order finite elements in space, we wish to design higher order time discretizations, while preserving some interesting mathematical properties as the dissipation of a discrete energy, and an efficiency close to the one observed for the second order scheme. More precisely, if $\theta = 0$ and B_h is diagonal, scheme (1) only requires the inversion of a diagonal matrix at each time step.

We want to use the technique of the modified equation, which consists in compensating the first term of the consistency error of a low order discretization, by adding a well chosen new term. If $\theta = 0$, this approach leads to the following fourth order accurate in time scheme

$$\left(I_h + \frac{\Delta t^2}{12} B_h \right) \frac{u_h^{n+1} - 2u_h^n + u_h^{n-1}}{\Delta t^2} + \left[B_h + \frac{\Delta t^2}{12} (B_h A_h - A_h B_h) \right] \frac{u_h^{n+1} - u_h^{n-1}}{2\Delta t} + A_h u_h^n - \frac{\Delta t^2}{12} A_h^2 u_h^n = \tilde{f}_h^n$$

Even if B_h is diagonal, A_h and B_h do not commute in general. We propose to replace the matrix $B_h A_h - A_h B_h$, potentially hard to invert, by an approximated matrix, easy to invert, without deteriorating the consistency of the scheme.

An article is being written and will be submitted soon.

6.4.2. *High order conservative explicit and implicit schemes for wave equations.*

Participants: Juliette Chabassier, Sébastien Imperiale.

In 2016 we have studied the space/time convergence of a family of high order conservative explicit and implicit schemes for wave equations. An original proof of convergence has been proposed and provides an understanding of the lack of convergence of some schemes when the time step approaches its greatest admissible value for stability (CFL condition). An article has been submitted.

6.4.3. *Efficient high order implicit time schemes for Maxwell's equations.*

Participants: H el ene Barucq, Marc Durufl e, Mamadou N'Diaye.

The Pad e approximant is well known to be one of the best approximation of an exponential function which is involved in the exact solution of the linear ODE (Ordinary Differential Equations):

$$y'(t) = Ay(t) + F(t)$$

where A is a given matrix (usually coming from finite element discretization) and F is a term source. The numerical solution can be constructed by approximating the exponential function using the diagonal Pad e approximant:

$$R(z) = \frac{P_m(z)}{Q_m(z)}$$

The function $R(z)$ is a fraction involving two polynomial P_m and Q_m of same degree and approximating the exponential. The corresponding scheme is implicit and A-stable in the sense of Dahlquist. The associated stability function is the same as the stability function of the Gauss-Runge-Kutta schemes. However, Gauss-Runge-Kutta schemes can be used to handle non-linear ODEs, but they are too expensive to use in practice. The diagonal Pad e schemes presented here can be seen as a simplification of Gauss-Runge-Kutta schemes in the case of linear ODE. We have proposed an efficient way to implement the diagonal Pad e schemes with an accurate approximation of the source term to keep the correct order of accuracy.

The main drawback of Pad e schemes is that the denominator $Q_m(z)$ has distinct roots. It implies that we have to solve distinct linear systems at each time step. As a result, we have also studied the case where the denominator has a unique real root γ :

$$R(z) = \frac{N(z)}{(1 - \gamma z)^m}$$

The numerator N is then found to obtain the "best" approximation of the exponential under the constraint of the A-stability property of the underlying schemes. The obtained schemes have been called Linear Singly Diagonal Implicit Runge-Kutta schemes (Linear SDIRK) since they share the same property as SDIRK (a unique linear system to solve several times) but they can be applied only to linear ODEs. We provide a performance assessment of different implicit schemes (Pad e schemes, SDIRK and Linear SDIRK). The comparison criteria are based on the amplitude and phase errors which are reliable gauges of accuracy when approximating waves problems. The Linear SDIRK schemes and the diagonal Pad e schemes have been implemented in the code Montjoie. We have performed numerical experiments in 1-D and 2-D for Maxwell's equations to validate these schemes and compare their efficiency.

This work has been presented at the conference ICOSAHOM [28], the colloquium Inter'Actions en Math ematiques Lyon 2016 and the Mathias annual Total seminar [27].

6.4.4. Optimized high-order explicit Runge-Kutta-Nyström schemes.

Participants: Marc Duruflé, Mamadou N'Diaye.

In this work we propose a high order time integration explicit scheme to solve a second order derivative non-linear ordinary differential equation (ODE)

$$y'' = f(t, y)$$

To solve this family of ODEs, explicit one-step Runge-Kutta-Nyström have been proposed by Hairer et al. The stability condition (CFL) associated with these schemes have been studied for order 3, 4 and 5 by Chawla and Sharma. In this work, we have extended the stability studies for high order. We proposed optimal coefficients for Runge-Kutta-Nyström schemes of order 6, 7, 8 and 10 which have been obtained by optimizing the CFL. With the obtained optimal CFL, these schemes are well suited for stiff problems where the stability condition is restrictive. These schemes have been implemented in the code Montjoie.

Numerical experiments have been conducted in 1-D for the non-linear Maxwell's equation and show that obtained Runge-Kutta-Nyström schemes of order 7 is quite efficient. This work has been presented at the conference ICOSAHOM [48].

7. Bilateral Contracts and Grants with Industry

7.1. Contracts with TOTAL

- Depth Imaging Partnership (DIP)
Period: 2014 May - 2019 April , Management: Inria Bordeaux Sud-Ouest, Amount: 120000 euros/year.
- Méthodes d'inversion sismique dans le domaine fréquentiel
Period: 2014 October - 2017 December , Management: Inria Bordeaux Sud-Ouest, Amount: 180000 euros.
- Portage de méthodes numériques de simulation de phénomènes complexes sur des architectures exascales
Period: 2016 January - 2017 December , Management: Inria Bordeaux Sud-Ouest, Amount: 150000 euros.
- Approximations hybrides par éléments finis discontinus pour l'élasto-acoustique
Period: 2016 November - 2018 October, Management: Inria Bordeaux Sud-Ouest, Amount: 165000 euros.

8. Partnerships and Cooperations

8.1. Regional Initiatives

8.1.1. Partnership with I2M in Bordeaux supported by Conseil Régional d'Aquitaine

title: Imaging complex materials.

Coordinator: Hélène Barucq

Other partners: I2M CNRS Université Bordeaux I

The detection, localization and monitoring of the defect evolution in composite materials, concrete and more generally heterogeneous materials is a challenging problem for Aeronautics and energy production. It is already possible to localize defects in homogeneous materials by using methods based on ultrasonic inspection and sometimes, they are usable in particular heterogeneous materials, most of the time in 2D. Classical methods rely on the correspondence between the distance and the propagation time of the wave traveling between the defect and the receivers. In complex media, such a correspondence may be lapsed, for instance when the velocity depends on the frequency (dispersion) or of the propagation direction (anisotropy). The defect signature can also be embedded in the acoustic field sent by the structure (multiple reflections). The complexity of the propagation in heterogeneous materials makes then difficult the accurate localization of the defect, in particular in 3D.

Topological imaging techniques can be applied to heterogeneous media. They can find the positions of defects from two simulations performed in a safe experimental medium. They have been developed at I2M laboratory to carry on 2D single/multi mode inspection in isotropic and anisotropic waveguides. They have also been applied to a highly reflecting medium observed with a single sensor. The objective of this work is to extend the technique to 3D problems. In particular, we are going to handle detection in composite plates and in highly heterogeneous media including a collection of small scatterers.

This project is supported by the Conseil Régional d'Aquitaine, for a duration of 2 years.

8.2. National Initiatives

8.2.1. 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 (Hiepac 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. 4 PhD students have defended their PhD in 2015 and they have now post-doctoral researchers in Europe. DIP is currently employing 2 PhD students and one post-doctoral researcher.

8.2.2. 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 in Strasbourg. The second one will be held in Paris in March 2017. The project is funded for 18 months starting from August 2016. The funding amounts 30000€.

8.3. European Initiatives

8.3.1. FP7 & H2020 Projects

8.3.1.1. GEAGAM

Title: Geophysical Exploration using Advanced Galerkin Methods

Program: H2020

Duration: January 2015 - December 2017

Coordinator: Universidad Del Pais Vasco (EHU UPV)

Partners:

Bcam - Basque Center for Applied Mathematics Asociacion (Spain)

Barcelona Supercomputing Center - Centro Nacional de Supercomputacion (Spain)

Total S.A. (France)

Universidad Del Pais Vasco Ehu Upv (Spain)

Pontificia Universidad Catolica de Valparaiso (Chile)

Universidad de Chile (Chile)

Universidad Tecnica Federico Santa Maria (Chile)

University of Texas at Austin (USA)

Inria contact: Hélène BARUCQ

The main objective of this Marie Curie RISE action is to improve and exchange interdisciplinary knowledge on applied mathematics, high performance computing, and geophysics to be able to better simulate and understand the materials composing the Earth's subsurface. This is essential for a variety of applications such as CO₂ storage, hydrocarbon extraction, mining, and geothermal energy production, among others. All these problems have in common the need to obtain an accurate characterization of the Earth's subsurface, and to achieve this goal, several complementary areas will be studied, including the mathematical foundations of various high-order Galerkin multiphysics simulation methods, the efficient computer implementation of these methods in large parallel machines and GPUs, and some crucial geophysical aspects such as the design of measurement acquisition systems in different scenarios. Results will be widely disseminated through publications, workshops, post-graduate courses to train new researchers, a dedicated webpage, and visits to companies working in the area. In that way, we will perform an important role in technology transfer between the most advanced numerical methods and mathematics of the moment and the area of applied geophysics.

8.3.1.2. *HPC4E*

Title: HPC for Energy

Program: H2020

Duration: December 2015 - November 2017

Coordinator: Barcelona Supercomputing Center

Partners:

Centro de Investigaciones Energeticas, Medioambientales Y Tecnologicas-Ciemat (Spain)

Iberdrola Renovables Energia (Spain)

Repsol (Spain)

Lancaster University (United Kingdom)

Total S.A. (France)

Fundação Coordenação de Projetos, Pesquisas e Estudos Tecnológicos, (Brazil)

National Laboratory for Scientific Computation, (Brazil)

Instituto Tecnológico de Aeronáutica, (Brazil)

Petrobras, (Brazil)

Universidade Federal do Rio Grande do Sul, (Brazil)

Universidade Federal de Pernambuco, (Brazil)

Inria contact: Stéphane Lanteri

This project aims to apply the new exascale HPC techniques to energy industry simulations, customizing them, and going beyond the state-of-the-art in the required HPC exascale simulations for different energy sources: wind energy production and design, efficient combustion systems for biomass-derived fuels (biogas), and exploration geophysics for hydrocarbon reservoirs. For wind energy industry HPC is a must. The competitiveness of wind farms can be guaranteed only with accurate wind resource assessment, farm design and short-term micro-scale wind simulations to forecast the daily power production. The use of CFD LES models to analyse atmospheric flow in a wind farm capturing turbine wakes and array effects requires exascale HPC systems. Biogas, i.e. biomass-derived fuels by anaerobic digestion of organic wastes, is attractive because of its wide availability, renewability and reduction of CO₂ emissions, contribution to diversification of energy supply, rural development, and it does not compete with feed and food feedstock. However, its use in practical systems is still limited since the complex fuel composition might lead to unpredictable combustion performance and instabilities in industrial combustors. The next generation of exascale HPC systems will be able to run combustion simulations in parameter regimes relevant to industrial applications using alternative fuels, which is required to design efficient furnaces, engines, clean burning vehicles and power plants. One of the main HPC consumers is the oil & gas (O&G) industry. The computational requirements arising from full wave-form modelling and inversion of seismic and electromagnetic data is ensuring that the O&G industry will be an early adopter of exascale computing technologies. By taking into account the complete physics of waves in the subsurface, imaging tools are able to reveal information about the Earth's interior with unprecedented quality.

8.4. International Initiatives

8.4.1. Inria International Partners

8.4.1.1. Declared Inria International Partners

8.4.1.1.1. 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 December 2016

8.5. International Research Visitors

8.5.1. Visits of International Scientists

- Antoine Chaigne (University of Music and Performing Arts Vienna) visited Magique 3D in November 2016.

- Rabia Djellouli (CSUN) visited Magique 3D in December 2016.

8.5.2. Visits to International Teams

8.5.2.1. Research Stays Abroad

- In the framework of the European project Geagam, Aralar Erdozain and Victor Péron visited Ignacio Muga, PUCV, Chile, in January and November 2016.
- In the framework of the European project Geagam, Florian Faucher and Ha Pham visited Henri Calandra, Total Houston, USA, in October 2016.

9. Dissemination

9.1. Promoting Scientific Activities

9.1.1. Scientific Events Organisation

9.1.1.1. General Chair, Scientific Chair

- Hélène Barucq organized the Fourth Workshop of Strategic Action DIP in Houston, October 10-11, 2016, <http://dip.inria.fr/workshops/fourth-workshop-of-the-strategic-action-dip/> and JOSO 2016 (Wave days in South-West) in Pau, March 9-11 <https://team.inria.fr/magique3d/conference-and-workshops/joso-2016-wave-days-in-south-west/>

9.1.1.2. Member of the Conference Program Committees

Victor Péron was member of the Program Committee of the Conference JOSO 2016 (Wave days in South-West) in Pau, March 9-11 <https://team.inria.fr/magique3d/conference-and-workshops/joso-2016-wave-days-in-south-west/>

9.1.2. Journal

9.1.2.1. Reviewer - Reviewing Activities

Members of Magique 3D have been reviewers for the following journals:

- Annales de l'Institut Henri Poincaré / Analyse non linéaire
- Applied Mathematics and Computation
- ESAIM : Mathematical Modelling and Numerical Analysis
- Geophysical Journal International
- IMA Journal of Numerical Analysis
- International Journal for Numerical Methods in Engineering
- Journal of Computational Physics
- Journal of Scientific Computing
- Journal of Sound and Vibration
- Journal of the Acoustical Society of America
- Siam Journal on Scientific Computing
- Zeitschrift fuer Angewandte Mathematik und Physik

9.1.3. Scientific Expertise

- Julien Diaz was expert for the evaluation of Millennium Science Initiative project for the government of Chile.

9.1.4. Research Administration

- H el ene Barucq has been the chairwoman of the local jury of Inria competitive selection for Young Graduate Scientists (CR2) in Bordeaux. She participated to the selection committee for an Assistant Professor position at the University of Nantes and Paris 13. She was also part of the hiring committee for a Professor position at the University of Rennes 1. She is member of the local bureau of Inria Bordeaux Sud-Ouest focusing on scientific questions arising from research teams and of the Center Committee dealing with general questions related to the whole Research Center. She is the scientific head of the project DIP since its creation in 2009.
- Juliette Chabassier is member of the Workgroup for sustainable development at Inria Bordeaux Sud-Ouest.
- Julien Diaz is elected member of the Inria Technical Committee and of the Inria Administrative and Scientific Boards. He is appointed member of the CDT (Commission de D veloppement Technologique)
- Mamadou N'Diaye is member of the Center Committee of Inria Bordeaux Sud-Ouest.
- Victor P eron is appointed member of the CJC (Commission Jeunes Chercheurs) of Inria Bordeaux Sud-Ouest.

9.2. Teaching - Supervision - Juries

9.2.1. Teaching

Licence : Izar Azpiroz, Fonctions et int egrales, 19.5 heures, MATH L1, UPPA, France

Master : Julien Diaz, Transform ees, 24h Eq. TD, M1, EISTIA, France

Master : Marc Durufl e, Calcul scientifique en C++, 96h Eq. TD, M1, Bordeaux INP, France

Licence : Marc Durufl e, Equations Diff erentielles, 20h Eq. TD, L3, Bordeaux INP, France

Licence : Marc Durufl e, Calcul scientifique en Fortran 90, 20h Eq. TD, L3, Bordeaux INP, France

Licence : Marc Durufl e, Algorithmique num erique, 30h Eq. TD, L3, Bordeaux INP, France

Licence : Mamadou N'Diaye, Compl ements d'alg bre, 19,5h Eq. TD, L1, UPPA, France

Licence : Mamadou N'Diaye, Fonction de la variable r elle, 19,5h Eq. TD, L1, UPPA, France

Licence : Mamadou N'Diaye, D veloppements limit s - suites et s ries, 19,5h Eq. TD, L2, UPPA, France

Licence : Mamadou N'Diaye, Analyse 3A et Analyse 3B, 19,5h Eq. TD, L2, UPPA, France

Master : Victor P eron, Analyse des EDP, 9 Eq. TD, M1, EISTI, France

Master : Victor P eron, Analyse num erique fondamentale, 70 Eq. TD, M1, UPPA, France

Master : Victor P eron, Analyse, 23 Eq. TD, M1, UPPA, France

Master : Victor P eron et S bastien Tordeux, Analyse Num erique 1: diff rences finies, 87 eq. TD, Master1, UPPA, FRANCE

Master : Victor P eron et S bastien Tordeux, Introduction aux ph nom nes de propagation d'ondes, 38 eq. TD, Master 2, UPPA, FRANCE

Licence : S bastien Tordeux, Statistique descriptive, 55 eq. TD, L1, UPPA, FRANCE

Licence : S bastien Tordeux, Analyse complexe , 20 eq. TD, niveau (M1, M2), L3, UPPA, France

9.2.2. Supervision

HDR : Julien Diaz, Modelling and advanced simulation of wave propagation phenomena in 3D geophysical media, Université de Pau et des Pays de l'Adour, April 7th, 2016 [9].

PhD : Aralar Erdozain, Fast inversion of 3D Borehole Resistivity Measurements using Model Reduction Techniques based on 1D Semi-Analytical Solutions, Université de Pau et des Pays de l'Adour, December 15th 2016, Hélène Barucq, David Pardo (BCAM) and Victor Péron. [10].

PhD : Vincent Popie, Modélisation asymptotique de la réponse acoustique de plaques perforées dans un cadre linéaire avec étude des effets visqueux, ISAE, January 14th 2016, Estelle Piot (ONERA) and Sébastien Tordeux. [11].

PhD in progress : Izar Azpiroz Irargorri, Approximation des problèmes d'Helmholtz couplés sur maillages virtuels, October 2014, Hélène Barucq, Julien Diaz and Rabia Djellouli (CSUN).

PhD in progress : Vincent Darrigrand, Etude d'erreur pour des problèmes d'Helmholtz approchés par des techniques de Petrov-Galerkin, October 2013, Hélène Barucq and David Pardo.

PhD in progress : Aurélien Citrain, Déformation 3D de maillages en imagerie sismique, Méthodes d'inversion sismique dans le domaine fréquentiel, October 2016, Hélène Barucq and Christian Gout.

PhD in progress : Florian Faucher, Méthodes d'inversion sismique dans le domaine fréquentiel, October 2014, Hélène Barucq.

PhD in progress : Hamza Alaoui Hafidi, Imagerie ultrasonore tridimensionnelle dans les milieux hétérogènes complexes, October 2015, Encadrement : Marc Deschamps, Michel Castaings, Eric Ducasse, Samuel Rodriguez (I2M), Hélène Barucq, Marc Duruflé, Juliette Chabassier (Magique 3D).

PhD in progress : Justine Labat, Diffraction d'une onde par des petits obstacles dans des milieux complexes, October 2016, Victor Péron and Sébastien Tordeux.

PhD in progress : Mamadou N'Diaye, Analyse et développement de schémas temporels hybrides pour les équations hyperboliques du premier ordre, January 2015, Hélène Barucq and Marc Duruflé.

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 (LFC).

PhD in progress : Elvira Shishenina, Approximations hybrides par éléments finis et éléments virtuels discontinus pour l'élasto-acoustique, October 2015, Hélène Barucq and Julien Diaz.

Master thesis : Aurélien Citrain, 2D hybrid meshes for a DG code, Insa de Rouen, Sept. 2016.

Master thesis : Alain Ha, High order time discretization for dissipative wave equations, Université de Rennes, Sept. 2016.

Master thesis : Justine Labat, Diffraction of an electromagnetic wave by small obstacles, Université de Pau et des Pays de l'Adour, Sept. 2016.

Master 1 internship : Baptiste Olivier, Modeling wave propagation in musical instruments, MatMeca, Sept. 2016.

9.2.3. *Juries*

- Hélène Barucq : Julien Diaz (Université de Pau et des Pays de l'Adour) "Modelling and advanced simulation of wave propagation phenomena in 3D geophysical media", HDR, April 7th 2016
- Hélène Barucq : Vincent Deymier (ONERA Toulouse) "Etude d'une méthode d'éléments finis d'ordre élevé et de son hybridation avec d'autres méthodes numériques pour la simulation électromagnétique instationnaire dans un contexte industriel", PhD thesis, December 8th 2016
- Hélène Barucq : Asma Toumi (Université Paul Sabatier Toulouse III) "Méthodes numériques asynchrone pour la modélisation de phénomènes multi-échelles", PhD thesis, September 21th 2016
- Hélène Barucq : Romain Brossier (Université de Grenoble) "Contributions to developments and applications of Full Waveform Modeling and Inversion", HDR, November 18th 2016

- Julien Diaz : Azba Riaz (Université de Cergy Pontoise) “A new discontinuous Galerkin formulation for time dependent Maxwell’s equations: a priori and a posteriori error estimation”, PhD thesis, April 4th 2016
- Julien Diaz : Valentin Vinales (Université de Paris Saclay) “ Problèmes d’interface en présence de métamatériaux : modélisation, analyse et simulations”, PhD thesis, September 8th 2016
- Julien Diaz (reviewer): Asma Toumi (Université Paul Sabatier Toulouse III) “Méthodes numériques asynchrone pour la modélisation de phénomènes multi-échelles”, PhD thesis, September 21th 2016

9.3. Popularization

- Juliette Chabassier took part in a round table around science professions in the high school of Valence d’Agen in March 2016.
- Juliette Chabassier shared her experience as a scientist during “Printemps de la Mixité” in May 2016.
- Juliette Chabassier participated in scientific “speed datings” during the “Filles et Maths” day in May 2016.
- Juliette Chabassier was co-responsible for a workshop around “Women in science” during Inria “Fête de la science” in October 2016.

10. Bibliography

Major publications by the team in recent years

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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), Laboratoire Photonique, Numérique et Nanosciences (LP2N)

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THEME

Interaction and visualization

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Project-Team MANAO

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- 5.4.4. - 3D and spatio-temporal reconstruction
- 5.5. - Computer graphics
- 5.5.1. - Geometrical modeling
- 5.5.2. - Rendering
- 5.5.3. - Computational photography
- 5.5.4. - Animation
- 5.6. - Virtual reality, augmented reality
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- 6.2.5. - Numerical Linear Algebra
- 6.2.6. - Optimization
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- 9.5.6. - Archeology, History
- 9.5.10. - Digital humanities

1. Members

Research Scientists

Pascal Barla [Inria, Researcher]
Gaël Guennebaud [Inria, Researcher]

Faculty Members

Xavier Granier [Team leader, IOGS, Professor, HDR]
Pierre Bénard [Univ. Bordeaux, Associate Professor]
Patrick Reuter [Univ. Bordeaux, Associate Professor]

Technical Staff

Romain Pacanowski [CNRS]

Brett Ridet [Inria, granted by ANR ISAR]

PhD Students

Boris Raymond [Univ. Bordeaux, Teaching Assistant, until Aug 2016]

Florian Canezin [Univ. Toulouse III, until Jan 2016]

Thomas Crespel [Inria]

Arthur Dufay [Technicolor]

Thibaud Lambert [Inria, granted by ANR RichShape]

Antoine Lucat [IOGS, granted by ANR Material]

Lois Mignard–Debise [Inria, granted by ANR ISAR & Deutsche Forschungsgemeinschaft e.V.]

David Murray [FEI]

John Restrepo Agudelo [Inria, until Jun 2016, granted by Deutsche Forschungsgemeinschaft e.V.]

Carlos Zubiaga Pena [Inria, until Nov 2016, granted by FP7 ITN PRISM]

Post-Doctoral Fellows

Elodie Lamothe [Inria]

Georges Nader [Inria, granted by ANR RichShape]

Administrative Assistant

Anne-Laure Gautier [Inria]

Others

Loic Barthe [Univ. Toulouse III, Professor, HDR]

Ivo Ihrke [Researcher, HDR]

Vincent Lepetit [Univ. Bordeaux, Professor]

Nicolas Mellado [CNRS, Research Scientist]

Mathias Paulin [Univ. Toulouse III, Professor, HDR]

David Vanderhaeghe [Univ. Toulouse III, Associate Professor]

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 [62], [39] 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 [75] and Light-Field rendering [37]). 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 [72], [76], 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 [97] 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.



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 [87], stereo displays or new display technologies [58], and physical fabrication [28], [45], [54]) the frontiers between real and virtual worlds are vanishing [41]. 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

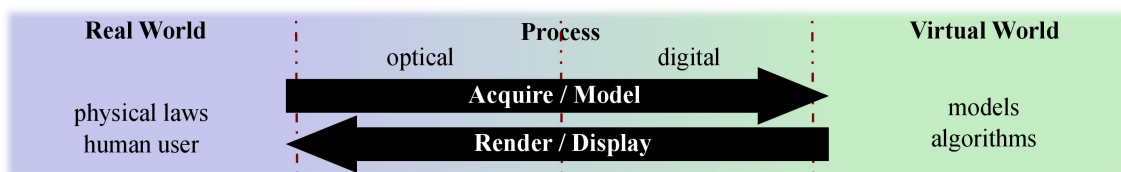


Figure 2. Interactions/Transfers between real and virtual worlds. One of our goal is to combine optical instruments with processes from computer science in order to blend the two worlds.

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 adaptation 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 [34] or geometric properties [103], as mastered by professional photographers;
- The modification of material characteristics or lighting conditions [104] to better understand shape features, for instance to decipher archaeological artifacts;
- The large influence of shape on the captured variation of shading [85] and thus on the perception of material properties [100].

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) [44] 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 specific 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 [71]. 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 [33], [41] and computational photography [86].
- **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 [97]. 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

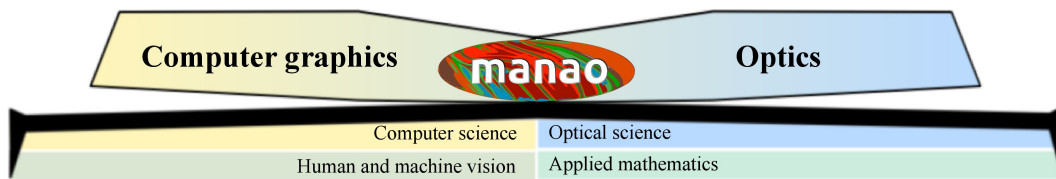


Figure 3. Related scientific domains of the MANAO project.

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 [46] 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 [59], [60] and display [58] 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 [48] or differential analysis [85], 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, see Section 6.3) 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 [89], 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 [55] in order to develop tailored strategies [101]. For instance, starting from simple direct lighting, more complex phenomena have been progressively introduced: first diffuse indirect illumination [53], [93], then more generic inter-reflections [62], [46] and volumetric scattering [90], [43]. 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 [42]. 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 [92] but are difficult to extend to non-piecewise-constant data [95]. More recently, researches prefer the use of Spherical Radial Basis Functions [98] or Spherical Harmonics [84]. For more complex data, such as reflective properties (e.g., BRDF [77], [63] - 4D), ray-space (e.g., Light-Field [73] - 4D), spatially varying reflective properties (6D - [88]), new models, and representations are still investigated such as rational functions [80] or dedicated models [31] and parameterizations [91], [96]. 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 [80].

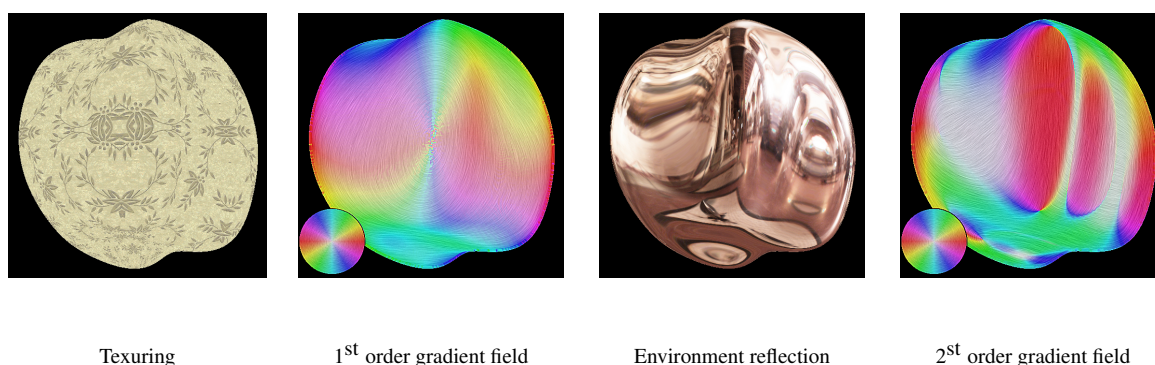


Figure 4. First-order analysis [102] have shown that shading variations are caused by depth variations (first-order gradient field) and by normal variations (second-order fields). These fields are visualized using hue and saturation to indicate direction and magnitude of the flow respectively.

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 [85] and frequency analysis [48]). Such an approach has led 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 [49] 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.

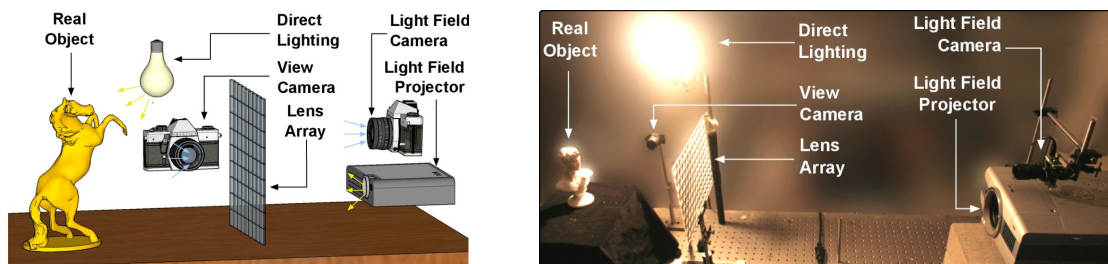


Figure 5. Light-Field transfer: global illumination between real and synthetic objects [41]

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 [73], [58]. We consider projecting systems and surfaces [38], for personal use, virtual reality and augmented reality [33]. 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 [52], [51]. These resulting systems have to acquire the different phenomena described in Axis 1 and to display them, in an efficient manner [56], [32], [57], [60]. 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 [61].

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 [60], [82]). Similarly, increasing the number of viewpoints is a way toward the creation of full 3D displays [73]. 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., [81], [107]).

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. [41]. 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 [70] are one of the key technologies to develop such acquisition (e.g., Light-Field camera⁰ [61] and acquisition of light-sources [52]), projection systems (e.g., auto-stereoscopic displays). Such an approach is versatile and may be applied to improve classical optical instruments [68]. More generally, by designing unified optical and digital systems [78], 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 [80]. Second, we have to integrate signals from multiple sensors (such as GPS, accelerometer, ...) to prevent some computation (e.g., [71]). Finally, the experience of the group in surface modeling help the design of optical surfaces [64] 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

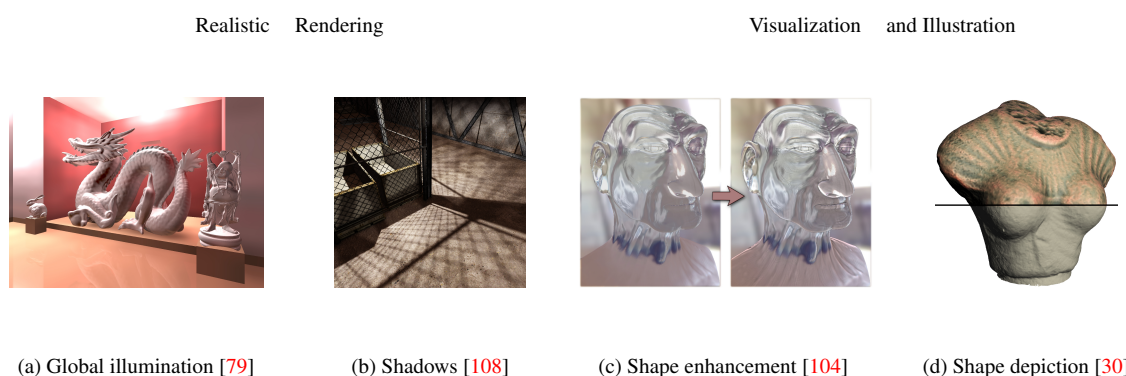


Figure 6. In the MANAO project, we are investigating rendering techniques from realistic solutions (e.g., inter-reflections (a) and shadows (b)) to more expressive ones (shape enhancement (c) with realistic style and shape depiction (d) with stylized style) for visualization.

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

⁰Lytro, <http://www.lytro.com/>

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 [105], [67] or stylized shading [36], [104] with various levels of abstraction. A clear representation of important 3D **object features** remains a 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 [29] 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 [106], motion blur [48], depth of field [94], 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 [69], [47]. 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 [40]. Independent image processing for each viewpoint may disturb the feeling of depth by introducing inconsistent information in each images. Finally, more dedicated displays [58] 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 [4] [35]. 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., [99]): 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 [99]), 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.

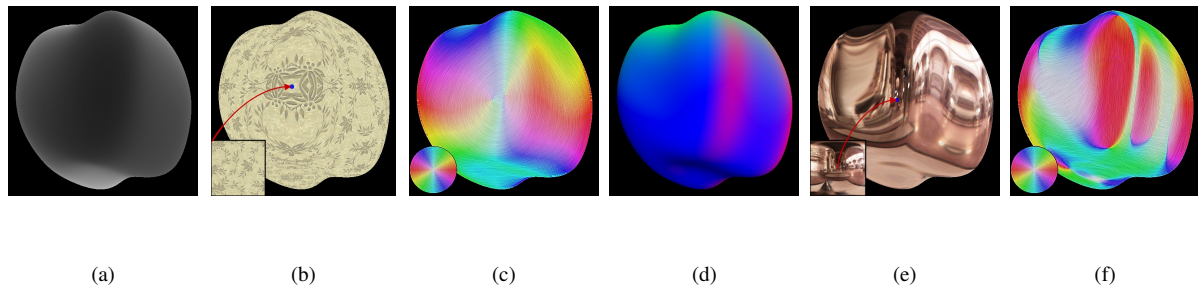


Figure 7. Based on our analysis [102] (Axis 1), we have designed a system that mimics texture (left) and shading (right) effects using image processing alone. It takes depth (a) and normal (d) images as input, and uses them to deform images (b-e) in ways that closely approximate surface flows (c-f). It provides a convincing, yet artistically controllable illusion of 3D shape conveyed through texture or shading cues.

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 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

In term of publication, we are regularly publishing our work at the prestigious conference SIGGRAPH. This year was particularly successful with two plain papers [17], [16] and one talk [19]. But this year more especially, an image from our work [16] were selected as the front cover of the corresponding special issue of ACM Transactions on Graphics.

Another great success is the creation, led by members of the LP2N, of a first workshop on nano-appearance. The goal of this workshop was to bring together people from the industry and the academia, and from domains that seem very different considering the scale they are interested in but close by the object of their studies: the appearance of materials. A rare initiative, this workshop took place during two days in November 2016.

6. New Software and Platforms

6.1. ALTA Lib

The ALTA Library

KEYWORDS: Statistic analysis - Fitting - Measures

FUNCTIONAL DESCRIPTION

ALTA is a multi-platform software library to analyze, fit and understand BRDFs. It provides a set of command line software to fit measured data to analytical forms, tools to understand models and data.

- Participants: Laurent Belcour, Romain Pacanowski, Xavier Granier and Pascal Barla
- Partner: LP2N (CNRS - UMR 5298)
- Contact: Romain Pacanowski
- URL: <http://alta.gforge.inria.fr/>

6.2. Elasticity Skinning

SCIENTIFIC DESCRIPTION

Geometric skinning techniques are very popular in the industry for their high performances, but fail to mimic realistic deformations. With elastic implicit skinning the skin stretches automatically (without skinning weights) and the vertices distribution is more pleasing. Our approach is more robust, for instance the angle's range of joints is larger than implicit skinning.

This software has been ported as a plugin for the Modo software (The Foundry) in collaboration with *Toulouse Tech Transfer*. This plugin has been bought by The Foundry, which maintains and sells it.

- Participants: Rodolphe Vaillant, Loïc Barthe, Florian Canezin, Gaël Guennebaud, Marie-Paule Cani, Damien Rohmer, Brian Wyvill, Olivier Gourmel and Mathias Paulin
- Partners: Université de Bordeaux - CNRS - INP Bordeaux - Université de Toulouse - Institut Polytechnique de Grenoble - Ecole Supérieure de Chimie Physique Electronique de Lyon
- Contact: Gaël Guennebaud
- URL: <http://rodolphe-vaillant.fr/?e=59>

6.3. Eigen

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, AVX, FMA, AVX512, AltiVec, VSX 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.

In 2016, we released three revisions of the 3.2 branch, as well as the new 3.3 version that leverages numerous major novel features and improvements. Those include, a novel evaluation mechanism of expressions, support for AVX, FMA, AVX512, VSX and ZVector vector instructions, unaligned vectorization, nvcc/CUDA, more OpenMP parallelism, a fast divide and conquer SVD algorithm, a CompleteOrthogonalDecomposition class for fast minimal norm solving, a LS-CG solver, a fast reciprocal condition number estimators in LU and Cholesky factorizations, LU::transpose()/adjoint() API, support for inplace decompositions, support for matrix-free iterative solvers, new array functions, support for any BLAS/LAPACK libraries as backend, improved support for mixing scalar types, eigenvectors in GeneralizedEigenSolver, a complete rewrite of LinSpaced, a non officially supported but massively used Tensor module with CUDA and OpenCL support, and **more**.

- Participant: Gaël Guennebaud
- Contact: Gaël Guennebaud
- URL: <http://eigen.tuxfamily.org/>

6.4. HDRSee

KEYWORDS: OpenGL-GLSL HDR/LDR Viewer **FUNCTIONAL DESCRIPTION** HDRSee is a OpenGL/GLSL software that displays High Dynamic Range (HDR) and Low Dynamic Range (LDR) images. It is based on several libraries (e.g., glut, see below for full dependencies). To display HDR images, HDRSee implements a few tone-mapping operators. Moreover, it is designed with a plugin mechanism that let developers add, as easily as possible, their own tone-mapping operator. All tone-mapping operations are done using Graphics Hardware through pixel shader operations. The GUI currently used is nvWidgets.

- Participants: Romain Pacanowski, Xavier Granier.
- Partner: LP2N (CNRS - UMR 5298)
- Contact: Romain Pacanowski
- URL: <http://mhdrviewer.gforge.inria.fr/>

6.5. Patate Lib

KEYWORDS: Expressive rendering - Multi-scale analysis - Material appearance - Vector graphics - 2D animation

FUNCTIONAL DESCRIPTION

Patate is a header only C++/CUDA library for graphics applications. It provides a collection of Computer Graphics techniques that incorporate the latest innovations from Inria research teams working in the field. It strives for efficiency and ease-of-use by focusing on low-level core operators and key algorithms, organized in modules, each tackling a specific set of issues. The central goal of the library is to drastically reduce the time and efforts required to turn a research paper into a ready-to-use solution, for both commercial and academic purposes.

The library is still in its infancy and we are actively working on it to include the latest of our published research techniques. Modules will be dealing with graphics domains as varied as multi-scale analysis, material appearance, vector graphics, expressive rendering and 2D animation.

- Participants: Gaël Guennebaud, Pascal Barla, Simon Boyé, Gautier Ciaudo and Nicolas Mellado
- Contact: Gaël Guennebaud
- URL: <http://patate.gforge.inria.fr/html/>

7. New Results

7.1. Analysis and Simulation

7.1.1. Principles of Light Field Imaging

Light field imaging offers powerful new capabilities through sophisticated digital processing techniques that are tightly merged with unconventional optical designs. This combination of imaging technology and computation necessitates a fundamentally different view of the optical properties of imaging systems and poses new challenges for the traditional signal and image processing domains. We aimed to provide a comprehensive review [14] of the considerations involved and the difficulties encountered in working with light field data during 25 years of research.

7.1.2. Physically-Based Reflectance Model Combining Reflection and Diffraction

Reflectance properties express how objects in a virtual scene interact with light; they control the appearance of the object: whether it looks shiny or not, whether it has a metallic or plastic appearance. Having a good reflectance model is essential for the production of photo-realistic pictures. Measured reflectance functions provide high realism at the expense of memory cost. Parametric models are compact, but finding the right parameters to approximate measured reflectance can be difficult. Most parametric models use a model of the surface micro-geometry to predict the reflectance at the macroscopic level. We have shown [26] that this micro-geometry causes two different physical phenomena: reflection and diffraction. Their relative importance is connected to the surface roughness. Taking both phenomena into account, we develop a new reflectance model that is compact, based on physical properties and provides a good approximation of measured reflectance.

7.1.3. Multi-Scale and Structured SV-BRDF Model for Scratched Materials

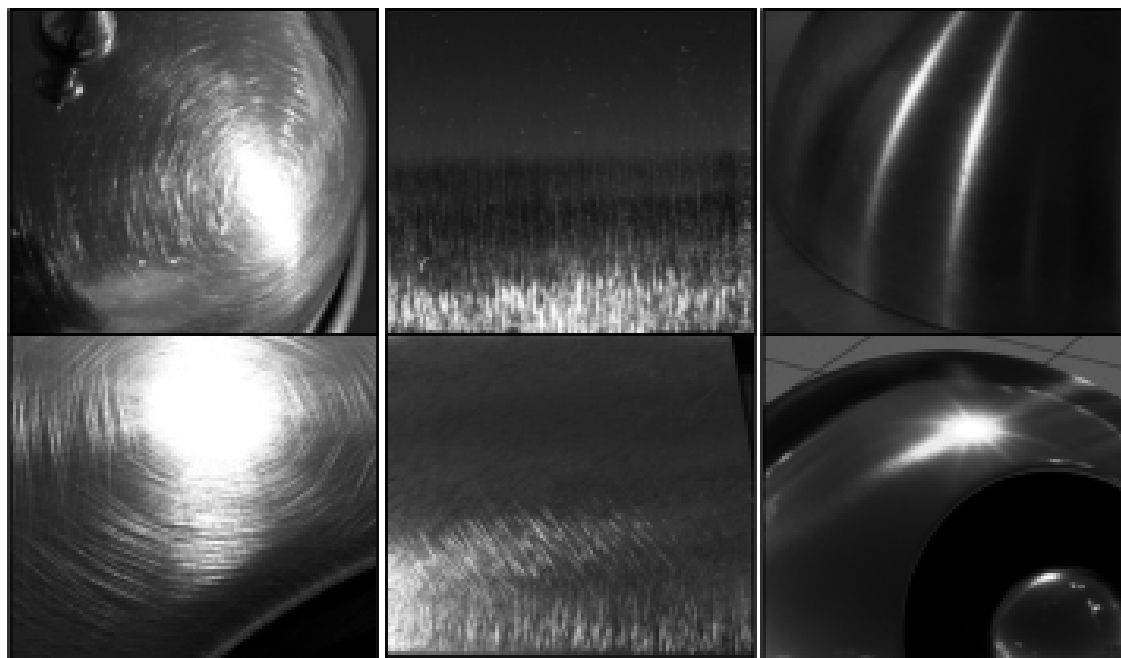


Figure 8. Our scratch BRDF (top) can reproduce several effects similar to real photographs (bottom).

We developed a Spatially-Varying BRDF model tailored to the multi-scale rendering of scratched materials such as metals, plastics or finished woods. Our approach takes advantage of the regular structure of scratch distributions to achieve high performance without compromising visual quality (fig. 8). The BRDF for a single scratch is simulated using an optimized 2D ray-tracer and compactly stored in a three-component 2D texture. In contrast to existing models, our approach takes into account all inter-reflections inside a scratch, including Fresnel effects. At render time, the SV-BRDF for the scratch distribution under a pixel or ray footprint is obtained by linear combination of individual scratch BRDFs. Our model can be evaluated using both importance and light sampling, in direct and global illumination settings. Our approach provides users with controls over the profile, micro-BRDF, density and orientation of scratches. All these material properties are updated at interactive rates. This work has been published at ACM Siggraph 2016 [16] and one our result has been selected as the cover of the ACM Siggraph 2016 proceedings. It is part of the PhD Thesis "Control of anisotropic materials appearance" [11] defended this year.

7.1.4. Cues for Perception of Appearance

Thanks for the FP7 ITN PRISM, we have participated to several user studies to understand the perception of an object appearance. First, for fluids and other deformable materials, we find [25] that observers show a high degree of constancy in matching the viscosity across the different variations. However, volume differences between test and match stimulus, especially with static stimuli, caused large effects of over- and under-estimation of viscosity. We also find that a number of cues related to curvatures, periodic movements of the liquids, and the way they spread out predict aspects of the observer's performance, but that humans achieve better constancy than the cues predict.

We have also investigated gloss haze [22]. The results reveals that haziness is a distinct visual dimension orthogonal to the commonly studied glossiness and blurriness. Coatedness appears to be nearly synonymous with haziness, as this is one of the main physical causes of haze in real world materials. Polish seems to be a combination of glossiness and haziness, as materials go from dull to hazy to highly glossy during the physical polishing process. The inferred tactile quality of friction is apparently uncorrelated with haziness. Our results demonstrate that haze is indeed a distinct perceptual dimension of gloss, which is systematically related to the kurtosis of the specular lobe.

7.2. From Acquisition to Display

7.2.1. Spatial Augmented Reality

Spatial augmented reality allows to improve or modify the perception of the reality with virtual information displayed directly in the real world, using video-projection. Many fields such as tourism, entertainment, education, medicine, industry or cultural heritage may benefit from it. Recent computer science techniques allow to measure, analyse and visualise the geometry of the surface of real objects, as for instance archeological artefacts. We have proposed a SAR interaction and visualisation technique (part of the PhD thesis "Interaction techniques, personalized experience and surface reconstruction for spatial augmented reality" [12] defended this year) that combines the advantages of the study of both real and 3D archeological artefacts. Thus, we superimpose on the object an expressive rendering based on curvatures with SAR, allowing for example to show details of engravings. Next, we simulate the use of a flashlight with the help of a 6-degree-of-freedom controller. The user can then specify the area on the object to be augmented and adjust the various necessary parameters of the expressive rendering. One of the main characteristics of SAR is to enable multiple users to simultaneously participate to the same experience. However, depending on the target application, this can be seen as a drawback.

We have also proposed a new display device [27] that allows to create experiences in SAR that are both multiuser and personalised by taking into account the user point of view. In order to do so, the projection display, set in front of the object to augment, is made from a material that is both retro-reflective and semi-transparent. We suggest two different uses of this new device, as well as two scenarios of application.

7.2.2. *Isotropic BRDF Measurements*

Image-based BRDF measurements on spherical material samples present a great opportunity to shorten significantly the acquisition time with respect to more traditional, non-multiplexed measurement methods for isotropic BRDFs. However, it has never been analyzed deeply, what measurement accuracy can be achieved in such a setup; what are the main contributing uncertainty factors and how do they relate to calibration procedures. We have developed [20] a new set of isotropic BRDF measurements with their radiometric and geometric uncertainties acquired within such an imaging setup. We have analyzed the most prominent optical phenomena that affect measurement accuracy and pave the way for more thorough uncertainty analysis in forthcoming image-based BRDF measurements. Our newly acquired data with their quantified uncertainties will be helpful for comparing the quality and accuracy of the different experimental setups and for designing other such image-based BRDF measurement devices.

7.3. **Rendering, Visualization and Illustration**

7.3.1. *Cache-friendly Sampling*

Monte-Carlo integration techniques for global illumination are popular on GPUs thanks to their massive parallel architecture, but efficient implementation remains challenging. The use of randomly de-correlated low-discrepancy sequences in the path-tracing algorithm allows faster visual convergence. However, the parallel tracing of incoherent rays often results in poor memory cache utilization, reducing the ray bandwidth efficiency. Interleaved sampling [65] partially solves this problem, by using a small set of distributions split in coherent ray-tracing passes, but the solution is prone to structured noise. On the other hand, ray-reordering methods [83] group stochastic rays into coherent ray packets but their implementation add an additional sorting cost on the GPU [74], [50]. We have introduced [19] a micro-jittering technique for faster multi-dimensional Monte-Carlo integration in ray-based rendering engines. Our method, improves ray coherency between GPU threads using a slightly altered low-discrepancy sequence rather than using ray-reordering methods. Compatible with any low-discrepancy sequence and independent of the importance sampling strategy, our method achieves comparable visual quality with classic de-correlation methods, like Cranley-Patterson rotation [66], while reducing rendering times in all scenarios.

7.3.2. *Multi-Resolution Meshes for Feature-Aware Hardware Tessellation*

Hardware tessellation is de facto the preferred mechanism to adaptively control mesh resolution with maximal performances. However, owing to its fixed and uniform pattern, leveraging tessellation for feature-aware LOD rendering remains a challenging problem. In [15], we relax this fundamental constraint by introducing a new spatial and temporal blending mechanism of tessellation levels, which is built on top of a novel hierarchical representation of multi-resolution meshes. This mechanism allows to finely control topological changes so that vertices can be removed or added at the most appropriate location to preserve geometric features in a continuous and artifact-free manner (cf. Figure 9). We then show how to extend edge-collapse based decimation methods to build feature-aware multi-resolution meshes that match the tessellation patterns. Our approach is fully compatible with current hardware tessellators and only adds a small overhead on memory consumption and tessellation cost. This work as been published at Eurographics 2016 [15].

7.3.3. *Shape Depiction for Transparent Objects*

Shading techniques are useful to deliver a better understanding of object shapes. When transparent objects are involved, depicting the shape characteristics of each surface is even more relevant. We have developed [21] a method for rendering transparent scenes or objects using classical tools for shape depiction in real time. Our method provides an efficient way to compute screen space curvature on transparent objects by using a novel screen space representation of a scene derived from Order Independent Transparency techniques. Moreover, we propose a customizable stylization that modulates the transparency per fragment, according to its curvature and its depth, which can be adapted for various kinds of applications.

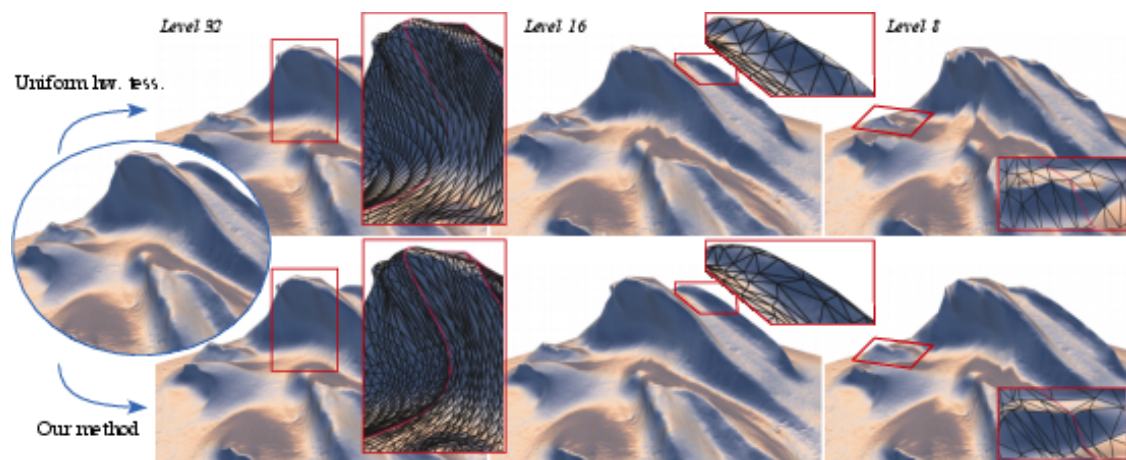


Figure 9. Uniform hardware tessellation (*top*) fails at representing accurately sharp features and areas of high curvature, such as the top and deep part of the drifts, which produces tessellation artifacts. Our method (*bottom*) better preserves those regions by adapting the triangle size and aligning their edges with those features.

7.4. Editing and Modeling

7.4.1. Flow-guided Warping for Image-based Shape Manipulation

Manipulating object shape in images usually require a-priori on their 3D geometry, and either user interactions or huge databases of 3D objects. In collaboration with the Maverick team (Inria Rhone Alpes), we have developed a method that manipulates perceived object shape from a single input color image without the need of additional 3D information, user input or 3D data. The key idea is to give the illusion of shape sharpening or rounding by exaggerating orientation patterns in the image that are strongly correlated to surface curvature (fig. 10). We build on a growing literature in both human and computer vision showing the importance of orientation patterns in the communication of shape, which we complement with mathematical relationships and a statistical image analysis revealing that structure tensors are indeed strongly correlated to surface shape features. We then rely on these correlations to introduce a flow-guided image warping algorithm, which in effect exaggerates orientation patterns involved in shape perception. We evaluate our technique by 1) comparing it to ground truth shape deformations, and 2) performing two perceptual experiments to assess its effects. Our algorithm produces convincing shape manipulation results on synthetic images and photographs, for various materials and lighting environments. This work has been published at ACM Siggraph 2016 [17].

7.4.2. Local Shape Editing at the Compositing Stage

Modern compositing software permit to linearly recombine different 3D rendered outputs (e.g., diffuse and reflection shading) in post-process, providing for simple but interactive appearance manipulations. Renderers also routinely provide auxiliary buffers (e.g., normals, positions) that may be used to add local light sources or depth-of-field effects at the compositing stage. These methods are attractive both in product design and movie production, as they allow designers and technical directors to test different ideas without having to re-render an entire 3D scene. In this work, we extended this approach to the editing of local shape: users modify the rendered normal buffer, and our system automatically modifies diffuse and reflection buffers to provide a plausible result. Our method is based on the reconstruction of a pair of diffuse and reflection prefiltered environment maps for each distinct object/material appearing in the image. We seamlessly combine the reconstructed buffers in a recompositing pipeline that works in real-time on the GPU using arbitrarily modified normals. This work as been published at the Eurographics Symposium on Rendering [24].



(a) Input image - ©Expertissim

(b) Shape sharpening

(c) Shape rounding

Figure 10. Our warping technique takes as input (a) a single image (Jules Benne, after Barye: “walking lion”) and modifies its perceived surface shape, either making it sharper in (b) or rounder in (c).

7.4.3. Topology-Aware Neighborhoods for Point-Based Simulation and Reconstruction

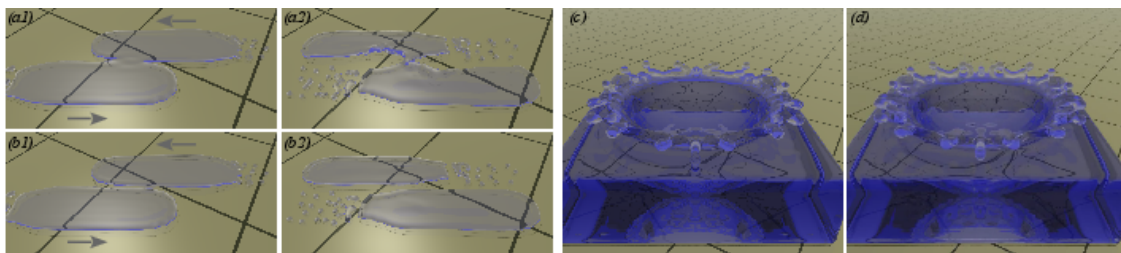


Figure 11. Two SPH fluid simulations using a standard Euclidean particle neighborhood (a,c), and our new topological neighborhood (b,d). On the left, two fluid components are crossing while moving in opposite directions.

Our new neighborhood performs accurate merging computations and avoids both unwanted fusion in the reconstruction and incorrect fluid interaction in the simulation. On the right, our accurate neighborhoods lead to different shape of the splash, and enable the reconstruction of the fluid with an adequate topology while avoiding bulging at distance.

Particle based simulations are widely used in computer graphics. In this field, several recent results have improved the simulation itself or improved the tension of the final fluid surface. In current particle based implementations, the particle neighborhood is computed by considering the Euclidean distance between fluid particles only. Thus particles from different fluid components interact, which generates both local incorrect behavior in the simulation and blending artifacts in the reconstructed fluid surface. In collaboration with IRIT, we developed a better neighborhood computation for both the physical simulation and surface reconstruction steps (fig. 11). Our approach tracks and stores the local fluid topology around each particle using a graph structure. In this graph, only particles within the same local fluid component are neighbors and other disconnected fluid particles are inserted only if they come into contact. The graph connectivity also takes into account the asymmetric behavior of particles when they merge and split, and the fluid surface is reconstructed accordingly, thus avoiding their blending at distance before a merge. In the simulation, this

neighborhood information is exploited for better controlling the fluid density and the force interactions at the vicinity of its boundaries. For instance, it prevents the introduction of collision events when two distinct fluid components are crossing without contact, and it avoids fluid interactions through thin waterproof walls. This leads to an overall more consistent fluid simulation and reconstruction. This work has been published at the Eurographics/ ACM SIGGRAPH Symposium on Computer Animation [18].

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

- CIFRE PhD contract with Technicolor (2014-2018)
Participants: A. Dufay, X. Granier, and R. Pacanowski
For this project, we aim at providing interactive previsualization of complex lighting with a smooth transition to the final solution.
- CIFRE PhD contract with FEI (2014-2018)
Participants: D. Murray, and X. Granier
For this project, we aim at providing expressive rendering techniques for volumes.

9. Partnerships and Cooperations

9.1. Regional Initiatives

9.1.1. Carer xD: "Caractérisation et restitution du réel xD"

Currently, the characterization and display of the real world are limited to techniques focusing on a subset of the necessary physical phenomena. A lot of work has been done to acquire geometric properties. However, the acquisition of a geometry on an object with complex reflection property or dynamic behavior is still a challenge. Similarly, the characterization of a material is limited to a uniform object for complex material or a diffuse material when one is interested in its spatial variations.

To reach full interaction between real and virtual worlds (augmented reality, mixed reality), it is necessary to acquire the real world in all its aspects (spatial, spectral, temporal) and to return it as in all these dimensions. To achieve this goal, a number of theoretical and practical tools will be developed around the development of mixed reality solutions and the development of some theoretical framework that supports the entire project.

9.2. National Initiatives

9.2.1. ANR

9.2.1.1. "Young Researcher" RichShape (2014-2018)

MANAO

Leader G. Guennebaud

This project aims at the development of novel representations for the efficient rendering and manipulation of highly detailed shapes in a multi-resolution context.

9.2.1.2. ALTA (2011-2016)

MAVERICK, REVES

Leader N. Holzschuch (MAVERICK)

The project ALTA aims at analyzing the light transport equations and at using the resulting representations and algorithms for more efficient computation. We target lighting simulations, either off-line, high-quality simulations or interactive simulations.

9.2.1.3. ISAR (2014-2017)

POTIOC, MANAO, LIG-CNRS-UJF, Diotasoft

Leader M. Hachet (POTIOC)

The ISAR project focuses on the design, implementation and evaluation of new interaction paradigms for spatial augmented reality, and to systematically explore the design space.

9.2.1.4. MATERIALS (2015-2019)

MAVERICK, LP2N-CNRS (MANAO), Musée d’Ethnographie de Bordeaux, OCÉ-Print

Leader N. Holzschuch (MAVERICK)

Local Leader R. Pacanowski (LP2N-CNRS)

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.

9.2.1.5. FOLD-Dyn (2016-2020)

IRIT, IMAGINE, MANAO, TeamTo, Mercenaries

Leader L. Barthe (IRIT)

Local Leader G. Guennebaud (Inria)

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.

9.2.2. Competitivity Clusters

9.2.2.1. LabEx CPU

IMB (UPR 5251), LABRI (UMR 5800), Inria (CENTRE BORDEAUX SUD-OUEST), I2M (NEW UMR FROM 2011), IMS (UMR 5218), CEA/DAM

Some members of *MANAO* participate in the local initiative CPU. As it includes many thematics, from fluid mechanics computation to structure safety but also management of timetable, safety of networks and protocols, management of energy consumption, etc., numerical technology can impact a whole industrial sector. In order to address problems in the domain of certification or qualification, we want to develop numerical sciences at such a level that it can be used as a certification tool.

9.3. European Initiatives

9.3.1. FP7 & H2020 Projects

9.3.1.1. PRISM

Title: Perceptual Representation of Illumination, Shape and Material

Programm: FP7

Duration: January 2013 - December 2016

Coordinator: JUSTUS-LIEBIG-UNIVERSITAET GIESSEN

Partners:

Justus-Liebig-Universitaet Giessen (Germany)

Katholieke Universiteit Leuven (Belgium)

Next Limit SI (Spain)

Technische Universiteit Delft (Netherlands)

the Chancellor, Masters and Scholars of The University of Cambridge (United Kingdom)

Bilkent Üniversitesi (Turkey)

Universite Paris Descartes (France)

The University of Birmingham (United Kingdom)

Local Leader: Pascal Barla

Visual perception provides us with a richly detailed representation of the surrounding world, enabling us to make subtle judgements of 1) 3D shape, 2) the material properties of objects, and 3) the flow of illumination within a scene. Together, these three factors determine the intensity of a surface in the image. Estimating scene properties is crucial for guiding action and making decisions like whether food is edible. Visual ‘look and feel’ also plays a key role in industrial design, computer graphics and other industries. Despite this, little is known about how we visually estimate the physical properties of objects and illumination. Previous research has mainly focussed on one or two of the three causal factors independently, and from the viewpoint of a specific discipline. By contrast, in PRISM we take an integrative approach, to understand how the brain creates a richly detailed representation of the world by looking at how all three factors interact simultaneously. PRISM is radically interdisciplinary, uniting experts from psychology, neuroscience, computer science and physics to understand both the analysis and synthesis of shape, shading and materials. PRISM is intersectoral by uniting researchers from seven leading Universities and two industrial partners, enabling impact in basic research, technology and the creative industries. Through research projects, cross-discipline visits, and structured Course Modules delivered through local and network-wide training events, we will endow PRISM fellows with an unusually broad overview and the cross-sector skills they need to become future leaders in European research and development. Thus, by delivering early-career training embedded in a cutting-edge research programme, we aim to 1) springboard the next generation of interdisciplinary researchers on perceptual representations of 3D scenes and 2) cement long-term collaborations between sectors to enhance European perception research and its applications.

9.4. International Initiatives

9.4.1. International Partners

9.4.1.1. Rainbow Particle Imaging Velocimetry

Partner : KAUST - King Abdullah University of Science & Technology

We propose a new approach for snapshot imaging of time-resolved, non-stationary 3D fluid flows, which we term Rainbow Particle Imaging Velocimetry (RainbowPIV). Using only a single camera, RainbowPIV will be able to track a dense set of particles advected in the flow. This is achieved by illuminating the flow volume with a stack of monochromatic light planes at different wavelengths (a “rainbow”). Particles are tracked in 3D by both following their 2D spatial position and their change in color, depending on which light plane they traverse.

RainbowPIV will provide dense measurements of 3D velocity vectors, thus obtaining a dense 3D representation of a 3D velocity field. This will allow us to accurately image and understand many new types of flow, including turbulent flows within complex 3D geometries and particle trajectories, with limited optical access. After the initial exploration stage covered in this proposal, RainbowPIV could find many applications in science and engineering, for example to help understand combustion processes or flow through catalytic converters, between turbine blades, and inside inlet manifolds.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

10.1.1.1. Member of the Organizing Committees

Expressive 2016 (NPAR-SBIM-CAe), Workshop on NanoAppearance

10.1.2. Scientific Events Selection

10.1.2.1. Member of the Conference Program Committees

ACM Siggraph 2016, ACM Siggraph Asia 2016, Symposium on Geometry Processing (SGP) 2016, Geometric Modeling and Processing (GMP) 2016, SIBGRAPI (Conference on Graphics, Patterns and Images) 2016

10.1.2.2. Reviewer

Eurographics 2016, Pacific Graphics 2016, High Performance Graphics 2016

10.1.3. Journal

10.1.3.1. Reviewer - Reviewing Activities

ACM Transactions on Graphics (TOG), IEEE Transactions on Visualization and Computer Graphics (TVCG), Computer Graphics Forum (CGF),

10.1.4. Invited Talks

Implicit Skinning : une méthode d’animation de personnages interactive avec contacts et étirements de la peau. Rencontres Animation Développement Innovation (RADI).

10.1.5. Research Administration

Inria Evaluation Committee

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

The members of our team are involved in teaching computer science at University of Bordeaux, ENSEIRB Engineering School, 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, Romain Pacanowski, Advanced Image Synthesis, 60 HETD, M2, Univ. Bdx, France.

Master : Gaël Guennebaud, Numerical Techniques, 45 HETD, M1, IOGS, France

Master : Xavier Granier, Image Synthesis, 14 HETD, M2, IOGS, France

Master : Gaël Guennebaud, Geometric Modeling, 22 HETD, M2, IOGS, France

Master : Romain Pacanowski, Thibaud Lambert, Antoine Lucat & Brett Ridet, Algorithmic and Object Programming, 60 HETD, M1, IOGS, France

Master : Xavier Granier, Romain Pacanowski, Colorimetry and Appearance Modeling, 20 HETD, M1, IOGS, France.

Master : Gaël Guennebaud and Pierre Bénard, High-performance 3D Graphics, 60 HETD, M1, Univ. Bdx and IOGS, France.

Master : Pierre Bénard, Virtual Reality, 24 HETD, M2, Univ. Bdx, France.

Master : Ivo Ihrke, Advanced Display Technology, 12 HETD, M1, IOGS, France

Master : Pierre Bénard, Image Synthesis and 3D modeling, 60 HETD, M2, ENSEIRB, France

Licence : Patrick Reuter, Digital Imaging, 36 HETD, L3, Univ. Bdx, France.

Some members are also in charge of some fields of study:

Master : Xavier Granier, M2, IOGS (Bordeaux), France.

License : Patrick Reuter, Science and Modeling, L2, Univ. Bdx, France.

10.2.2. Supervision

PhD : Boris Raymond, Rendering and manipulation of anisotropic materials, Univ. Bordeaux, P. Barla & G. Guennebaud & X. Granier

PhD : John Restrepo, Plenoptic Imaging and Computational Image Quality Metrics, Inria & Univ. Bordeaux, I. Ihrke

PhD : Brett Ridet, Interactive spatial augmented reality, Inria & Univ. Bordeaux, P. Reuter & X. Granier

PhD : Carlos Zubiaga Pena, Image-space editing of appearance, Inria & Univ. Bordeaux, P. Barla & X. Granier

PhD : Florian Canezin, Implicit Modeling, Univ. Toulouse III, G. Guennebaud & Loic Barthe

PhD : Arthur Dufay, Adaptive high-quality of virtual environments with complex photometry, Technicolor & Univ. Bordeaux, J.-E. Marvie R. Pacanowski & X. Granier

PhD : Thibaud Lambert, Real-time rendering of highly detailed 3D models, Inria & Univ. Bordeaux, G. Guennebaud & P. Bénard

PhD : Loïs Mignard-Debize, Plenoptic function and its application to spatial augmented reality, Inria & Univ. Bordeaux, P. Reuter & I. Ihrke

PhD : Antoine Lucat, Appearance Acquisition and Rendering, IOGS & Univ. Bordeaux, R. Pacanowski & X. Granier

PhD : David Murray, Expressive Rendering of Volumetric Data, FEI & Univ. Bordeaux, J. Baril & X. Granier

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Major publications by the team in recent years

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- [12] B. RIDEL. *Interaction techniques, personalized experience and surface reconstruction for spatial augmented reality*, Université de bordeaux, October 2016, <https://hal.inria.fr/tel-01414792>.

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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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- 2.2.1. - Cardiovascular and respiratory diseases
- 4.3.2. - Hydro-energy
- 4.3.3. - Wind energy
- 5.2.1. - Road vehicles
- 5.2.3. - Aviation
- 5.2.4. - Aerospace
- 5.5. - Materials
- 8.4. - Security and personal assistance
- 8.4.1. - Crisis management

1. Members

Research Scientist

Michel Bergmann [Inria, Researcher, HDR]

Faculty Members

Angelo Iollo [Team leader, Univ. Bordeaux, Professor, HDR]

Afaf Bouharguane [Univ. Bordeaux, Associate Professor]

Charles-Henri Bruneau [Univ. Bordeaux, Professor]

Lisl Weynans [Univ. Bordeaux, Associate Professor]

Technical Staff

Florian Bernard [Inria]

Andrea Valenti [Univ. Bordeaux, until Apr 2016]

PhD Students

Emanuela Abbate [Universita degli Studi dell'Insubria / Universite de Bordeaux]

Mathias Braun [IRSTEA]

Meriem Jedouaa [Inria]

Baptiste Lambert [Univ. Bordeaux]

Claire Morel [VALEOL]

Alice Raeli [Univ. Bordeaux]

Federico Tesser [Inria]

Post-Doctoral Fellow

Andrea Ferrero [Inria]

Administrative Assistant

Anne-Laure Gautier [Inria]

Others

Mohsen Broumand [Inria, Intern, from Oct 2016 until Dec 2016]

Marco Cisternino [Univ. Bordeaux, Engineer, from Nov 2014 until Feb 2016]

Antoine Fondaneche [Corwave, Assistant Engineer, from Sept 2016]

Pierre-Jakez Lebreton [Inria, Intern, from Jun 2016 until Jul 2016]

Nadia Loy [Inria, Intern, from Oct 2015 until March 2016]

Martin Maurey [Inria, Intern, from Jun 2016 until Sep 2016]

Jean-Christophe Ricklin [Univ. Bordeaux, Intern, from May 2016 until Jul 2016]

Sebastien Riffaud [Inria, Intern, until Aug 2016]

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 derived from first principles or be data-driven. With ROMs one trades accuracy for speed and scalability, and counteracts the curse of dimension by significantly reducing the computational complexity. ROMs represent an ideal building block of 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. 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 [55], [47] and boundary conditions are imposed using appropriate interpolation methods [33], [57], [52]. 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 non-structured 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 presently virtually absent at Inria, are among the main scientific challenges of our team.

3.2. Reduced-order models

Massive parallelization and rethinking of numerical schemes will allow the solution of new problem in physics and the prediction of new phenomena thanks to simulation. However, in industrial applications fast on line responses are needed for design and control. For instance, 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 at a large number of conditions to give an estimate of the maximum loads, and hence stresses, that the structure of the detailed aircraft design will experience in service. A simplistic estimate of the number of analyses required would multiply the numbers of conditions to give 10^7 . 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 loads conditions, meaning that approximately 10^5 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 [44], our interest will be focused on two axis. On the one hand, we start from the consideration that small, highly non-linear 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 close to the walls at the scale of a millimeter for computational domains that are of the order of hundreds of meters. In this context our approach is characterized by 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) [48], [56], [36] we can accurately approximate large solution databases using a small base. Recent techniques to investigate the temporal evolution of the POD modes (Koopman modes [50], [34], Dynamic Mode Decomposition [54]) allow a dynamic discrimination of the role played by each of them. This in turn can be exploited to interpolate between the modes in parameter

space, thanks to ideas relying on optimal transportation [58], [40] that we have started developing in the FP7 project FFAST and H2020 AEROGUST. In the following we precise these ideas on a specific example.

4. Application Domains

4.1. Energy conversion

We consider applications in the domain of wind engineering and sea-wave converters. As an example of application of our methods, we show a recent realization where we model a sea-wave energy converter, see figure 1. In this unsteady example, the full interaction between the rigid floater, air and water is described by a monolithic model, the Newton's law, where physical parameters 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 [55]. The background method for fluid structure interface is the volume penalization method [33] where the level set functions is used to improve the degree of accuracy of the method [38] and also to follow the object. The simulations are unsteady, three dimensional, with $O(10^8)$ grid points on 512 CPUs.

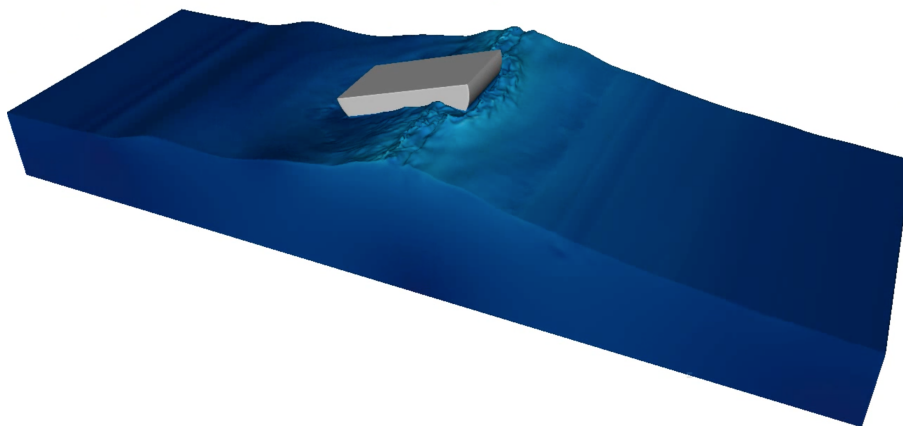


Figure 1. Numerical modeling of a sea-wave converter by a monolithic model and Cartesian meshes.

4.2. Impacts

The numerical modelling of multimaterial rapid dynamics in extreme conditions is an important technological problem for industrial and scientific applications. Experiments are dangerous, need heavy infrastructures and hence are difficult and expensive to realize. The simulation of such phenomena is challenging because they couple large deformations and displacements in solids to strongly non-linear behaviour in fluids. In what follows, we privilege a fully Eulerian approach based on conservation laws, where the different materials are characterized by their specific constitutive laws. This approach was introduced in [46] and subsequently pursued and extended for example in [51], [45], [35], [59].

We study hyper-velocity phenomena where several materials are involved. An example of this approach is the impact of a projectile immersed in air over a shield, see figure 2. Using the same set of equations across the entire domain, we model the compressible fluid, the hyperelastic material and the interaction at the interface that models possible rebounds. Only the constitutive laws characterize the different materials.

The simulation is performed over a 4000^2 fixed Cartesian grid so that the resulting numerical scheme allows an efficient parallelization (512 processors in this case) with an isomorphism between grid partitioning and processor topology. The challenge for our team is to increase the accuracy of the simulation thanks to grid refinement in the vicinity of the moving interfaces, still guaranteeing scalability and a simple computational set up.

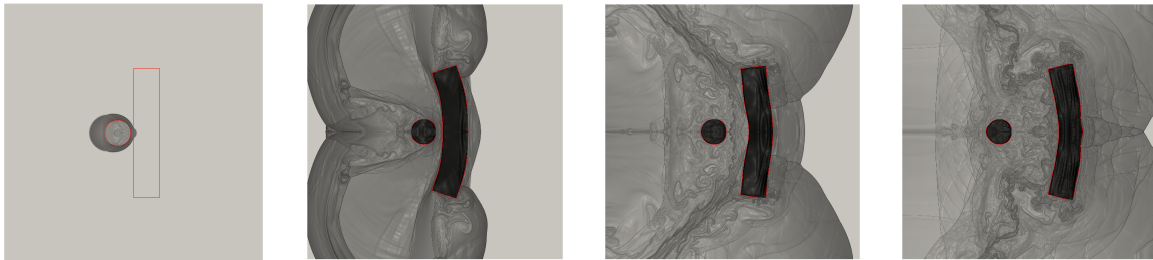


Figure 2. Impact and rebound of a copper projectile on a copper plate. Interface and schlieren at $50\mu s$, $199\mu s$, $398\mu s$ and $710\mu s$. From left to right, top to bottom.

4.3. New materials

Thanks to the multi-scale schemes that we develop, we can characterize new materials from constituents. As an example, consider the material presented in figure 3 left. It is a picture of a dry foam that is used as dielectric material. This micrography is taken at the scale of the dry bubbles, where on the surface of the bubble one can observe the carbon nanotubes as white filaments. The presence of nanotubes in the dry emulsion makes the electrical capacitance of this material significantly affected by its strain state by creating aligned dipoles at a larger scale compared to the size of the dielectric molecules. It is a typical multi-scale phenomenon in presence of widely varying physical properties. This material is used to generate micro currents when it undergoes vibrations. The schemes that we devise allow to model this multi-scale irregular material by a monolithic model (same equation in the whole domain), in this case a variable coefficient diffusion equation. In order to recover adequate accuracy, the numerical scheme is adapted near the interfaces between the different subdomains. The computational hierarchical mesh is directly derived by the micrography of the material (figure 3 right).

4.4. Bio-inspired robotic swimming

In bioinspired robotic swimming the aim is of simulating a three-dimensional swimmer starting from pictures. The first step is to build the three-dimensional fish profile based on two-dimensional data retrieved from the picture of an undeformed fish at rest. This is done by a skeleton technique and a three-dimensional level set function describing the body surface. Then the skeleton is deformed using an appropriate swimming law to obtain a sequence of level set functions corresponding to snapshots of the body surface uniformly taken at different instants.

Thanks to skeleton deformation we typically reconstruct 20% of the snapshots necessary to simulate a swimming stroke, since the time scale of the simulation is significantly smaller than the time step between two subsequent reconstructed snapshots. Also, the surface deformation velocity is required to set the boundary conditions of the flow problem. For this reason it is necessary to build intermediate level set functions and to compute the deformation velocity field between subsequent fish snapshots. Optimal transportation is well suited to achieve this goal providing an objective model to compute intermediate geometries and deformation velocities.

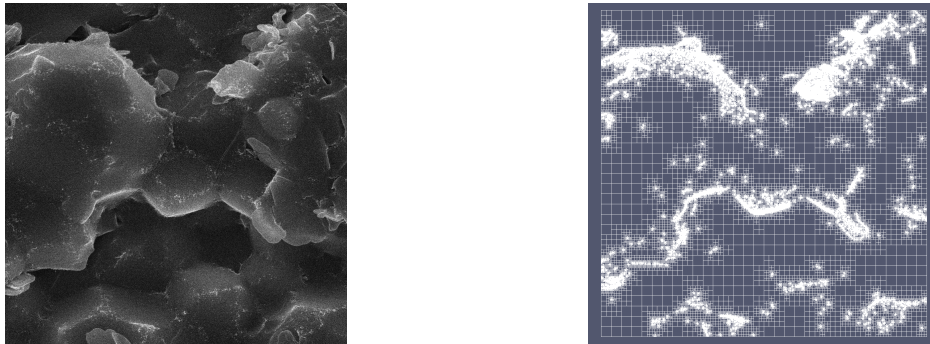


Figure 3. A micrography of an electrostrictive material is shown on the left: the bright regions visualize the carbon nanotubes. The hierarchical grid adapted to the nanotubes is shown on the right. The ratio between the largest and the smallest cell side is 2^7 . Project developed in collaboration with the CRPP physics and chemistry lab of the CNRS in Bordeaux (Annie Colin, Philippe Poulin).

Numerical simulations have been performed in 3D, see figure 4. However, it has been observed that these algorithms do not preserve the physics/features of the represented objects. Indeed, the fish tends to compress during the deformation.

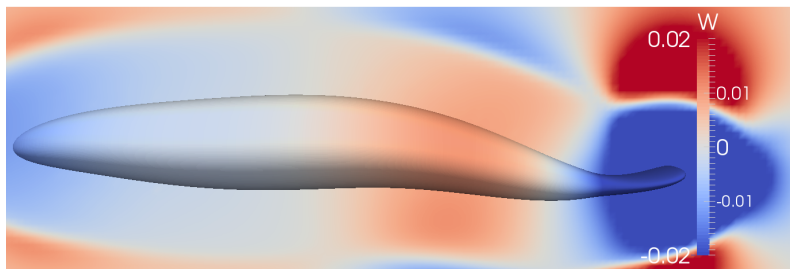


Figure 4. Comparison of the exact deformation velocity (presented inside the swimmer) and the approximated velocity identified using optimal transport (represented outside the fish). The error of the identification scheme is negligible for this component of the velocity, as it can be inferred by comparing the two velocities on the boundary of the swimmer.

For this reason, we will consider incompressible or rigid transports. Another example of bio-inspired swimming is presented in the highlights section.

5. Highlights of the Year

5.1. Highlights of the Year

Numerical simulation of zebrafish larvae C-bend

This part is performed in collaboration with the MRGM laboratory (Laboratoire Maladies Rares : Génétique et Métabolisme, <https://mrgm.u-bordeaux.fr/>). They are interested in the swimming of a zebrafish larvae under genetic modifications. One aim is to quantify the power spent by such fishes to swim after a stimuli reaction. The numerical simulation we develop can help computing integral quantities such the power [39]. This simulation is challenging due to coupling several methods like image treatment (from movies given by MRGM), optimal transport [58] and numerical simulations.

First 2D numerical results have been performed from a series of 615 pictures obtained at a rate equal to 15 000 images per second. The fish is a 8-day zebrafish larvae (length is $\ell = 7\text{ mm}$) presented in figure 5.

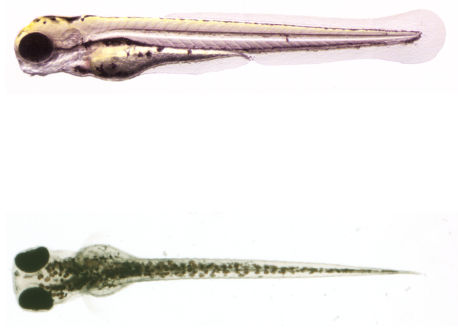


Figure 5. Pictures of a 8-day zebrafish larvae. Source: MRGM.

All the 615 pictures have been post-processed to remove the displacement of the center of mass (due to the hydrodynamic forces) as well as the rotation angle (due to the hydrodynamic torques) to isolate the kinematic of the deformation. Indeed, the displacement of the mass center and the rotation angle have to be computed as being the results of the flow effects generated by the fish deformation. The numerical solver requires however more than 615 images for the overall simulation due to small times steps limitation. The missing images are thus computed using optimal transportation with the algorithm presented in [40]. This method gives also the deformation velocity inside the body that is necessary for our numerical simulation based on the penalty method (see figure 4 for an example of deformation velocity computation).

A comparison between experimental and numerical swimming behaviors is presented in figure 6. The qualitative behaviors look quite similar. In a more quantitative way, figures 7 and 8 show the temporal evolution of the rotating angle as well as the position of the center of mass. The numerical results (displacement of the mass center and the rotation) are quite close to the experimental ones (the ones removed in the post-processed of the original pictures).

The small differences can be explained by the fact the the actual simulation is only two-dimensional. Another explanation is that the deformation velocity obtained by optimal transportation is by definition irrotational and *a priori* non divergence free. We are now working on the 3D simulation as well as a modified (sub-)optimal transportation including rotational effects for a divergence free field.

6. New Software and Platforms

6.1. COCOFLOW

FUNCTIONAL DESCRIPTION

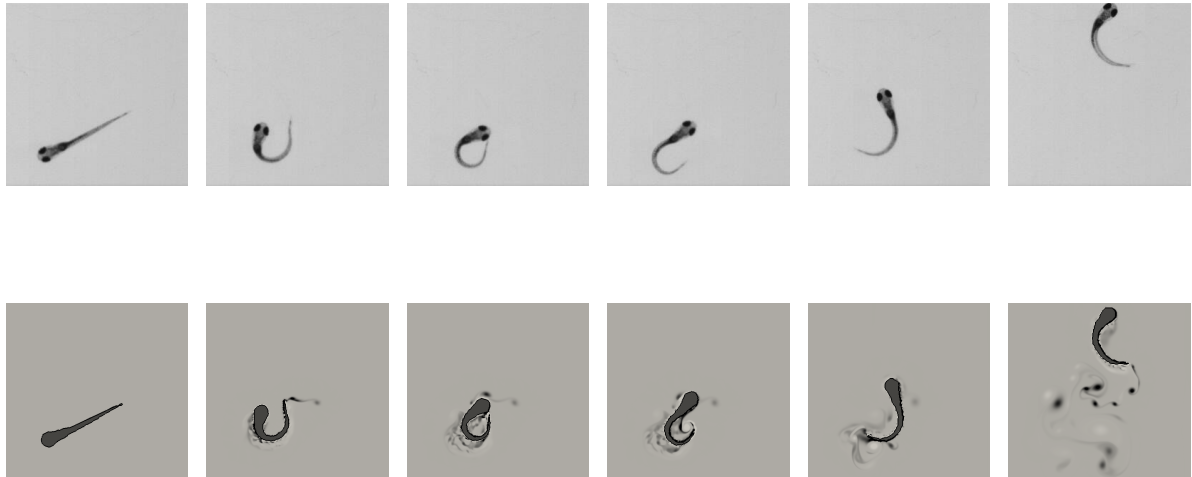


Figure 6. Comparison between experimental (top) and numerical results (bottom) at t_0 , $t_0 + 0.7$ ms, $t_0 + 1.1$ ms, $t_0 + 1.3$ ms, $t_0 + 2$ ms and $t_0 + 4.1$ ms from left to right. Experiments results given by MRGM.

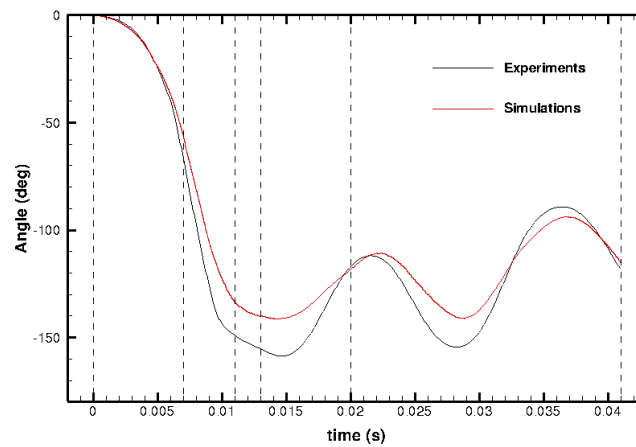
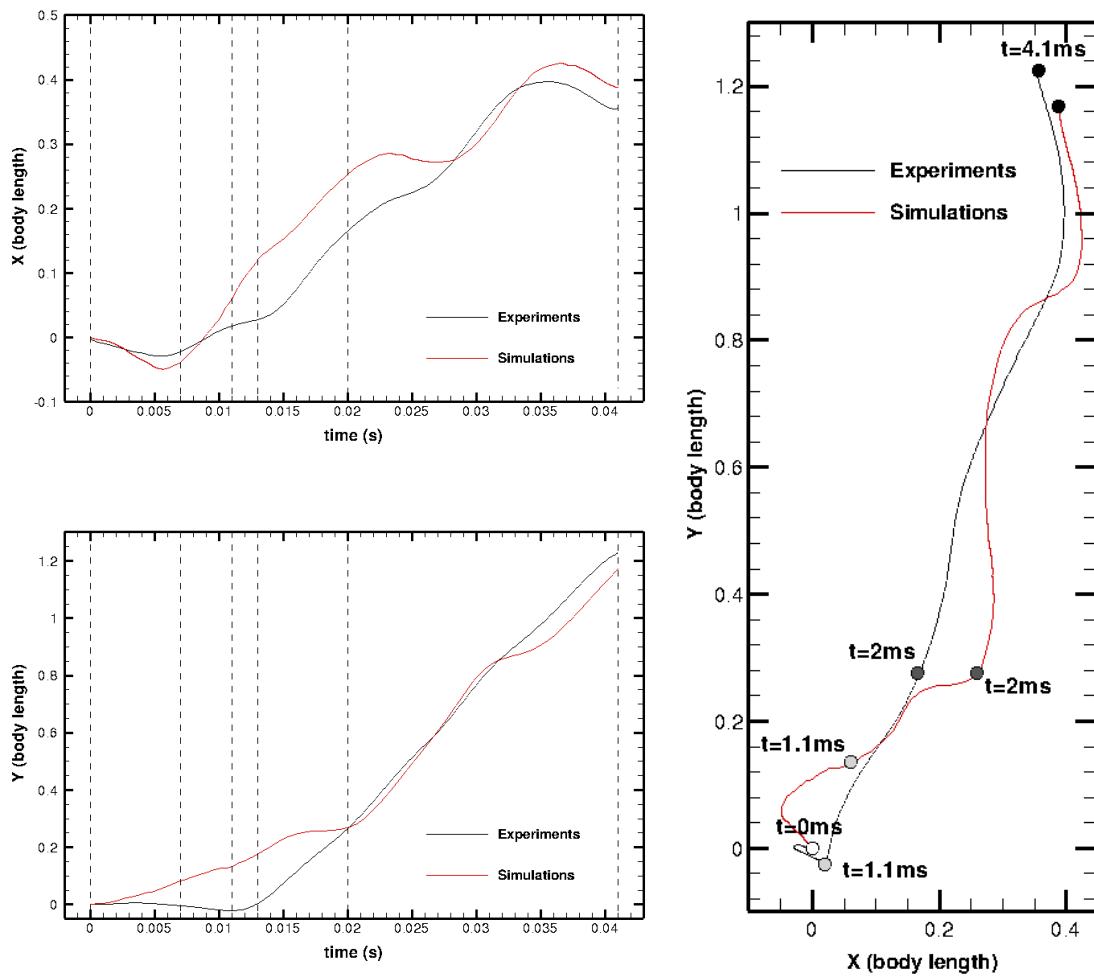


Figure 7. Temporal evolution of the rotation angle.



(a) Temporal evolution of the center of mass.

(b) Position of the center of mass.

Figure 8. Kinematic results for the zebrafish swimming.

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.

- Contact: Florian Bernard
- URL: <https://gforge.inria.fr/projects/cocoflow>

6.2. KOPPA

Kinetic Octree Parallel PolyAtomic
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
- Contact: Florian Bernard
- URL: <https://git.math.cnrs.fr/gitweb/?p=plm/fbernard/KOPPA.git;a=summary>

6.3. 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

6.4. 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
- Contact: Michel Bergmann
- URL: <https://gforge.inria.fr/projects/nascar/>

7. New Results

7.1. Hybrid POD/DNS: application to aeroelastic windturbine blade

Some new techniques related to Reduced Order Modelling have been developed in the framework of the EU project AEROGUST. The first proposed approach is based on a domain decomposition method in which a POD [56], [43], [44], [37], [36] model is dynamically coupled with a CFD solver [39], [38]. This tool can be used to perform predictive simulations thanks to the fact that the non-linear effects related to new working conditions are directly captured by the CFD solver while the far field region can be efficiently described by the POD model. The hybrid technique has been extended to gust simulations by the introduction of forcing terms which can describe perturbations coming from the far field.

The domain decomposition approach has been proposed also inside an iterative procedure named "numerical zoom" which is based on the use of several mesh levels. This procedure is repeated several times in order to focus the degrees of freedom of the discretisation in the region close to the body.

Finally, the POD method has been proposed also for the acceleration of CFD solver for incompressible flows. The solution of the Poisson problem on the pressure variable which appears in incompressible solvers can be quite time consuming. The proposed approach consists in searching the solution of the Poisson problem in the space spanned by the POD basis. This is done by substituting the POD expansion in the Poisson equation and minimizing the residuals. The robustness of the method has been improved by introducing a check on the quality of the Poisson solution (based on the divergence of the velocity field at the end of the correction step) and a dynamic update of the POD basis.

The domain decomposition approach with the forcing terms has been used to simulate the effects of a gust on a wind turbine blade in a simplified configuration at low Reynolds number. The numerical zoom procedure is applied by coupling a DNS simulation with a POD description of the far field. The solution obtained on three levels of mesh is reported in Figure 9 in which the vortex structures are shown according to the q -criterion. The bending of the blade is described by a non-linear beam model. Figure 10 shows the shapes of the blade without loads, in the chosen working condition and during the gust.

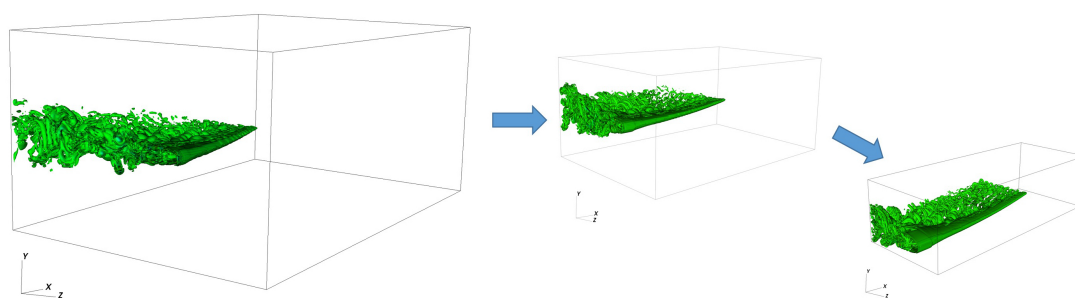


Figure 9. Numerical zoom on the wind turbine blade simulation (vortex structure visualised by q -criterion)

7.2. Discretization of the Laplacian operator using a multitude of overlapping cartesian grids

A new finite-difference approach to solve a Laplacian operator has been developed, using patches of overlapping grids where a fined level is needed, leaving coarser meshes in the rest of the computational domain. These overlapping grids will have generic quadrilateral shapes (as shown in figure 11).



Figure 10. Blade shape without loads (top), in the chosen working condition (middle) and during the gust (bottom)

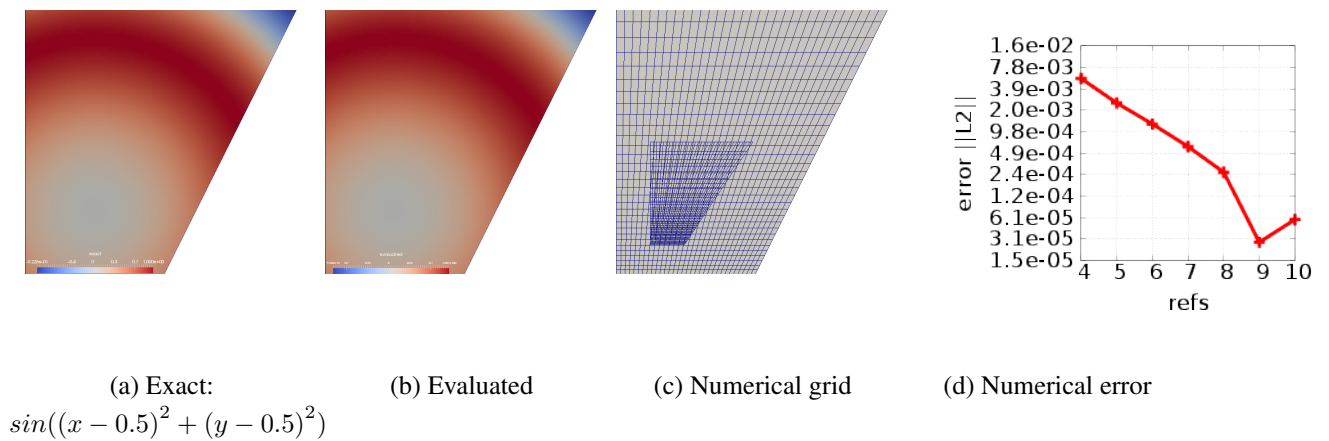
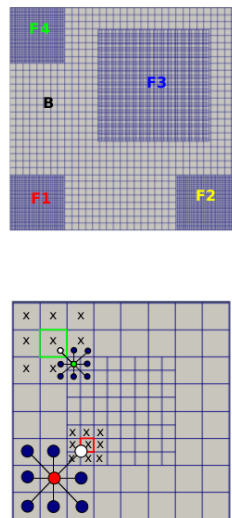


Figure 11. results

A monolithic approach is used to solve the algebraic equations, applying restriction and prolongation operators to fill the non-diagonal blocks of the resulting matrix. These operators work on data structures communicated between the different grids using ad hoc parallel inter-communicators, as shown in figure 12. 12.



$$\begin{bmatrix} D & R & R & R & R \\ P & D & 0 & 0 & 0 \\ P & 0 & D & 0 & 0 \\ P & 0 & 0 & D & 0 \\ P & 0 & 0 & 0 & D \end{bmatrix} \times \begin{bmatrix} x \\ x \\ x \\ x \\ x \end{bmatrix} = \begin{bmatrix} f \\ f \\ f \\ f \\ f \end{bmatrix}$$

Blocks D are the discretization matrices onto each grid
(parallel intra-communications).

Blocks R and P are the restriction and prolongation operators between the grids
(parallel inter-communications).

Figure 12. Monolithic approach

Works are going on to change the solver from the finite-difference approach to a finite-volume one, and to implement the 3D case. The use of a finite-volume solver can benefit from the usage of octree patches instead of cartesian grids, obtaining a more accurate refining and a greater precision.

7.3. Numerical simulation of a biomimetic LVAD developed by CorWave

We just started a collaboration with the PME CorWave. The CorWave LVAD utilizes an undulating disc wave pumping mechanism, replacing the high speed, high shear impeller of current continuous flow rotary pumps. Louis de Lillers, the CorWave project manager, has contacted MEMPHIS to perform numerical simulations and optimizations of their LVAD. This collaboration has started with an industrial PhD (Cifre, Antoine Fondaneche). Figure 13 shows preliminary results (proof of concept) for the CorWave LVAD obtained with the code NaSCar described in [38].

7.4. A sharp Cartesian method for incompressible flows with large density ratios

We have developed and validated a new Cartesian method for bifluid incompressible flows with high density ratios. The specificity of the method relies on a sharp second order numerical scheme for the spatial resolution of the discontinuous elliptic problem for the pressure, that was developed in [42]. The Navier-Stokes equations are integrated in time thanks to a fractional step method based on the Chorin scheme and discretized in space on a Cartesian mesh. The bifluid interface is implicitly represented using a level set function. The numerical tests show the improvements due to this sharp method compared to classical first order methods. As an illustration, we present here numerical results for the dam break test case.

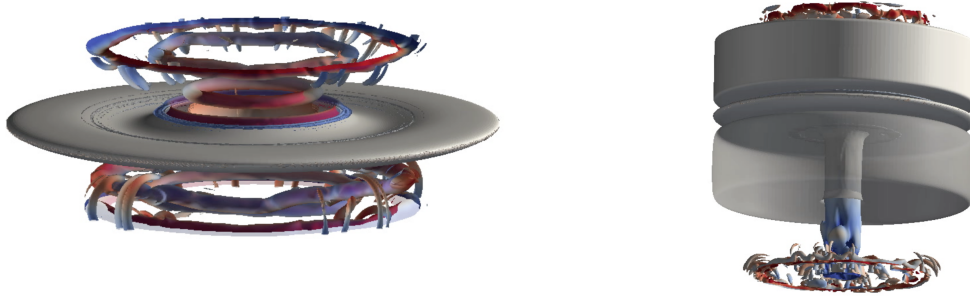


Figure 13. Preliminary results (proof of concept) for the CorWave LVAD. Left: oscillating membrane, right: the whole pump system.

This test case is studied in [53] and [41], and based on experiments conducted in [49]. The initial configuration is a water column at rest in air. The initial height and width of the column are both 5.715 cm. The domain size is 40 cm \times 10 cm. The value of the physical parameters are

$$\left\{ \begin{array}{l} \rho_{water} = 1000 \text{ kg/m}^3, \\ \mu_{water} = 1.137 \times 10^{-3} \text{ kg/ms}, \\ \rho_{air} = 1.226 \text{ kg/m}^3, \\ \mu_{air} = 1.78 \times 10^{-5} \text{ kg/ms}, \\ \sigma = 0.0728 \text{ kg/s}^2 \\ g = -9.8 \text{ m/s}^2 \end{array} \right. \quad (6)$$

We present in Figure 14 the interface evolution at non-dimensional times $T = t\sqrt{g/h} = 0, 1, 2, 3, 4$, with h the initial height of the water column. The computations are performed with 256×64 points.

In Figure 15, we plot the evolution in time of the water front, compared to the experimental results of [49], and to the results obtained for the Ghost-Fluid method and the conservative method of Raessi and Pitsch [53]. We observe that the front propagation is in agreement with the experimental results and the results of the conservative method presented in [53]. It means that, though the method is not strictly conservative, the numerical errors due to momentum transfer across the interface are not large enough to slow down the propagation of the front. It is not the case for instance for the Ghost-Fluid method, as it can be noticed in Figure 15 and has been reported in [53].

7.5. Platooning of trucks on highways

In the context of energy saving, the platooning of ground vehicles on top of a road, in particular highways has been studied. The numerical simulations are performed in 2D and 3D for up to 10 billions unknowns on 384 cores. The goal is to have trucks autonomously following their leader to form a road train in order to improve traffic flow efficiency and to reduce oil consumption. Thus the distance between trucks is short. For instance a gain of about 40% can be obtained on the drag coefficient of the followers when the distance between trucks is equal to 1.8125 their height (see the figure 16), that is approximately eight meters. Even the leader has a lower drag coefficient (-10%) as the first follower compresses the flow in its wake. In the figure it is clearly shown that the pressure gradients inside the gap between the vehicles are much lower than in front of the leader.

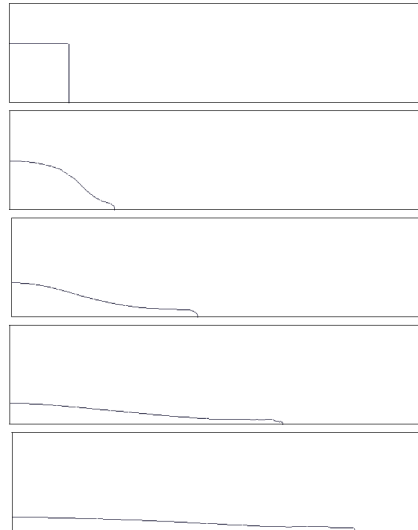


Figure 14. Evolution of the interface for the dam break problem at non-dimensional times $T = t\sqrt{g/h} = 0, 1, 2, 3, 4$.

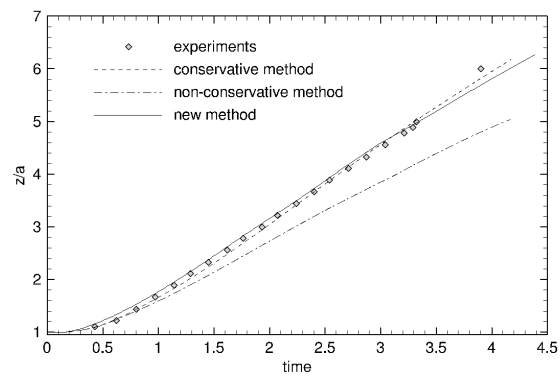


Figure 15. Evolution of the front of propagation: comparison between experimental data and several numerical methods: the Ghost Fluid method (non-conservative method), the conservative method of Raessi and Pitsch and our new method, The dimensionless location of the front $\frac{z}{a}$ is plotted as a function of the dimensionless time $t\sqrt{qh}$.

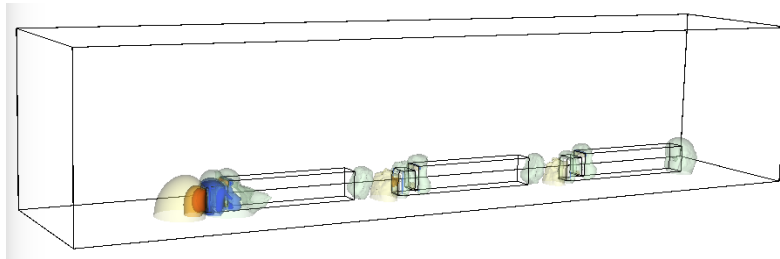


Figure 16. Mean pressure contours of the mean flow around three simplified European tractor-trailer geometries with a distance equal to 1.8125 their height on top of a road in three dimensions.

7.6. Non-linear elasto-plastic dynamics of compressible materials

We describe a numerical model to simulate the non-linear elasto-plastic dynamics of compressible materials. The model is fully Eulerian and it is discretized on a fixed Cartesian mesh. The hyperelastic constitutive law considered is neo-hookean and the plasticity model is based on a multiplicative decomposition of the inverse deformation tensor. The model is thermodynamically consistent and it is shown to be stable in the sense that the norm of the deviatoric stress tensor beyond yield is non-increasing. The multimaterial integration scheme is based on a simple numerical flux function that keeps the interfaces sharp. Numerical illustrations in one to three space dimensions of high-speed multimaterial impacts in air are presented.

In TC4 an iron sphere is impacting an aluminium plate immersed in air. The computational domain is $[-0.3, 0.7] \times [-0.4, 0.4] \times [-0.4, 0.4]$ m. The initial velocity of the projectile is 1000 m.s^{-1} . The computation is performed on a $500 \times 400 \times 400$ mesh with 216 processors. Homogeneous Neumann conditions are imposed on the left and right borders and cantilever on the others.

The results are given in Fig 17 where we present the Schlieren results on the vertical symmetry plane and the material interfaces. As in the 2D case the projectile perforates the aluminium plate which is strongly stretched. The breaking of the plate at final time is due to the level set function resolution.

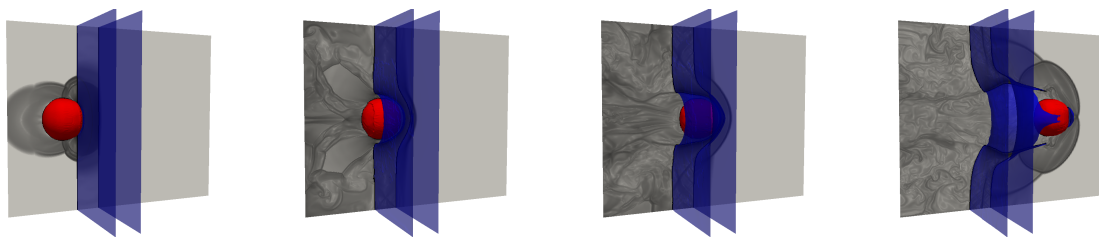
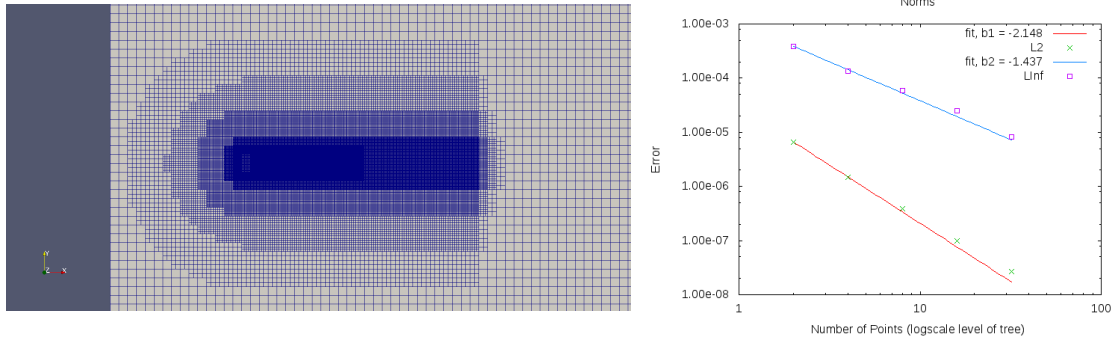


Figure 17. Schlieren representation on the vertical symmetry plane and the material interfaces.

7.7. Hierarchical grids: applications with quadtrees/octrees

A first application with a specific method is the resolution of the incompressible Navier-Stokes equations. A Navier-Stokes solver dealing with quadtrees has been implemented in parallel this year. The overall aim will be to model in 3D the flow over a wind turbine using an Octree grid. On the figure 18 can be seen an example of QuadTree mesh. A Finite Volume Semi-Lagrangian scheme is used.



(a) Example of QuadTree mesh for circular cylinder (b) Norms as a function of number of points on grid

Figure 18.

First, the order of convergence of the Laplacian Solver discretization on QuadTrees has been computed and compared with those obtained with other schemes as explained previously. The method for solving the Laplacian Solver is named Diamond method and consists in using a dual mesh and considering that the Gradients are constants inside. The order of convergence of 2 has been obtained. The order of convergence of the overall Navier-Stokes resolution on QuadTree meshes has been computed and the order of 2 is get as can be seen on figures 18. For the L_∞ norm, the order of 2 can't be reach caused by the loss of accuracy when a gap in refinement level occurs.

For now the grid is fixed, so the next step will be to refine and coarsen the grid following the position of the obstacle and the "interesting" areas. The work will then go on with the implementation of this Navier-Stokes solver with adaptive QuadTree meshes in 3D.

A second application is phase changing material. We consider problems governed by linear elliptic equations with discontinuity interfaces across the domain. The equation coefficients, the solution and its normal derivative can undergo a jump across these internal boundaries. We present a compact second-order finite-difference scheme on a tree-based adaptive grid that can be efficiently solved in parallel. The main idea is to optimize the truncation error of the discretization as a function of the local grid configuration.

The variable coefficient heat diffusion problem we consider is modeled by:

$$-\operatorname{div}(\kappa(\vec{x})\nabla u(\vec{x})) = g(\vec{x}), \quad \text{in } D, \quad (7)$$

$$R(\kappa\partial_{\vec{n}}u(\vec{x}))_S = [u], \quad \text{on } \gamma \quad (8)$$

$$[\kappa(\vec{x})\partial_{\vec{n}}u(\vec{x})] = 0, \quad \text{on } \gamma \quad (9)$$

Where $\vec{x} = (x, y, z)$ are the spatial coordinates and $\kappa(\vec{x})$ is piecewise continuous on each subdomain but it may be discontinuous across γ (the boundary of the D subdomain that contains the discontinuities through). A cell-centered investigation often leads to a symmetric linear system, since the relation between two neighbors is reflective. Considering the configuration in Fig. 19 it is natural to define the discretization at c_4 in terms of the others.



Figure 19. A test configuration centered in c_4 .

Let h be the side length of the cell c_4 . To obtain the existence of a linear consistent scheme we must be able to find the coefficients a_i such that:

$$u_{xx} + u_{yy} = a_1u_1 + a_2u_2 + a_3u_3 + a_4u_4 + a_5u_5 + a_6u_6 + a_7u_7 + O(h)$$

A complete Taylor's analysis on all the involved neighbors, applying them relative linear combinations of the expansions, implies that the coefficients a_i must satisfy the following linear system:

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & -h & 0 & -h & \frac{3h}{2} & -\frac{h}{2} & \frac{3h}{2} \\ 0 & h & h & 0 & \frac{h}{2} & -\frac{3h}{2} & -\frac{3h}{2} \\ 0 & \frac{h^2}{2} & 0 & \frac{h^2}{2} & \frac{9h^2}{8} & \frac{h^2}{8} & \frac{9h^2}{8} \\ 0 & -h^2 & 0 & 0 & \frac{3h^2}{4} & \frac{3h^2}{4} & -\frac{9h^2}{4} \\ 0 & \frac{h^2}{2} & \frac{h^2}{2} & 0 & \frac{h^2}{8} & \frac{9h^2}{8} & \frac{9h^2}{8} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \\ a_6 \\ a_7 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 1 \end{pmatrix}$$

In the example above there are seven concerned points, so, we can determine infinite solutions of the complete system but we search a unique one. Let M be the constraints matrix, \vec{a} the weights vector, \vec{f} the right hand side vector for consistency and $F(\vec{a})$ a weights function. The problem to minimize has the Lagrangian form:

$$\mathcal{L} = F(\vec{a}) - \vec{\lambda}(M\vec{a} - \vec{f}) \quad (10)$$

We write the minimization problem (5) in matrix form like:

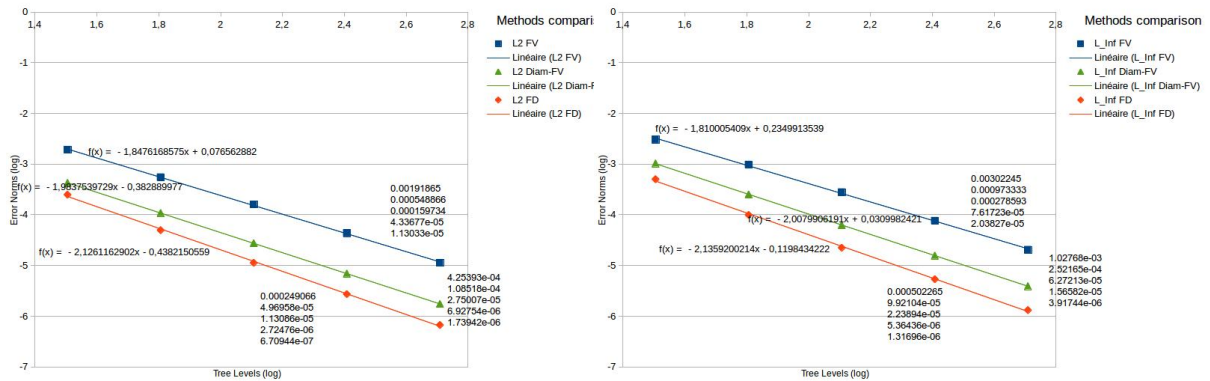
$$Ax = b \Leftrightarrow \begin{cases} \frac{\partial F(\vec{a})}{\partial \vec{a}} - M^T \vec{\lambda} = 0 \\ M\vec{a} = \vec{f} \end{cases}$$

This choice allows us to implement a scheme always consistent case by case.

Following a consistence proof several tests have been produced to strenghten our method like penalization and different kinds of model until a modeling of the problem (7.7) step by step. We built a new cell centered finite difference method able to:

- be consistent and locally convergent to second order on balanced grids;
- simplify and promote an AMR approach along discontinuity;
- solve the coupled problems (2)-(3) and (2)-(4);
- a first consistent result on the complete model (2)-(3)-(4).

The finite different method presented here has been compared with two other methods finite volume scheme (Fig. 20). The first one has been implemented by Marco Cisternino and the diamonds one by Claire Taymans (see previous sections). All the three methods stick on the same grid and they use PABLO’s data structure with its parallel balance.



(a) L_2 norm comparison

(b) L_∞ norm comparison

Figure 20. Comparison between several numerical approaches.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

We intend to pursue our partnership with Valeol, a wind turbine contractor in Aquitaine. Valeol poses simulation problems that cannot be addressed with standard tools. We have developed for them simplified PDE models for design in the frame of an industry funded PhD (CIFRE). We are currently adapting octree and Chimera approaches to the design of aerodynamic appendices to improve performance of existing installations. This is done in the frame of yet another CIFRE PhD thesis and the corresponding research contract. Moreover, thanks to this technology readiness, Valeol could join for the first time an H2020 research project, AEROGUST, that we are promoting with several academic and industrial institutions across Europe.

This year, we have also developed an new collaboration with the CorWave (<http://www.corwave.fr>). CorWave develops blood pumps based on a unique and patented wave membrane pumping technology. This collaboration has begun with an industry funded PhD (CIFRE), officially for the early 2017. Antoine Fondaneche, the PhD candidate, is now employed by CorWave on a basis of a two-month CDD contract.

We continue to deploy our effort in flow control and drag reduction for ground vehicles. After a fruitful collaboration with Renault, we are in the phase of negotiating a new collaboration. A new collaboration is starting with Valeo to optimize car cooling devices. DNS simulations are performed and compared to the industrial results obtained with URANS and LES methods and an EU network about this subject is going to be proposed.

9. Partnerships and Cooperations

9.1. Regional Initiatives

The project members are actively participating to the CPU cluster of excellence of Idex Bordeaux (<http://cpu.labex.u-bordeaux.fr/>)

9.2. National Initiatives

We belong to the GDR AMORE on ROMs.

9.2.1. Starting grants

A PEPS project ("Programme Exploratoire Premier Soutien"), initiated by Afaf Bouharguane, about Optimal Transport Theory. Angelo Iollo and Lisl Weynans are also involved in this project.

A PEPS project ("Programme Exploratoire Premier Soutien") on the numerical simulation of the biomimetic undulatory swimming for both under water vehicle optimisation and the Modeling of human locomotor system, initiated by Michel Bergmann with the MRGM laboratory (Laboratoire Maladies Rares : Génétique et Métabolism, <https://mrgm.u-bordeaux.fr/>). Afaf Bouharguane and Angelo Iollo are also involved in this project.

NEMO (A Numerical Enabler for MultiPhysics Simulations on Octrees) is an action to improve and merge all the main MEMPHIS numerical codes. To achieve this goal we have a 12 months financial support (Inria BSO FRM) for a young engineer. This work will be done with strong interaction the the local Inria BSO SED as well as Philippe Depouilly from the IMB "SED".

SMecH is a start-up project in software edition, carried on by Florian Bernard, research engineer in the MEMPHIS team. The project aims at porting to an industrial level the numerical codes developed by the MEMPHIS team. The different collaboration with industrial partners have highlighted the need of new numerical tools to simulate high complexity phenomena such as atmospheric reentries, multi-material flows or fund-structure interactions, but also to highly automatize the numerical simulation workflow to save engineer time. The research codes developed in the MEMPHIS team could match perfectly to this need thanks to:

- the various innovative multi-physics models implemented
- the use of Hierarchical Cartesian schemes that automatize the treatment of moving geometry with accuracy
- the development of schemes suitable for High Parallel Computing.

This year, the project has been submitted to the DGD, the Inria department in charge of technological transfert, and has been granted an engineer for 6 months as well as the support of IT-Translation.

9.3. European Initiatives

9.3.1. FP7 & H2020 Projects

EU research projects were and will be a privileged instrument of diffusion and transfer of our results. The AEROGUST H2020 project involves aeronautical industry (Airbus, Dassault, Piaggio..) and research labs (University of Bristol, DLR, NLR, University of Cape Town) and is dedicated to modeling of aerodynamic gust response for applications. We take part in this project by developing simulation models for unsteady aeroelastic problems and data-driven reduced-order models. We played a similar role for the past in the FP7 project FFAST with the same partners.

9.3.1.1. AEROGUST

Title: Aeroelastic Gust Modelling

Programm: H2020

Duration: May 2015 - April 2018

Coordinator: University of Bristol

Partners:

Airbus Defence and Space (Germany)

University of Cape Town (South Africa)

Dassault Aviation (France)

Deutsches Zentrum für Luft - und Raumfahrt Ev (Germany)

Stichting Nationaal Lucht- en Ruimtevaartlaboratorium (Netherlands)
Numerical Mechanics Applications International (Belgium)
Optimad Engineering S.R.L. (Italy)
Piaggio Aero Industries Spa (Italy)
The University of Liverpool (United Kingdom)
University of Bristol (United Kingdom)
Valeol (France)

Inria contact: Angelo IOLLO and Michel Bergmann

Encounters with atmospheric turbulence are a vitally important in the design and certification of many manmade structures such as aircraft and wind turbines. Gusts cause rapid changes in the flow about the structures which leads to rigid and flexible unsteady responses. Knowledge of aircraft/gust interactions is therefore vital for loads estimation during aircraft design as it impacts on control systems and often defines the maximum loads that these structures will experience in service. At present industry typically uses the linear doublet lattice method with static loads corrections from expensive wind tunnel data. The wind tunnel data is created using the final aerodynamic surface in the predicted cruise shape. This means that gust loads come relatively late when the design options have been narrowed. Increased competition and environmental concerns are likely to lead to the adoption of more flexible materials and the consideration of novel configurations, in which case the linear assumptions of the current gust loads process will become unacceptable. To introduce non-linearity into the gust loads process without significantly increasing the cost and time, this project has three main objectives: to carry out investigations using CFD so that the non-linearities in gust interactions are understood; to create a gust loads process that does not require wind tunnel data and hence reduces the need for wind tunnel testing; to develop updated reduced order models for gust prediction that account for non-linearity at an acceptable cost. These investigations will reduce the need for expensive wind tunnel testing and hence lead to time and cost savings at the design stage therefore ensuring that the European aerospace and defense industry remain competitive in the future. The wind turbine industry has similar concerns, with gusts and wind shear restricting the locations available for wind farms. The project will also address these issues using common methodology.

9.3.2. Collaborations with Major European Organizations

Partner 1: Chalmers University (Sweden)

This activity is complemented by several international interactions, in particular with Chalmers University in order to converge towards the real implementation of new control technologies on cars, buses and trucks.

Partner 2: Optimad Engineering , Torino (Italy)

We have a crucial partnership with Optimad Engineering, a spin-off of the Politecnico di Torino. This society has implemented in industrial codes several schemes that we have developed for the past. In exchange, we have access to these codes. One example is Pablo, an octree managing parallel library (<http://www.optimad.it/products/pablo/>). Three former PhD students at Inria are presently employed in Optimad and several others have spent or will spend a research period in this company in order to get acquainted with code architecture and massive parallelism. This company represents for us an ideal partner for the actual industrial feedback on our methods. As mentioned, we plan to create a local start-up in close collaboration with Optimad. This start-up will respond to actual industrial needs by specific software packages built starting from open source tools that are made available to the applied research community via a consortium. Florian Bernard has been recruited in Memphis for two years with the objective of bringing to a higher maturity level a set of modules developed within the team. He plans to fully invest himself in the creation of the start-up. As for the consortium, we are discussing with several partners including Cineca (Italy HPC center) and Optimad about how to structure such a mutual effort. The Storm Inria team is included in the discussions as a possible partner.

Partner 3: W4E (Wave for Energy) (Italy)

One project is the design of an ISWEC (Inertial Sea Wave Energy Converter) in collaboration with W4E (Wave for Energy), Optimad and others. The ISWEC is a floater prototype that can extract energy from the sea waves. The mechanism is based on a gyroscope that is rotating due to the passive motion of the floater. This prototype is actually tested in the Mediterranean sea in Italy. We will develop the numerical simulation as well as the shape optimization of the ISWEC.

Partner 4: MRGM (Maladies Rares : Génétique et Métabolisme), Bordeaux University (France)

We develop a collaboration with the MRGM lab. They are interested in the swimming of a zebrafish larvae under genetic modifications. One aim is to quantify the power spent by such fishes to swim after a stimuli reaction. The numerical simulation we develop can help computing integral quantities such as the power. This simulation is challenging due to the coupling several methods like image treatment (from movies given by MRGM), optimal transport and numerical simulations.

Partner 5: CRPP (Centre de recherche Paul Pascal), LOF (Laboratoire du Futur) and LOMA (Laboratoire Ondes et Matière d'Aquitaine) labs, Bordeaux University, France.

We established collaborations with physics and chemistry labs in Bordeaux, namely the CRPP, the LOF and the LOMA. They are concerned with the behavior of many passive (CRPP and LOF) and active (LOMA) particles in an incompressible flow. With these partners, we intend to use a combined experimental and computational approach to calibrate models in the case of dilute and concentrated suspensions. The numerical simulations of such particles can help to understand some underlying phenomena at the particles scale and thus to develop mesoscopic models for the whole system (PhD of Baptiste Lambert, oct. 2015).

9.4. International Initiatives

9.4.1. Inria International Labs

9.4.1.1. Declared Inria International Partners

Collaboration with Optimad Engineering.

9.5. International Research Visitors

9.5.1. Visits of International Scientists

Giovanni Russo, Professor at the Catane university, has visiting our team several times this year.

Johnny Guzman, associate professor, Université de Brown, USA, one week.

9.5.1.1. Internships

Mohsen Broumand, a PhD visitor from Winnipeg university, has a collaboration with Lisl Weynans for bi-fluid simulations (from October 2016).

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Selection

10.1.1.1. Reviewer

Charles-Henri Bruneau has reviewed several papers for the 9th International Conference on Computational Fluid Dynamics, July 10th-15th, Istanbul.

10.1.2. Journal

10.1.2.1. Member of the Editorial Boards

Angelo Iollo is in the advisory board of Acta Mechanica.

10.1.2.2. 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.

10.1.3. Invited Talks

The invited talks are [15], [16], [17], [18].

10.1.4. Leadership within the Scientific Community

Angelo Iollo is responsible of the scientific policy of the scientific computing departement of the LabEx CPU. This department gathers 60 researchers of the math lab IMB, of the computer science lab LaBRI, of the mechanics lab I2M and of the CEA.

10.1.5. Scientific Expertise

Michel Bergmann: reviewer of the PhD defense *Apprentissage d'estimateurs sans modèle avec peu de mesures - Application à la mécanique des fluides* de Kévin Kasper, Ecole normale supérieure de Cachan, 12/10/2016.

Michel Bergmann: member of the Inria Young Researchers Commission, which allocates PhD and Postdoc grants.

Lisl Weynans has participated to the *Comités de sélection* Cnam and Paris 5 Descarte, may 2016.

Angelo Iollo: Président du jury d'HDR de Heloise Beaugendre, Institut de Mathématiques de Bordeaux, université de Bordeaux, mars 2016.

Angelo Iollo: Membre Jury HDR de Laurent Cordier, Institut P', université de Poitiers, novembre 2016.

Angelo Iollo: Membre du Jury de thèse de Loic Lacouture « Modélisation et simulations de mouvement de structures fines » département de mathématiques, juin 2016, Université Paris Sud.

Angelo Iollo: Président du jury de thèse de Olivier Gallinato, « Modélisation du processus cancéreux et méthodes superconvergentes de résolution de problèmes d'interface sur maillage cartésien », Institut de Mathématiques de Bordeaux, université de Bordeaux, novembre 2016.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

Four members of the team are Professors or Assistant Professors at Bordeaux University and have a teaching duty, which consists in courses and practical exercises in numerical analysis and scientific computing. Michel Bergmann (CR) also teaches around 64 hours per year (practical exercises in programmation for scientific computing).

10.2.2. Supervision

PhD in progress : Alice Raeli, Numerical Modelling for Phase Changing Materials, 12/06/2014, Azaiez M., Bergmann M., Iollo A.

PhD in progress : Claire Morel, Modélisation aérodynamique 3D d'une turbine éolienne, 01/01/2015, M., Bergmann M., Iollo A.

PhD in progress : Federico Tesser, Identification of dense suspensions rheology, 01/11/2014, Bergmann M., Iollo A.

PhD in progress : Baptiste Lambert, modélisation et simulations numériques des contacts dans des écoulements chargés en particules, 01/10/2015, Bergmann M., Weynans L.,

PhD in progress : Emanuela Abbate, Méthodes numériques pour problèmes stiff en mécanique des fluides et élasticité, 01/11/2015, Iollo, A.

PhD in progress : Mathias Braun, Modèles réduits et problèmes inverses pour l'étude de la résilience des réseaux d'eau potable, 01/10/2015, Iollo A. and Mortazavi I.

PhD in progress : Meriem Jedoua, Introduction d'une méthode efficace de capture d'interface permettant la localisation d'un grand nombre d'objets immergés dans un fluide. Applications à des solides rigides et des vésicules (membranes élastiques) immergés dans un fluide incompressible, 01/10/2013, Bruneau C.-H. and Maitre E.

2012-2016. Dr. Hervé Ung. Ancien ENSEIRB-MATMECA. Problèmes inverses dans les réseaux d'eau potable. Angelo Iollo, Iraj Mortazavi, Bourse Irstea.

10.2.3. Juries

Michel Bergmann has been reviewer of the PhD defense *Apprentissage d'estimateurs sans modèle avec peu de mesures - Application à la mécanique des fluides* de Kévin Kasper, Ecole normale supérieure de Cachan, 12/10/2016.

Lisl Weynans has participated to the PhD defense of Andrea Filippini, Inria Bordeaux, 14/12/2016.

Angelo Iollo: Président du jury d'HDR de Heloise Beaugendre, Institut de Mathématiques de Bordeaux, université de Bordeaux, mars 2016.

Angelo Iollo: Membre Jury HDR de Laurent Cordier, Institut P', université de Poitiers, novembre 2016.

Angelo Iollo: Membre du Jury de thèse de Loic Lacouture « Modélisation et simulations de mouvement de structures fines » département de mathématiques, juin 2016, Université Paris Sud.

Angelo Iollo: Président du jury de thèse de Olivier Gallinato, « Modélisation du processus cancéreux et méthodes super-convergentes de résolution de problèmes d'interface sur maillage cartésien », Institut de Mathématiques de Bordeaux, université de Bordeaux, novembre 2016,

10.3. Popularization

Lisl Weynans has co-organized the Journée "Filles et Maths, une équation lumineuse": may 11t 2016

Lisl Weynans has co-organized Journée Emploi Maths de l'Unité de Formation "Mathématiques et Interaction"

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- [2] M. BERGMANN, A. IOLLO. *Modeling and simulation of fish-like swimming*, in "Journal of Computational Physics", 2011, vol. 230, n^o 2, p. 329 - 348.
- [3] M. BERGMANN, A. IOLLO. *Bioinspired swimming simulations*, in "Journal of Computational Physics", 2016, vol. 323, p. 310 - 321.
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- [7] A. DE BRAUER, A. IOLLO, T. MILCENT. *A Cartesian Scheme for Compressible Multimaterial Models in 3D*, in "Journal of Computational Physics", 2016, vol. 313, p. 121-143.
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- [11] M. BERGMANN, A. IOLLO. *Bioinspired swimming simulations*, in "Journal of Computational Physics", 2016, vol. 323, p. 310 - 321 [DOI : 10.1016/j.jcp.2016.07.022], <https://hal.inria.fr/hal-01405039>.
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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 Medecine

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Project-Team MNEMOSYNE

Creation of the Team: 2012 February 01, updated into Project-Team: 2014 July 01

Keywords:

Computer Science and Digital Science:

- 1.1.12. - Non-conventional architectures
- 1.5. - Complex systems
- 3.1.1. - Modeling, representation
- 3.1.7. - Open data
- 3.2.2. - Knowledge extraction, cleaning
- 3.2.5. - Ontologies
- 3.3. - Data and knowledge analysis
- 3.3.2. - Data mining
- 3.4.1. - Supervised learning
- 3.4.2. - Unsupervised learning
- 3.4.3. - Reinforcement learning
- 3.4.4. - Optimization and learning
- 3.4.6. - Neural networks
- 3.4.8. - Deep learning
- 5.1.1. - Engineering of interactive systems
- 5.1.2. - Evaluation of interactive systems
- 5.2. - Data visualization
- 5.3.3. - Pattern recognition
- 5.4.1. - Object recognition
- 5.4.2. - Activity recognition
- 5.7.1. - Sound
- 5.7.3. - Speech
- 5.7.4. - Analysis
- 5.8. - Natural language processing
- 5.9.1. - Sampling, acquisition
- 5.10.5. - Robot interaction (with the environment, humans, other robots)
- 5.10.7. - Learning
- 5.10.8. - Cognitive robotics and systems
- 5.11.1. - Human activity analysis and recognition
- 7.1. - Parallel and distributed algorithms
- 8.2. - Machine learning
- 8.5. - Robotics

Other Research Topics and Application Domains:

- 1.3. - Neuroscience and cognitive science
- 1.3.1. - Understanding and simulation of the brain and the nervous system
- 1.3.2. - Cognitive science
- 2.2.6. - Neurodegenerative diseases

- 8.5.2. - Crowd sourcing
- 9.1.1. - E-learning, MOOC
- 9.4.1. - Computer science
- 9.5.8. - Linguistics
- 9.6. - Reproducibility
- 9.7. - Knowledge dissemination
- 9.9.1. - Environmental risks

Mnemosyne hosted by Institut des Maladies Neurodégénératives, IMN, Bordeaux NeuroCampus.

1. Members

Research Scientists

- Frédéric Alexandre [Team leader, Inria, Senior Researcher, HDR]
- Xavier Hinaut [Inria, Researcher, from Feb 2016]
- Randa Kassab [Inria, Starting Research position, from Sep 2016, FUI Sumatra]
- Nicolas Rougier [Inria, Researcher, HDR]
- Thierry Viéville [Inria, Senior Researcher (part-time (20%) in the project-team), HDR]

Faculty Member

- André Garenne [Univ. Bordeaux, Associate Professor]

PhD Students

- Maxime Carrere [Univ. Bordeaux]
- Ikram Chraïbi Kaadoud [Univ. Bordeaux, granted by CIFRE]
- Thalita Firmo Drumond [Inria, from Oct 2016]
- Charlotte Héricé [Univ. Bordeaux]
- Bhargav Teja Nallapu [Inria, from Nov 2016]
- Meropi Topalidou [Inria+Region]

Post-Doctoral Fellow

- Fabien Benureau [Inria]

Visiting Scientist

- Sabyasachi Shivkumar [IIT Madras, India, from Jun 2016 until Jul 2016]

Administrative Assistant

- Chrystel Plumejeau [Inria, part time in the team]

Others

- Rachel Confiant-Dute [Inria, Licence Univ. Bordeaux, Jun 2016]
- Louis Devers [Inria, Licence Univ. Bordeaux, from May 2016 until Aug 2016]
- Emeline Duquenne [IMS, Master Univ. Bordeaux, from Jan 2016 until Jun 2016]
- Lylia Fauvel [Inria, Licence Univ. Bordeaux, Jun 2016]
- Pramod Kaushik [Inria, IIIT Hyderabad, India, from Jun 2016 until Dec 2016]
- Erwan Le Masson [Inria, Master Enseirb, Bordeaux INP, from Apr 2016 until Sep 2016]
- Adrian Palacios [Univ. Valparaiso, Associate member]
- Romain Pastureau [Inria, Licence Univ. Bordeaux, Jun 2016]
- Remy Portelas [Inria, Licence Univ. Bordeaux, May 2016]
- Camille Soetaert [Inria, Master UTC, from Sep 2016]
- Alexia Souvane [Inria, Master Univ. Bordeaux, from Jun 2016 until Jul 2016]

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 mnemonic 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 (*cf.* § 6.1). 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 protocols.

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 [54]. 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 undoubtedly 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 [56], [43]. 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 mimic 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 homunculus or any central clock. Numerical schemes developed for distributed dynamical systems and algorithms elaborated for distributed computations are of central interest here [40], [49] and were the basis for several contributions in our group [55], [52], [57]. 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 [41]; the associated formalism [46] 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 [38], that demonstrated a richness of behavior

[42] 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 [52], [53] and their use for observing the emergence of typical cortical properties [45]. 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 (*cf.* § 6.1). 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, as we will discuss in § 6.1).

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 [44], [37]. 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 episodes and supervising the training of a procedural memory in the cortex.

At the behavioral level, as mentioned 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 continuous re-arrangement is supposed to involve several kinds of learning, at different time scales (from msec to years in humans) and to interfere 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 protocols 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* [39]). 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 mimic 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.

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 mnemonic 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 undoubtedly 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

5.1.1. *First PhDs defended*

2016 is a very special year for our young team Mnemosyne, since our first three PhDs have been defended in October and November [1], [2], [3].

6. New Software and Platforms

6.1. Positioning

Our previous works in the domain of well-defined distributed asynchronous adaptive computations [55], [52], [57] have already made us define a library (DANA [51]), closely related to both the notion of artificial neural networks and cellular automata. From a conceptual point of view, the computational paradigm supporting the library is grounded on the notion of a unit that is essentially a (vector of) potential that can vary along time under the influence of other units and learning. Those units can be organized into layers, maps and networks.

We will also have to interact with the High Performance Computing (HPC) community, since having large scale simulations at that mesoscopic level is an important challenge in our systemic view of computational neuroscience. Our approach implies to emulate the dynamics of thousands, or even millions, of integrated computational units, each of them playing the role of a whole elementary neural circuit (e.g. the microcolumn for the cortex). Mesoscopic models are considered in such an integrative approach, in order to exhibit global dynamical effect that would be hardly reachable by compartment models involving membrane equations or even spiking neuron networks.

The vast majority of high performance computing softwares for computational neuroscience addresses sub-neural or neural models [41], but coarser grained population models are also demanding for large scale simulations, with fully distributed computations, without global memory or time reference, as it is specified in (cf. § 3.2).

6.2. DANA

Distributed Asynchronous Numerical & Adaptive computing framework

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/>

6.3. ENAS

Event Neural Assembly Simulation

KEYWORDS: Neurosciences - Health - Physiology

SCIENTIFIC DESCRIPTION

As one gains more intuitions and results on the importance of concerted activity in spike trains, models are developed to extract potential canonical principles underlying spike coding. These methods shed a new light on spike train dynamics. However, they require time and expertise to be implemented efficiently, making them hard to use in a daily basis by neuroscientists or modelers. To bridge this gap, we developed the license free multiplatform software ENAS (<https://enas.inria.fr>) integrating tools for individual and collective spike analysis and simulation, with some specificities devoted to the retina. The core of ENAS is the statistical analysis of population codes. One of its main strength is to provide statistical analysis of spike trains using Maximum Entropy-Gibbs distributions taking into account both spatial and temporal correlations as constraints, allowing to introduce causality and memory in statistics. ENAS also generates simulated spike trains. On one hand, one can draw a population raster from an user-specified Gibbs distribution. On the other hand, we have integrated in ENAS our retina simulator VIRTUAL RETINA, extended here to include lateral connections in the IPL. We hope that ENAS will become a useful tool for neuroscientists to analyse spike trains and we hope to improve it thanks to user feedback. Our goal is to progressively enrich it with the latest research results, in order to facilitate transfer of new methods to the community.

FUNCTIONAL DESCRIPTION

As one gains more intuitions and results on the importance of concerted activity in spike trains, models are developed to extract potential canonical principles underlying spike coding. These methods shed a new light on spike train dynamics. However, they require time and expertise to be implemented efficiently, making them hard to use in a daily basis by neuroscientists or modelers. To bridge this gap, we developed the license free multiplatform software ENAS integrating tools for spike trains analysis and simulation. These tools are accessible through a friendly Graphical User Interface that avoids any scripting or writing code from the user. Most of them have been implemented to run in parallel to reduce the time and memory consumption. ENAS offers basic visualizations and classical analysis for statistics of spike trains analysis. It also proposes statistical analysis with Maximum Entropy-Gibbs distributions taking into account both spatial and temporal correlations as constraints, allowing to introduce causality and memory in statistics. ENAS also includes specific tools dedicated to the retina: Receptive Field computation and a virtual retina simulator. Finally, ENAS generates synthetic rasters, either from known statistics or from the VIRTUAL RETINA simulator. We expect ENAS to become a useful tool for neuroscientists to analyse spike trains and we hope to improve it thanks to users feedback. From our perspective, our goal is to progressively enrich ENAS with the latest research results, in order to facilitate transfer of new methods to the community.

- Participants: Bruno Cessac, Salim Kraria, Hassan Nasser, Thierry Viéville, Rodrigo Cofre Torres, Geoffrey Portelli, Pierre Kornprobst, Theodora Karvouniari and Daniela Pamplona
- Contact: Bruno Cessac
- URL: <https://enas.inria.fr>

6.4. Virtual Enaction

KEYWORDS: Neurosciences - Simulation - Health

FUNCTIONAL DESCRIPTION

VirtualEnaction: A Platform for Systemic Neuroscience Simulation. The computational models studied in our team 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 have deployed an existing open-source video game middleware (Minecraft) in order to be able to shape the survival situation to be studied and we have begun to revisit some models in order to be able to integrate them as an effective brainy-bot. This was made as a platform associated to a scenario that is the closest possible to a survival situation (foraging, predator-prey relationship, partner approach to reproduction). We could integrate in the platform 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 was corresponding to the major anatomical regions studied in the team.

Nevertheless, we have seen recently that a major entertainment company (Microsoft) bought Minecraft to make similar (but larger) adaptations to what was being targeted by our VirtualEnaction project. We are currently studying the resulting product (the Malmö project) in order to adapt our strategy.

- Participants: André Garenne, Frédéric Alexandre, Nicolas Rougier and Thierry Viéville
- Contact: Frédéric Alexandre
- URL: <http://virtualenaction.gforge.inria.fr/>

7. New Results

7.1. Overview

This year we first explored two main loops of cerebral architecture, the limbic and motor loops, and their associated memory mechanisms. The limbic loop (*cf.* § 7.2) concerns the taking into account of the emotional and motivational aspects by the respondent and operant conditioning and their relations with the semantic and episodic memories. The motor loop (*cf.* § 7.3) considers the evolution of sensorimotor learning, from goal-directed behaviors to habitual behaviors.

We also began this year to study some characteristics of the systemic integration of our models (*cf.* § 7.4), raising the question of the conditions of autonomous learning and certain global characteristics such as neuromodulation.

Finally, we study the links between our bio-inspired modeling work and Machine Learning (*cf.* § 7.5), revisiting this latter domain in the light of the principles highlighted by our models.

7.2. The limbic loop

We explored the limbic loop by describing a series of neural mechanisms that propose how responding conditioning results from interactions between the amygdala, the nucleus accumbens and the limbic pole of the frontal cortex. In our models [1], this learning is also fed by exchanges with the hippocampus (episodic memory) and the sensory cortex (semantic memory) and we studied the major role of acetylcholine in these exchanges. This also allowed us to address the difficult question of the articulation between the respondent and operant conditioning in particular in the nucleus accumbens. We proposed an original mechanism whereby noradrenaline could modulate the balance between exploration and exploitation [12] based on an assessment of the level of uncertainty and its impact on performance [13].

Also in connection with this loop, we studied the dynamics of dopamine release in the midbrain, considered to play an essential role in the coding of the prediction error. This model developed in the framework of our collaboration with India (*cf.* § 9.3) proposes to introduce into the classical circuit, new actors (such as the pedunculopontine tegmental nucleus in the brainstem) and new functions (dissociation of amplitude and timing of the reward), that we will seek to corroborate in the future.

Lastly, we carried out a thorough study about the behavior of our model of associative memory in the hippocampus [23], and particularly about its resistance to interference.

7.3. The motor loop

The nervous system structures involved in decision making constitute a circuit formed by the basal ganglia, the cortex, the thalamus and their numerous interconnections. This circuit can be described as a set of loops operating in parallel and interacting at different points. The decisions and therefore the actions of an individual emerge from the interactions between these loops and the plasticity of their connections. These emerging behaviors and arising learning processes are addressed through a closed-loop approach in which the theoretical model is in constant interaction with the environment of the task. To this end, neural modeling and dedicated analysis software tools were developed in the laboratory, at the level of the neuronal circuit. We have explored this year the dynamics of information flows within this circuit through a computational model described at the neuron and synapse level. Taking into account previous experimental observations from primates and earlier computational models, we incrementally developed a network capable of learning to perform behavioral tasks under several protocols and conditions [5]. The development of this computational model was conducted in parallel with the development of an experimental model of decision making in the salamander (*Pleurodeles waltlii*) [2]. The result here is a computational model of learning and decision making in the basal ganglia that allows for the testing of experimental hypotheses and also to conduct *in silico* pathophysiological or pharmacological investigations at the cellular level.

7.4. Systemic integration

We have worked this year on the integration of goal-oriented and habitual behaviors, two modes of learning associated to the motor loop. There is an apparent contradiction between experimental data showing that the basal ganglia are involved in goal-oriented and routine behaviors and clinical observations. Lesion or disruption by deep brain stimulation of the globus pallidus interna has been used for various therapeutic purposes ranging from the improvement of dystonia to the treatment of Tourette's syndrome. None of these approaches has reported any severe impairment in goal-oriented or automatic movement. To solve this conundrum, we trained two monkeys to perform a variant of a two-armed bandit-task (with different reward contingencies). Bilateral inactivation of the globus pallidus interna, by injection of muscimol, prevents animals from learning new contingencies while performance remains intact, although slower for the familiar stimuli. We replicate *in silico* these data by adding lateral competition and Hebbian learning in the cortical layer of the theoretical model of the cortex–basal ganglia loop that provided the framework of our experimental approach [7]. These results suggest that a behavioral decision results from both the cooperation (acquisition) and competition (expression) of two distinct but entangled memory systems, the goal-directed system and the habitual system that may represent the two ends of the same graded phenomenon.

We began our first works of systemic integration associating our models developed in the limbic and motor loops, for the study of the taking into account of the uncertainty in the selection of the action [1]. This preliminary work using the VirtualEnaction platform (*cf.* § 6.4) will be continued this year with a PhD that begins.

We have more generally proposed a study [11], analyzing the role of neuromodulation in adaptation to uncertainty, whose potential systemic impact is evident, particularly because it provides precious characteristics for autonomous learning [10].

7.5. Machine Learning

In Machine Learning, we were interested this year in two phenomena for which we consider classical paradigms of modeling and for which we wonder how they could be adapted by bio-inspiration.

The first paradigm concerns the manipulation of temporal sequences. In a perspective of better understanding how brain learn structured sequences we extended a model on syntax acquisition using the Reservoir Computing framework (using random recurrent networks) [16], [9], [19], [20]. The extended model is also used in a Human-Robot Interaction architecture to enable users to use more natural language with robots [14], [15], [18]. This work will be extended with our collaborators at the University of Hamburg (*cf.* § 9.3).

In an industrial application for the representation of electrical diagrams (*cf.* § 8.1), we also study how recurrent layered models can be trained to run through these schemes for prediction and sequence representation tasks.

The second paradigm concerns the extraction of characteristics and the use of hierarchical networks, as in the case of deep networks. An industrial application whose study has just begun (*cf.* § 9.2) will lead us to revisit these models to make them more easily usable in constrained frameworks, for example with limited size corpuses.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

8.1.1. Contract with Algotech

Participants: Frédéric Alexandre, Ikram Chraïbi Kaadoud, Nicolas Rougier, Thierry Viéville.

Algotech is a SME working in the domain of CADD software edition for electrical circuit diagram interpretation and design. Its activity is interesting for our team because they are also interested in the design, by learning, of perception (for diagram identification) and action aspects of loops (for diagram genesis) with the

specificity of working at a small scale, considering the variety of items to be manipulated. This is consequently a very interesting benchmark for transferring our bio-inspired models to the domain of classical machine learning, as we have begun this year.

9. Partnerships and Cooperations

9.1. Regional Initiatives

9.1.1. *PsyPhiNe: Cogito Ergo Es*

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 to explore 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. Early results (analysis not yet finished) tend to show that people have a tendency to over-interpret any kind of behavior as intentional and meaningful. We also organized our second national conference in Nancy gathering speakers from philosophy, robotics, art and psychology and hired a new post-doc to work on the new experimental setup (<http://poincare.univ-lorraine.fr/fr/manifestations/psyp hine-2016>)

9.1.2. *Project of the Aquitaine Regional Council: Decision making, from motor primitives to action*

Participants: Nicolas Rougier, Meropi Topalidou.

This project has ended with the PhD defense of Meropi Topalidou on October 10th, 2016. Using a computational model, we investigated the classic hypothesis of habits formation and expression in the basal ganglia and proposed a new hypothesis concerning the respective role for both the basal ganglia and the cortex. Inspired by previous theoretical and experimental works [47], we designed a computational model of the basal ganglia- thalamus-cortex system that uses segregated loops (motor, cognitive and associative) and makes the hypothesis that basal ganglia are only necessary for the acquisition of habits while the expression of such habits can be mediated through the cortex. This work leads to several publications including an important article in "Movement disorders" [7] explaining some counter-intuitive clinical observations. Furthermore, the early work during the first year of the PhD led N.Rougier to create the ReScience journal.

9.1.3. *Collaboration with the Neurocentre Magendie on parameter optimization: Neurobees*

Participant: André Garenne.

The development of computational models of neurons and networks typically involves tuning the numerical parameters to fit experimental results. Parameter tuning can sometimes be manually completed, it is more convenient to use automated optimization algorithms at least for two reasons: (i) to apply an homogeneous processing to all the calculation and parameter space exploration which alleviates operator influence and (ii) to avoid a tedious and uncertain result from human operators when the dimensionality increases. A multi-agent algorithm in line with ABC (Artificial Bee Colony) paradigm has been applied to new benchmark tests in order to ensure its robustness and better performances, especially when compared to evolutionary and swarm algorithms and this has recently been confirmed, thanks to the local Plafrim computation facilities.

9.2. National Initiatives

9.2.1. *FUI Sumatra*

Participants: Frédéric Alexandre, Thalita Firmo Drumond, Xavier Hinaut, Randa Kassab, 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 describing 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 heterogeneous 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 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.

9.2.3. *Project Motus of the ANSES*

Participant: André Garenne.

The MOTUS project (MODulation dU Signal RF et effets sur le cerveau : approche in vivo et in vitro) is financed by the ANSES (the french national agency for health security). This 3 years project is studying the effects of GSM-RF on living matter and especially neuronal activity and development. Our main involvement concerns electrophysiological data and spike trains analysis as well as the development of pharmacological protocols to test GSM-RF effects hypotheses.

9.2.4. *Project Mimacore of the CNRS Challenge Imag'In*

Participants: Frédéric Alexandre, Nicolas Rougier.

Better understanding the resting states (regional interactions and corresponding functional networks in the brain when the subject is at rest) is of central interest for a systemic approach of brain understanding. As we think that this domain is not mature enough for a direct functional modeling approach, we try to get familiar with it, through this imaging study. In this exploratory study funded by the CNRS, we are associated with three teams in neuroscience developing three imaging techniques (MRS, MRI, Clarity), to explore resting states in rodents and learn more about their genesis.

9.3. International Initiatives

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

9.3.1.1. *Braincraft*

Title: Braincraft

International Partner (Institution - Laboratory - Researcher):

University of Colorado, Boulder (United States) - Computational Cognitive Neuroscience
- Randall O'Reilly

Start year: 2015

We develop with this team a computationally-based understanding of the neural circuits involved in decision making, namely basal ganglia and prefrontal cortex. More precisely, we want to understand what are the processes by which animals and humans select their actions based on their motivations and on the consequences of past actions. This is a fundamental question in neurosciences, with implications to ethology, psychology, economics, sociology and computer science. Through a unique combination of expertise in cognitive psychology, neurosciences and computer science, this associate team will foster a collaboration for developing a computationally-based understanding of the neural circuits involved in decision making, namely basal ganglia and prefrontal cortex. One of the key question is to know the overall contribution of these structures and their function in the decision process.

9.3.2. Participation in Other International Programs

9.3.2.1. *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.

9.3.2.2. *Project BGaL with India*

In the 3-years project "Basal Ganglia at Large (BGaL)", funded by the CNRS and the CEFIPRA, we collaborate with the computer science department of IIIT Hyderabad and the biomedical department of IIT Madras, for the design of models of basal ganglia and for their implementation at large scale as well as for their relation with other brain structures. This year we have developed a model of a dopaminergic region, VTA, central for reinforcement learning in the basal ganglia.

9.3.2.3. *Project ECOS-Sud with Chile*

In the 3-years project "A network for computational neuroscience, from vision to robotics", funded by ECOS-Sud and Conicyt, we collaborate with University Santa Maria and University of Valparaiso in Chile, and also with another Inria EPI, NeuroMathComp. The goal of the project is to rely on our experience of previous collaborations with these teams, to develop original tools and experimental frameworks to open our scientific domains of investigation to new fields of valorization, including medical (neurodegeneration) and technological aspects (robotics). This year, in addition to the visits of a Professor and a PhD student, we have written a chapter book that will be published next year and have prepared together a summer school to be held in Chile in January 2017 (<http://www.laconeu.cl/>).

9.4. International Research Visitors

9.4.1. Visits of International Scientists

Prof. Palacios Adrian

Date: Sep 2016

Institution: Univ. Valparaiso (Chile)

Ravello Cesar (PhD student)

Date: Nov 2016

Institution: Univ. Valparaiso (Chile)

Prof O'Reilly Randall

Date: June 2016

Institution: U. Colorado Boulder (USA)

Mollick Jessica (PhD student)

Date: Jul 2016 - Aug 2016

Institution: U. Colorado Boulder (USA)

9.4.1.1. Internships

Kaushik Pramod

Date: June 2016 - Dec 2016

Institution: IIIT Hyderabad (India)

Sabyasachi Shivkumar

Date: June 2016 - July 2016

Institution: IIIT Madras (India)

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

10.1.1.1. General Chair, Scientific Chair

X. Hinaut : Co-organiser of the 2nd Autumn Day of the Working Group (GT8) "Robotique et Neurosciences" of Groupe de Recherche (GDR) Robotique (CNRS), at LaBRI, 17th November 2016.

10.1.1.2. Member of the Organizing Committees

Projections, Interactions, Emotions - Journées PsyPhINe, 2016 (<http://poincare.univ-lorraine.fr/fr/manifestations/psyphine-2016>, N. Rougier)

10.1.2. Scientific Events Selection

10.1.2.1. Member of the Conference Program Committees

F. Alexandre: SAB 2016

10.1.2.2. Reviewer

F. Alexandre reviewer for AMINA 2016; X. Hinaut for CogSci 2016.

10.1.3. Journal

10.1.3.1. Member of the Editorial Boards

- Frédéric Alexandre: Review Editor for Frontiers in Neurorobotics;
- Nicolas Rougier: Editor in chief for ReScience, review editor for Frontiers in Neurorobotics.

10.1.3.2. Reviewer - Reviewing Activities

- F. Alexandre: Frontiers in Human Neuroscience; npj Science of Learning; European Journal of Neuroscience; PLoS ONE;
- A. Garenne: Journal of Integrative Neuroscience
- X. Hinaut: PLoS ONE, Neural Networks, Intellectica, Frontiers in Neurorobotics, ReScience, Cognitive Computation.

10.1.4. Invited Talks

F. Alexandre: invited talk at the conference: “Modeling: success and limitations” (<http://www.cnrs.fr/inismi/spip.php?article1876>), Dec 6th and interview for the journal of the CNRS (<https://lejournel.cnrs.fr/articles/modeliser-plus-pour-simuler-moins>).

X. Hinaut: “Reservoir Computing for Robot Language Acquisition”, at IROS Workshop on Machine Learning Methods for High-Level Cognitive Capabilities in Robotics. Daejeon, South Korea, October 2016 [9].

N. Rougier:

- Open Science, AdaWeek, November 2016, Paris
- ReScience, "La loi numérique, et après ?", November 2016, Meudon
- "One actor, two critics", Robotiques et Neurosciences, November 2016, Bordeaux
- "Advanced Scientific Programming in Python", July 2016, Austin, USA.
- "Computational Neuroscience", International School of Bioelectromagnetics, Erice, April 2016, Italy.

10.1.5. Leadership within the Scientific Community

X. Hinaut:

- member of the Administration Committee of Fresco association (French Federation of students in Cognitive Science)
- member of “open citizen labs” : MindLaBdx (Bordeaux), IA*lab and CogLab (La Paillasse, Paris).

10.1.6. 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.

10.1.7. Research Administration

- F. Alexandre is member of the Inria Evaluation Committee; Deputy Scientific Delegate and Vice-head of the Project Committee of Inria Bordeaux Sud-Ouest; Corresponding scientist for Bordeaux Sud-Ouest of the Inria COERLE ethical committee; Member of the national Inria committee for international chairs; Member of the local Inria committee for young researchers hiring; 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'
- N. Rougier is vice-head of the Mnemosyne team-project; elected member of the Inria Evaluation Committee; Responsible of the local Inria committee for invited professors; Member of the steering committee for the BioComp CNRS consortium; Editor in chief and co-founder of ReScience.

- Thierry Viéville is in charge, at the Inria national level till October 2016, of the institute science outreach actions and depends on the Direction Générale Déléguée à la Science for this part of his work. He is, for Inria, in charge of the <http://classcode.fr> project.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

Advanced scientific python summer school, University of Reading, September 2016 (N. Rougier).

F. Alexandre: Teaching at the IBRO Advanced School in Neuroscience “Basal Ganglia, Parkinson’s disease And Related Disorders”, May 9-21, 2016, Faculty of Sciences, Rabat (Morocco)

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 since 2009 in charge of formations of high-school teachers in popular computer science.

10.2.2. Juries

We participate to many juries each year.

10.3. Popularization

For a multi-disciplinary team as Mnemosyne, science popularization is not only a nice and useful contribution to the dissemination of scientific knowledge but also a necessity since we work with colleagues from bio-sciences with whom sharing profound ideas in computer science is mandatory for a real collaboration.

- Thierry Viéville is for 80% of his time involved in popularization actions.
- Frédéric Alexandre: Article in the journal La Tribune in January 2016 about robots and emotions; Article in tribute to Marvin Minsky (Blog Binaire <http://binaire.blog.lemonde.fr/2016/01/29/lintelligence-artificielle-debraillee/>; Bulletin of the French Society of Computer Science <http://www.societe-informatique-de-france.fr/bulletin/1024-numero-8/>); Article about learning in the magazine of the University of Bordeaux (<http://www.u-bordeaux.fr/Universite/U-magazine>)
- Xavier Hinaut: “Apprentissage de la grammaire par un cerveau positronique”. CogTalk organised by the association Ascoergo, Bordeaux, March 2016.
- Nicolas Rougier: "Le Grand Remue-Méninges", October 2016, Bordeaux; "Les neurosciences au coeur des innovations", May 2016, Lyon; Interview for the "Verge of Discovery" March 2016; Intervention for the "Artificial Intelligence forum", Bordeaux.
- For all the team: participation to the “Fête de la Science” in an exhibition in the Scientific Museum Cap Sciences: <http://www.bordeaux-neurocampus.fr/fr/divers/toutes-les-communications/com-2016/fete-de-la-science.html>

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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

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- 6.2.4. - Statistical methods
- 6.2.6. - Optimization
- 6.2.7. - High performance computing
- 6.3. - Computation-data interaction
 - 6.3.1. - Inverse problems
 - 6.3.2. - Data assimilation
 - 6.3.3. - Data processing
 - 6.3.4. - Model reduction
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 - 2.6.1. - Brain imaging
 - 2.6.3. - Biological Imaging

1. Members

Research Scientists

Olivier Saut [Team leader, CNRS, Senior Researcher, HDR]
Sebastien Benzekry [Inria, Researcher]
Clair Poinard [Inria, Researcher, HDR]

Faculty Members

Thierry Colin [Bordeaux INP, Professor, HDR]
Annabelle Collin [Bordeaux INP, Associate Professor]

Technical Staff

Marie Martin [Inria]
Jean Mercat [Inria]
Boris Raymond [Inria]
Vivien Pianet [Inria]

PhD Students

Perrine Berment [Univ. Bordeaux, until Oct 2016]
Sergio Corridore [Univ. Bordeaux, from Nov 2016]
Manon Deville [Univ. Bordeaux]
Olivier Gallinato-Contino [Inria]
Thibaut Kritter [Univ. Bordeaux]
Thomas Michel [Univ. Bordeaux, until Nov 2016]
Chiara Nicolo [Inria, from Oct 2016]
Agathe Peretti [Univ. Bordeaux]
Cynthia Perier [Univ. Bordeaux]
Etienne Baratchart [Inria, until Jul 2016]

Post-Doctoral Fellows

Guillaume Dechrste [Inria]
Benjamin Taton [CHU Bordeaux, Medical Doctor]

Administrative Assistant

Sylvie Embolla [Inria]

Others

Mikaël Antoine [Institut Bergonié, Radiotherapy Physician, from Nov 2016]
Francois Cornelis [APHP, Radiologist, HDR]
Laura Lumale [Inria, Intern, from Jul 2016 until Sep 2016]
Louise Missenard [Institut Bergonié, Medical Student, from Oct 2016]
Claudia Pouypoudat [CHU Bordeaux, Medical Student]

2. Overall Objectives

2.1. Objectives

The MONC project-team aims at developing new mathematical models built on partial differential equations and statistical methods and based on precise biological and medical knowledge. The goal is ultimately to be able to help clinicians and/or biologists to better understand, predict or control tumor growth and possibly evaluate the therapeutic response, in a clinical context or for pre-clinical studies through quantitative numerical tools. We develop patient-specific approaches (mainly based on medical images) as well as population-type approaches in order to take advantage of large databases. We claim that we can have a clinical impact that can change the way of handling certain pathologies.

In vivo modeling of tumors is limited by the amount of information obtainable. 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 growth, assess tumor status as well as anatomical or functional details. Using different techniques 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 and medical doctors now have access to a wide spectrum of therapies (surgery, mini-invasive techniques, radiotherapies, chemotherapies, targeted therapies...).

Our project aims at supporting the decision process of oncologists in the definition of therapeutic protocols via quantitative methods. 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 growth 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?

In addition, 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 critical need of integrating biological knowledge into mathematical models based on clinical or experimental data. The main purpose of our project is 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

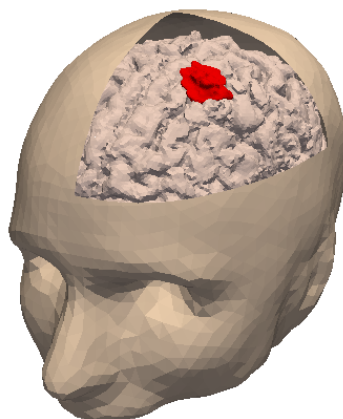


Figure 1. 3D numerical simulation of a meningioma. The tumor is shown in red.

The general strategy consists of the interactions of several stages:

- **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 microenvironment

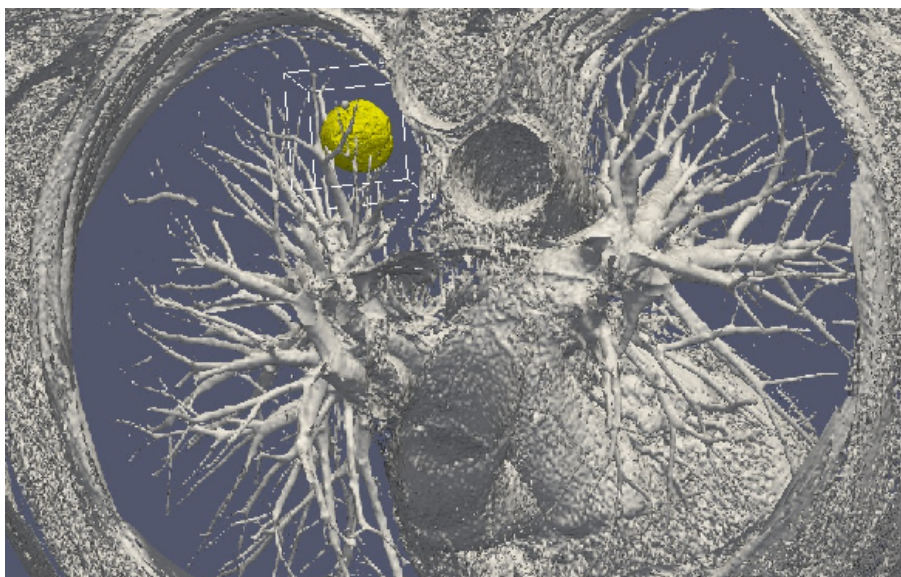


Figure 2. 3D numerical simulation of a lung tumor. The tumor is shown in yellow.

(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. It is also a crucial point: we need longitudinal data in time in order to be able to understand the time course of the disease. The data may also be obtained from analyses of blood samples or biopsies. A close collaboration with clinicians is required for selecting the specific cases to focus on, the understanding of the key points and of the key 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.
- **Stage 3: Adaptation of the model to data.** The model has to be adapted to the data: it is useless to have a model taking many biological features of the disease into account 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. Due to the complexity of the data - 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. Presently, most of the inverse problems - developed in the team - are solved using a gradient method coupled with some Monte-Carlo type algorithm. More efficient methods could be used as for example the sequential methods, *i.e.* the Kalman type filters or the so-called Luenberger filter (nudging). Using sequential methods can 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.
- Stage 4': 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 [9], 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: Simulation and prediction. Once the models have been parametrized, the simulation part can be done. We also need to include a quantification of uncertainties and to produce 3D simulations that can be confronted to reality.

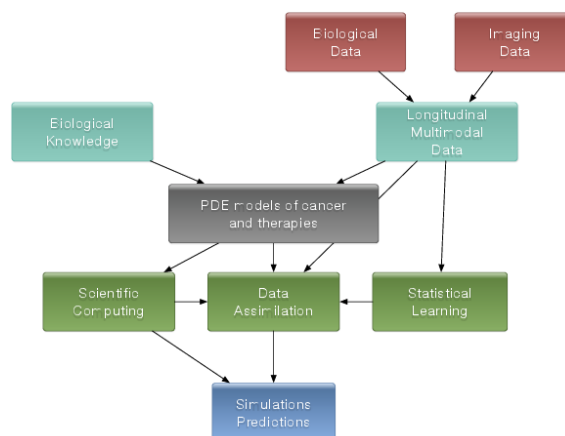


Figure 3. General strategy of the team to build meaningful models in oncology.

3. Research Program

3.1. Introduction

Our research on mathematical oncology is three-fold:

- Axis 1: Tumor modeling for patient-specific simulations.
- Axis 2: Bio-physical modeling for personalized therapies.
- Axis 3: Quantitative cancer modeling for biological and preclinical studies.

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 radiotherapies, but also thermo-ablations, radio-frequency ablations or electroporation that play a crucial role in the case of a relapse or for a metastatic disease, which is precisely the clinical context where the techniques of axis 1 will be applied.

The third axis, even if not directly linked to clinical perspectives, 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 will 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 forecast, 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. But it is an aspect that we keep in mind on a long term one.

The scientific challenge is therefore as follows: knowing the history of the patient, the nature of the primitive tumor, its histopathology, knowing the treatments that patients have undergone, knowing 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 the image 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 O.D.E. or a P.D.E 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 an 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.

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 –

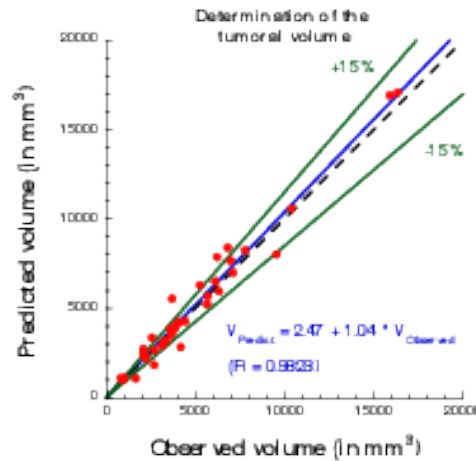


Figure 4. Plot showing the accuracy of our prediction on meningioma volume. Each point corresponds to a patient whose two first exams were used to calibrate our model. A patient-specific prediction was made with this calibrated model and compared with the actual volume as measured on a third time by clinicians. A perfect prediction would be on the black dashed line. Medical data was obtained from Prof. Loiseau, CHU Pellegrin.

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 bioelectromagneticians 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 these 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.

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 potentiate 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 makers (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'Angiogenèse 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),
- Meningioma (intracranial tumors),
- Metastases to the lung, liver from various organs,
- Soft-tissue sarcoma,
- Hepatocellular Carcinoma (primary liver tumors),

with starting works on kidney cancer, EGFR-mutated lung cancer and pancreas cancer.

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.

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

Last year saw a net increase in the diffusion of our work outside our own academic circle. Perrine Berment has clinched a seat in the national final of *Ma thèse en 180 secondes* after winning regional competition. Research achieved in the team was mentioned in popular radio shows like https://www.franceinter.fr/emissions/futur-proche/futur-proche-28-octobre-2016?xtmc=kurde_medecin&xtnp=1&xtr=14. This opens new collaboration opportunities locally and nationally for the team.

On a scientific point of view, the team has significantly increased its work on modeling tumor heterogeneity and texture analysis with very promising results so far, particularly in the thesis of Thibaut Kritter, Agathe Peretti, Cynthia Perier. We have developed a model for texture evolution over time which may offer a much better insight than approaches using statistical methods on texture features (*e.g.* radiomics).

5.1.1. Awards

Julien Jouganous has won *Prix Le Monde de la Recherche Universitaire*, http://www.lemonde.fr/sciences/article/2016/11/23/prix-le-monde-de-la-recherche-2016-1-evolution-du-cancer-en-equations_5036804_1650684.html.

6. New Software and Platforms

6.1. CADMOS

KEYWORDS: Health - Cancer - Partial differential equation - Cartesian grid

- Participants: Olivier Saut, Julien Jouganous, Annabelle Collin and Olivier Gallinato
- Partners: CNRS - INP Bordeaux - Université de Bordeaux
- Contact: Olivier Saut
- URL: <https://team.inria.fr/monc/software/>

6.2. Carcinom

Computer-Assisted Research about Cancer growth and INSights on Oncological Mechanisms

KEYWORDS: Cancer - Data modeling - Regression

- Participants: Vivien Pianet and Simon Evain
- Contact: Sébastien Benzekry
- URL: <https://team.inria.fr/monc/software/>

6.3. MetaPoumon

KEYWORDS: Health - Evolution - Cancer - Medical imaging

FUNCTIONAL DESCRIPTION

The software evaluates the aggressiveness of pulmonary metastasis or response to treatment for predictive goal. To do this, we use a mathematical model based on a set of equations to nonlinear partial differential equations. This model is calibrated to the patient data using a longitudinal sequence of CT or MRI of the patient.

- Participants: Olivier Saut, Thierry Colin, Marie Martin and Julien Jouganous
- Partners: CNRS - IPB - Université de Bordeaux
- Contact: Olivier Saut
- URL: <https://team.inria.fr/monc/software/>

6.4. Nenuphar

KEYWORDS: Modeling - Oncologie - Cancer - Partial differential equation - Medical - Medical imaging

FUNCTIONAL DESCRIPTION

The goal of project is to evaluate the aggressiveness of a tumor or its response to therapy. For that purpose, we use a mathematical model based on a set of nonlinear partial differential equations. This model is calibrated on patient data using a longitudinal sequence of CT Scan or MRI of the patient. This approach has been validated on about 35 clinical cases of lung metastases from various primary tumors (kidney, bladder, thyroid). Using two initial images showing the targeted lesion, we recover the patient-specific parameters of the model. The evolution of the disease is then predicted by letting the model run for later times with these parameters.

- Partners: CNRS - INP Bordeaux - Université Bordeaux 1
- Contact: Marie Martin
- URL: <https://team.inria.fr/monc/software/>

6.5. PapriK

- Contact: Cynthia Perier
- URL: <https://team.inria.fr/monc/software/>

6.6. SESAR

Monitor of the effect of RT on Retroperitoneal Sarcoma

KEYWORDS: Segmentation - Health - DICOM - Cancer - Medical imaging

- Partner: Institut Bergonié
- Contact: Cynthia Perier
- URL: <https://team.inria.fr/monc/software/>

6.7. SegmentIt

KEYWORDS: Health - Signal - Registration of 2D and 3D multimodal images - 3D - Image analysis - Image - Processing - Medical imaging

FUNCTIONAL DESCRIPTION

Image processing software for anatomical and functional data. Segmentation, registration and digital filtering. Assessment of the kidney perfusion and the kidney function (to be continued).

- Participants: Thierry Colin, Olivier Saut, Vivien Pianet, Agathe Peretti, Marie Martin, Sébastien Benzekry, Baudoin Denis De Senneville, Cynthia Perier, Benjamin Taton, Nicolas Grenier and Christian Combe
- Contact: Benjamin Taton
- URL: <https://team.inria.fr/monc/software/>

7. New Results

7.1. Free boundary problem for cell protrusion formations: theoretical and numerical aspects

Authors: Olivier Gallinato, Masahito Ohta, Clair Poignard, Takashi Suzuki

In this paper, a free boundary problem for cell protrusion formation is studied theoretically and numerically. The cell membrane is precisely described thanks to a level set function, whose motion is due to specific signalling pathways. The aim is to model the chemical interactions between the cell and its environment, in the process of invadopodia or pseudopodia formation. The model consists of Laplace equation with Dirichlet condition inside the cell coupled to Laplace equation with Neumann condition in the outer domain. The actin polymerization is accounted for as the gradient of the inner signal, which drives the motion of the interface. We prove the well-posedness of our free boundary problem under a sign condition on the datum. This criterion ensures the consistency of the model, and provides conditions to focus on for any enrichment of the model. We then propose a new first order Cartesian finite-difference method to solve the problem. We eventually exhibit the main biological features that can be accounted for by the model: the formation of thin and elongated protrusions as for invadopodia, or larger protrusion as for pseudopodia, depending on the source term in the equation. The model provides the theoretical and numerical grounds for single cell migration modeling, whose formulation is valid in 2D and 3D. In particular, specific chemical reactions that occurred at the cell membrane could be precisely described in forthcoming works. Journal: *Journal of Mathematical Biology*, Springer Verlag (Germany), 2016, <10.1007/s00285-016-1080-7> lien hal: <https://hal.inria.fr/hal-01412264v1>

7.2. Mathematical model for transport of DNA plasmids from the external medium up to the nucleus by electroporation

Authors: Michael Leguèbe, M Notarangelo, Monika Twarogowska, Roberto Natalini, Clair Poignard

This work is devoted to modelling gastrointestinal stromal tumour metastases to the liver, their growth and resistance to therapies. More precisely, resistance to two standard treatments based on tyrosine kinase inhibitors (imatinib and sunitinib) is observed clinically. Using observations from medical images (CT scans), we build a spatial model consisting in a set of non-linear partial differential equations. After calibration of its parameters with clinical data, this model reproduces qualitatively and quantitatively the spatial tumour evolution of one specific patient. Important features of the growth such as the appearance of spatial heterogeneities and the therapeutical failures may be explained by our model. We then investigate numerically the possibility of optimizing the treatment in terms of progression-free survival time and minimum tumour size reachable by varying the dose of the first treatment. We find that according to our model, the progression-free survival time reaches a plateau with respect to this dose. We also demonstrate numerically that the spatial structure of the tumour may provide much more insights on the cancer cell activities than the standard RECIST criteria, which only consists in the measurement of the tumour diameter. Finally, we discuss on the non-predictivity of the model using only CT scans, in the sense that the early behaviour of the lesion is not sufficient to predict the response to the treatment. Journal: *Mathematical Medicine and Biology*, Oxford University Press (OUP), 2016, <10.1093/imammb/dqw002> lien hal: <https://hal.inria.fr/hal-01380292>

7.3. Free boundary problem for cell protrusion formations: theoretical and numerical aspects

Authors: Olivier Gallinato, Masahito Ohta, Clair Poignard, Takashi Suzuki

In this paper, a free boundary problem for cell protrusion formation is studied theoretically and numerically. The cell membrane is precisely described thanks to a level set function, whose motion is due to specific signalling pathways. The aim is to model the chemical interactions between the cell and its environment, in the process of invadopodia or pseudopodia formation. The model consists of Laplace equation with Dirichlet condition inside the cell coupled to Laplace equation with Neumann condition in the outer domain. The actin polymerization is accounted for as the gradient of the inner signal, which drives the motion of the interface. We prove the well-posedness of our free boundary problem under a sign condition on the datum. This criterion ensures the consistency of the model, and provides conditions to focus on for any enrichment of the model. We then propose a new first order Cartesian finite-difference method to solve the problem. We eventually exhibit the main biological features that can be accounted for by the model: the formation of thin and elongated protrusions as for invadopodia, or larger protrusion as for pseudopodia, depending on the source term in the equation. The model provides the theoretical and numerical grounds for single cell migration modeling, whose formulation is valid in 2D and 3D. In particular, specific chemical reactions that occurred at the cell membrane could be precisely described in forthcoming works. Journal: *Journal of Mathematical Biology*, Springer Verlag (Germany), 2016, <10.1007/s00285-016-1080-7> lien hal: <https://hal.inria.fr/hal-01412264v1>

7.4. Spatial modelling of tumour drug resistance: the case of GIST liver metastases *Mathematical Medicine and Biology Advance*

Authors: Guillaume Lefebvre, François Cornelis, Patricio Cumsille, Thierry Colin, Clair Poignard, Olivier Saut

This work is devoted to modelling gastrointestinal stromal tumour metastases to the liver, their growth and resistance to therapies. More precisely, resistance to two standard treatments based on tyrosine kinase inhibitors (imatinib and sunitinib) is observed clinically. Using observations from medical images (CT scans), we build a spatial model consisting in a set of non-linear partial differential equations. After calibration of its parameters with clinical data, this model reproduces qualitatively and quantitatively the spatial tumour evolution of one specific patient. Important features of the growth such as the appearance of spatial heterogeneities and the therapeutical failures may be explained by our model. We then investigate numerically the possibility of optimizing the treatment in terms of progression-free survival time and minimum tumour size reachable by varying the dose of the first treatment. We find that according to our model, the progression-free survival time reaches a plateau with respect to this dose. We also demonstrate numerically that the spatial structure of the tumour may provide much more insights on the cancer cell activities than the standard RECIST criteria, which only consists in the measurement of the tumour diameter. Finally, we discuss on the non-predictivity of the model using only CT scans, in the sense that the early behaviour of the lesion is not sufficient to predict the response to the treatment. Journal: *Mathematical Medicine and Biology*, Oxford University Press (OUP), 2016, <10.1093/imammb/dqw002> lien hal: <https://hal.inria.fr/hal-01380292>

7.5. Mathematical modeling of cancer immunotherapy and synergy with radiotherapy

Team participant: S. Benzekry Other participants: R. Serre, N. André, J. Ciccolini, D. Barbolosi (SMARTc, Inserm, Marseille, FR), L. Padovani, X. Muracciole (Radiotherapy Unit, La Timone Hospital, Marseille, FR), F. Barlési (Multidisciplinary Oncology and Therapeutic Innovations Unit, AP-HM, Marseille, FR) and C. Meille (Roche Pharmaceuticals, Basel, Switzerland)

Combining radiotherapy with immune checkpoint blockade may offer considerable therapeutic impact if the immunosuppressive nature of the tumor microenvironment (TME) can be relieved. In this study, we used mathematical models, which can illustrate the potential synergism between immune checkpoint inhibitors and radiotherapy. A discrete-time pharmacodynamic model of the combination of radiotherapy with inhibitors of the PD1–PDL1 axis and/or the CTLA4 pathway is described. This mathematical framework describes how a growing tumor first elicits and then inhibits an antitumor immune response. This antitumor immune response is described by a primary and a secondary (or memory) response. The primary immune response appears first and is inhibited by the PD1–PDL1 axis, whereas the secondary immune response happens next and is inhibited by the CTLA4 pathway. The effects of irradiation are described by a modified version of the linear-quadratic model. This modeling offers an explanation for the reported biphasic relationship between the size of a tumor and its immunogenicity, as measured by the abscopal effect (an off-target immune response). Furthermore, it explains why discontinuing immunotherapy may result in either tumor recurrence or a durably sustained response. Finally, it describes how synchronizing immunotherapy and radiotherapy can produce synergies. The ability of the model to forecast pharmacodynamic endpoints was validated retrospectively by checking that it could describe data from experimental studies, which investigated the combination of radiotherapy with immune checkpoint inhibitors. In summary, a model such as this could be further used as a simulation tool to facilitate decision making about optimal scheduling of immunotherapy with radiotherapy and perhaps other types of anticancer therapies.

7.6. Non-Standard Radiotherapy Fractionations Delay the Time to Malignant Transformation of Low-Grade Gliomas

Team participant: S. Benzekry. Other participants: A. Henares-Molina, V.M. Perez-Garcia and A. Martinez-Gonzalez (Môlab, Universidad de Castilla-La Mancha, Ciudad Real, Spain) P.C. Lara (Radiation Oncology, Las Palmas University Hospital, Las Palmas, Spain), M. Garcia-Rojo (Pathology department, Jerez de la Frontera Hospital, Jerez de la Frontera, Spain)

Grade II gliomas are slowly growing primary brain tumors that affect mostly young patients. Cytotoxic therapies (radiotherapy and/or chemotherapy) are used initially only for patients having a bad prognosis. These therapies are planned following the “maximum dose in minimum time” principle, i. e. the same schedule used for high-grade brain tumors in spite of their very different behavior. These tumors transform after a variable time into high-grade tumors, what decreases significantly the patient’s life expectancy. In this paper we study mathematical models describing the growth of grade II gliomas in response to radiotherapy. We find that protracted metronomic fractionations, *i.e.* therapeutical schedules enlarging the time interval between low-dose radiotherapy fractions, may lead to a better tumor control without an increase in toxicity. Other non-standard fractionations such as protracted or hypoprotracted schemes may also be beneficial. The potential survival improvement depends on the tumor proliferation rate and can be even of the order of years. A conservative metronomic scheme, still being a suboptimal treatment, delays the time to malignant progression of at least one year when compared to the standard scheme.

7.7. Model-driven optimization of antiangiogenics + cytotoxics combination in breast cancer mice treated with bevacizumab and paclitaxel

Team participant: S. Benzekry. Other participants: S. Mollard (CRUK, Cambridge, UK), J. Ciccolini, D-C Imbs, R. El Cheikh, D. Barbolosi (SMARTc, Inserm, Marseille, FR)

Bevacizumab is the first-in-class antiangiogenic drug administrated concomitantly with cytotoxics. Several reports have shown that antiangiogenics could induce a transient phase of vascular normalization, thus ensuring a better drug delivery provided that cytotoxics administration is delayed. However, determining this best sequence is challenging. We have developed a simple mathematical model describing the impact of antiangiogenics on tumor vasculature. A 3.4 days delay between bevacizumab and paclitaxel was first proposed by the model as an optimal sequence. To test its relevance, 84 mice were orthotopically xenografted with human MDA-231Luc+ breast cancer cells. Two different sets of experiments were performed, based

upon different bevacizumab dosing (10 or 20 mg/kg) and inter-cycle intervals (7 or 10 days), comprising several combinations with paclitaxel. Results showed that scheduling bevacizumab administration 3 days before paclitaxel improved antitumor efficacy (48% reduction in tumor growth as compared with concomitant dosing, $p < 0.05$) while reducing metastatic spreading. Additionally, bevacizumab alone could lead to more aggressive metastatic disease with shorter survival in animals. Our phenomenological model was able to fit experimental data and provided insight on the underlying dynamics of vasculature's ability to deliver the cytotoxic agent. Final simulations suggested a new, data-informed optimal sequence of 2.4 days. Our data suggest that concomitant dosing between bevacizumab and paclitaxel could be a sub-optimal strategy at bedside. In addition, this proof of concept study suggests that mathematical modelling could help to identify the best sequence among a variety of possible alternate treatment modalities, thus refining the way experimental or clinical studies are conducted.

7.8. Dynamics of concomitant resistance: data, theories and mathematical modeling

Team participant: S. Benzekry Other participants: C. Lamont, L. Hlatky, P. Hahnfeldt (Center of Cancer and Systems Biology, Boston, USA)

In mice bearing two tumors implanted simultaneously, tumor growth was suppressed in one of the two tumors. Three theories of this phenomenon were advanced and assessed against the data. As formalized, the two models of competition for nutrients and indirect angiogenesis-regulated inhibition were not able to explain the growth behavior as well as a third model based on direct systemic inhibition. The superior model offers a depiction of concomitant resistance that provides an improved theoretical basis for tumor growth control that may also find utility in therapeutic planning to avoid post-surgery metastatic acceleration.

7.9. Modeling spontaneous metastasis following surgery: an in vivo-in silico approach

Team participant: S. Benzekry. Other participants: A. Tracz, M. Mastro, R. Corbelli and J. Ebos (Roswell Park Cancer Institute, Buffalo, USA) D. Barbolosi (SMARTc, Inserm, Marseille, FR)

Rapid improvements in the detection and tracking of early-stage tumor progression aim to guide decisions regarding cancer treatments as well as predict metastatic recurrence in patients following surgery. Mathematical models may have the potential to further assist in estimating metastatic risk, particularly when paired with in vivo tumor data that faithfully represent all stages of disease progression. Herein we describe mathematical analysis that uses data from mouse models of spontaneous metastasis developing after surgical removal of orthotopically implanted primary tumors. Both presurgical (primary tumor) and postsurgical (metastatic) growth was quantified using bioluminescence and was then used to generate a mathematical formalism based on general laws of the disease (*i.e.* dissemination and growth). The model was able to fit and predict pre-/post-surgical data at the level of the individual as well as the population. Our approach also enabled retrospective analysis of clinical data describing the probability of metastatic relapse as a function of primary tumor size. In these data-based models, inter-individual variability was quantified by a key parameter of intrinsic metastatic potential. Critically, our analysis identified a highly nonlinear relationship between primary tumor size and postsurgical survival, suggesting possible threshold limits for the utility of tumor size as a predictor of metastatic recurrence. These findings represent a novel use of clinically relevant models to assess the impact of surgery on metastatic potential and may guide optimal timing of treatments in neoadjuvant (presurgical) and adjuvant (postsurgical) settings to maximize patient benefit.

7.10. Computational Trials: Unraveling Motility Phenotypes, Progression Patterns, and Treatment Options for Glioblastoma Multiforme

Team participants: Thierry Colin, Olivier Saut. Other participants: Fabio Raman, Elizabeth Scribner, Olivier Saut, Cornelia Wenger, Hassan Fathallah-Shaykh.

Glioblastoma multiforme is a malignant brain tumor with poor prognosis and high morbidity due to its invasiveness. Hypoxia-driven motility and concentration-driven motility are two mechanisms of glioblastoma multiforme invasion in the brain. The use of anti-angiogenic drugs has uncovered new progression patterns of glioblastoma multiforme associated with significant differences in overall survival. Here, we apply a mathematical model of glioblastoma multiforme growth and invasion in humans and design computational trials using agents that target angiogenesis, tumor replication rates, or motility. The findings link highly-dispersive, moderately-dispersive, and hypoxia-driven tumors to the patterns observed in glioblastoma multiforme treated by anti-angiogenesis, consisting of progression by Expanding FLAIR, Expanding FLAIR + Necrosis, and Expanding Necrosis, respectively. Furthermore, replication rate-reducing strategies (e.g. Tumor Treating Fields) appear to be effective in highly-dispersive and moderately-dispersive tumors but not in hypoxia-driven tumors. The latter may respond to motility-reducing agents. In a population computational trial, with all three phenotypes, a correlation was observed between the efficacy of the rate-reducing agent and the prolongation of overall survival times. This research highlights the potential applications of computational trials and supports new hypotheses on glioblastoma multiforme phenotypes and treatment options.

N

8. Partnerships and Cooperations

8.1. National Initiatives

8.1.1. Plan Cancer

8.1.1.1. NUMEP

Plan Cancer NUMEP: 2016–2019. Numerics for Clinical Electroporation Funding: 460 k€ Partners: Inria Team MONC, Institut de Pharmacologie de Toulouse, CHU J. Verdier de Bondy Duration: Octobre 2016—Septembre 2019 Project leader: C. Pognard Co-PI: M-P. Rols (IPBS), O. Séror (CHU J. Verdier)

8.1.1.2. Dynamo

Plan Cancer DYNAMO: 2015–2018. Dynamical Models for Tissue Electroporation Funding: 370 k€ Partners: Laboratoire Ampère, Lab. Vectorology and Anticancerous Therapies (IGR), Inria Team MONC Duration: Octobre 2015—Septembre 2018 Project leader: R. Scorretti (Laboratoire Ampère) Co-PI: L.M. Mir (IGR), C. Pognard (Inria Team MONC)

8.1.1.3. Moglimaging

- Project acronym - Moglimaging: Modeling of Glioblastoma treatment-induced resistance and heterogeneity by multi-modal imaging.
- Partners -
- Duration - from Nov. 2016 to Nov 2019.
- Coordinator - E. Cohen-Jonathan Moyal, Institut Universitaire du Cancer Toulouse / Local coordinator - O. Saut.
- Team participants - S. Benzekry, A. Collin, C. Pognard, O. Saut.

8.1.1.4. MIMOSA

- Project acronym - Plan Cancer MIMOSA (Physique, Mathématiques et Sciences de l'ingénieur appliqués au Cancer)
- Partner - Laboratory of Biology, Bordeaux University
- Duration - from 2014 to 2017
- Coordinator - Th. Colin
- Team participants - S. Benzekry, Th. Colin, C. Pognard, O. Saut

- Title - Mathematical modeling for exploration of the impact of mechanical constraints on tumor growth

8.1.2. A*Midex MARS

- Project acronym - A*Midex MARS
- Partner - Service d'Oncologie Multidisciplinaire & Innovations Thérapeutiques, Hopitaux de Marseille
- Duration - from 2014 to 2016
- Coordinator - F. Barlesi
- Team participant - S. Benzekry
- Title - Modeling Anticancer Research & Simulation

8.1.3. PEPS CNRS

- PEPS CNRS "Jeune chercheur" Acronym: Metamat Partners: J. Ebos, Roswell Park Cancer Institute, Buffalo, USA Duration: October - November 2016 PI: S. Benzekry

8.1.4. Competitvity 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.

8.2. International Initiatives

8.2.1. Inria International Partners

8.2.1.1. Informal International Partners

- LEA EBAM on electroporation <http://lea-ebam.cnrs.fr>,
- JSPS Core-to-Core "Establishing Network in Mathematical Medicine" granted by Japan, led by T. Suzuki, Osaka University, (local PI: C. Poignard).

8.3. International Research Visitors

8.3.1. Visits of International Scientists

Clair Poignard and the team had visits from the following scientists:

- T. Suzuki, Osaka University, Japan,
- R. Natalini, IAC, Rome (PhD co-supervision of M. Deville)
- F. Gibou, UCSB, Santa Barbara (Numerical methods for cell aggregate electroporation).
- Rouzaimaimati Makemuti (Associate professor at Xingiang University, China);

Thierry Colin and Olivier Saut had the pleasure to welcome Hassan Fathallah-Shaykh (neuro-oncologist, Univ. Alabama at Birmingham) for two weeks to work on ours models for glioblastoma.

9. Dissemination

9.1. Promoting Scientific Activities

9.1.1. Scientific Events Organisation

9.1.1.1. Member of the Organizing Committees

Thierry Colin was in the organizing committee of the *6th International Conference in Computational Surgery and Dual Training* in Bordeaux. The whole team (particularly A. Collin and C. Poignard) was involved in the organization of this event.

9.1.2. Journal

9.1.2.1. Reviewer - Reviewing Activities

- S. Benzekry - biomathematical modeling journals: Journal of Theoretical Biology, Mathematical Biosciences, Bulletin of Mathematical Biology, Theoretical Biology and Medical Modeling, Mathematical Biosciences and Engineering, Journal of Biological Informatics, Journal of Biological Systems, ESAIM:Proc, Mathematics and Computers in Simulation; and medical/biological journals about cancer: Clinical Pharmacokinetics, BMC Cancer
- A. Collin - Computer Methods in Applied Mechanics and Engineering.
- T. Colin - Too much to list...
- C. Poignard - SIAM Journal on Mathematical Analysis, IEEE Trans on Mag, J. Math. Biology, J. Theoretical Biology
- O. Saut - IEEE Trans. Med. Imaging, PLOS Computational Biology, PLOS One, Medical Image Analysis, Nature Comm.

9.1.3. Invited Talks

- Sébastien Benzekry:
 - Integrated Mathematical Oncology Department, Moffitt Cancer Center, Tampa, Florida, USA.
 - Department of Genetics, Roswell Park Cancer Institute, Buffalo, NY, USA.
 - Mathematics Department Colloquium, Ryerson University, Toronto, Canada.
 - Metronomics @ Mumbai, Mumbai, India.
- Thierry Colin:
 - Second French-Korean congress, July 2016, Bordeaux.
 - Treatment optimization for glioblastomas, October 2016, Cuenca, Spain.
 - Keio University Hospital, Japan,
 - Tokyo University of Science, Japan,
 - Osaka University, Japan.
- Olivier Saut: ALGORITHMY 2016, Conference on Scientific Computing, Podbanske, Slovakia (<http://www.math.sk/alg2016>).

9.1.4. Leadership within the Scientific Community

- O. Saut is the head of the CNRS GDR 3471 Metice (<http://metice.math.cnrs.fr>).

9.1.5. Scientific Expertise

- S. Benzekry was a reviewer for research projects of the CETIC (Centre d'Excellence Africain en Technologies de l'Information et de la Communication) and for the Erwin Schroedinger-Fellowship of the Austrian Science Fund (FWF).
- O. Saut is an expert for the French Ministry of Research (for various programs including PHC and EGIDE programs).
- O. Saut was a reviewer for Research Career Development Fellowship program of Dublin City University.
- O. Saut is a reviewer for project proposals in IGSSE (International Graduate School of Science and Engineering), Technical University of Munich.

9.1.6. Research Administration

- C. Poignard is elected member of the Inria evaluation committee.
- O. Saut is a member of the Steering Committee of Labex TRAIL (<http://trail.labex.u-bordeaux.fr>).

9.2. Teaching - Supervision - Juries

9.2.1. Teaching

Licence: S. Benzekry, Equations différentielles ordinaires, 20h, ENSEIRB-Matmeca, France.

Master: T. Colin, Last year of Engineering school Enseirb-Matmeca: multiphysics modelling

Licence: T. Colin, First Year of the Engineering school of chemistry of Bordeaux, specialization in structures and composite material: basic mathematics.

Licence and Master: A. Collin did a full service as MdC at the Engineering school ENSEIRB-Matmeca.

Licence: Clair Poignard, Engineering school ENSCPB. L3 undergraduate course on numerical analysis (50h).

Licence: Clair Poignard, Engineering school ENSEIRB-Matmeca: undergraduate lecture on numerical analysis (18h).

Master : Olivier Saut, Outils Numériques pour la Mécanique, 20h, M1, ENSEIRB-Matmeca, France.

9.2.2. Supervision

- PhD : P. Berment, Mathematical modelling evaluating radiotherapy outcome for colorectal tumor with Pet Scan, Univ. Bordeaux, July 2016, Thierry Colin and Olivier Saut.
- PhD : E. Baratchart, Quantitative study of the dynamics and spatial aspects of metastatic development using mathematical models, Univ. Bordeaux, February 2016, S. Benzekry, Th. Colin and O. Saut.
- PhD in progress : M. Deville, Modeling of electroporation and gene transfection across tissue. Theoretical and numerical aspects., Sep 2014, C. Poignard and R. Natalini (IAC, CNR Roma).
- PhD : O. Gallinato, Invasive process modeling of the tumor metastatic cells, Univ. Bordeaux, C. Poignard and T. Suzuki (Osaka University). (PhD defended November 22, 2016)
- PhD in progress : T. Ritter, Primary tumors modelling with a view to the gliomas and adenocarcinomas study, Sep 2015, C. Poignard and O. Saut
- PhD : T. Michel, Analysis of mathematical growth tumor models, Univ. Bordeaux, C. Poignard and Th. Colin. (PhD defended November 18, 2016)
- PhD in progress : A. Perreti, Anti-angiogenic traitements modeling using medical imaging, Oct 2014, Th. Colin and O. Saut.
- PhD in progress : S. Corridore, 2016-2019, A. Collin and C. Poignard.
- PhD in progress : C. Perier, 2016-2019, B. Denis de Senneville and O. Saut.
- PhD in progress: C. Nicolò, Mathematical modeling of systemic aspects of cancer and cancer therapy, Oct 2016, S. Benzekry and O. Saut.

9.2.3. Juries

- O. Saut was a reviewer of the PhD of Matthieu Lê "Modélisation de la croissance de tumeurs cérébrales, application à la radiothérapie", Univ. Nice, Inria Sophia Antipolis, July 2016.

9.3. Popularization

- Popularization article in a special edition of the journal "Tangente" devoted to mathematics in medicine. (S. Benzekry).
- S. Benzekry was interviewed by the journal "Sciences et Avenir".
- A. Collin is an active member of "Femmes et Sciences" and gave several talks in this context (Printemps de la Mixité, talks in high schools...).
- O. Saut is a regular speaker at Entretien de l'Excellence (<http://www.lesentretiens.org>).

- O. Saut was a speaker at the "Forum des Métiers" in Collège Montaigne, Lormont.

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Project-Team PHOENIX

Programming Language Technology For Communication Services

IN COLLABORATION WITH: Laboratoire Bordelais de Recherche en Informatique (LaBRI)

IN PARTNERSHIP WITH:

CNRS

Université de Bordeaux

RESEARCH CENTER

Bordeaux - Sud-Ouest

THEME

Distributed programming and Software engineering

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- 1.4. - Ubiquitous Systems
- 2.1. - Programming Languages
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- 2.5. - Software engineering
- 2.6.2. - Middleware
- 5.1. - Human-Computer Interaction
- 5.11. - Smart spaces

Other Research Topics and Application Domains:

- 1.3.2. - Cognitive science
- 2.1. - Well being
- 2.5.2. - Cognitive disabilities
- 2.5.3. - Assistance for elderly
- 4.5. - Energy consumption
- 8. - Smart Cities and Territories

1. Members

Research Scientist

Eugene Volanschi [Inria, Advanced Research position]

Faculty Members

Charles Consel [Team leader, Bordeaux INP, Professor, HDR]

Helene Sauzeon [Univ. Bordeaux, Professor, HDR]

Bernard N Kaoua [Univ. Bordeaux, Professor, External collaborator, HDR]

Technical Staff

Quentin Barlas [Inria, Engineers, from Feb 2016]

Benjamin Bertran [Inria, Engineers, until Feb 2016]

Julien Durand [Inria, Engineers]

Ludovic Fornasari [Inria, Engineers]

PhD Students

Adrien Carteron [Inria, PhD Student, granted by Conseil Régional d'Aquitaine]

Quentin Chisin [Inria, PhD Student, until Sep 2016]

Lucile Dupuy [Inria, PhD Student, until Oct 2016, granted by Conseil Régional d'Aquitaine]

Audrey Landuran [Univ. Bordeaux, PhD Student]

Cécile Mazon [Inria, PhD Student]

Antoine Riche [Inria, PhD Student, from Oct 2016]

Post-Doctoral Fellows

Charlotte Froger [Inria, Post-Doctoral Fellow]

Maxime Lussier [Inria, Post-Doctoral Fellow, until Jan 2016]

Administrative Assistants

Cecile Boutros [Inria, Assistant]
Catherine Cattaert Megrat [Inria, Assistant]

Others

Rafik Belloum [Inria, pre-PhD Student, from Nov 2016]
Amandine Delage [RPDAD, Research technician]
Amandine Desrozier [Inria, Research technician, from Feb 2016]
Pauline Fontagne [Inria, Research technician]
Flora Gallet [Inria, Research technician, from Aug 2016]
Maelle Joulin [Inria, Research technician, from Apr 2016]
Milan Kabac [Inria, Engineer, until Aug 2016]
Sebastien Marot [CNAM, Intern, until Feb 2016]
Anthony Miramont [Inria, Research technician, from Aug 2016 until Oct 2016]
Edwin Poumarat [Inria, Intern, from Feb 2016 until Jun 2016]
Clelia Raynaud [Univ. Bordeaux, Intern, from Apr 2016 until Jun 2016]
Joan Rieu [Inria, Intern, from Mar 2016 until Aug 2016]
Corinne Toupin [RPDAD, Research technician, until Jan 2016]
Flavie Valriviere [RPDAD, Research technician, from Mar 2016 until Jun 2016]

2. Overall Objectives

2.1. Context

A host of networked entities (devices and services) are populating smart spaces that become prevalent (*e.g.*, building management, personal assistance, avionics) and large scale (*e.g.*, train station, city, highway network). These smart spaces are becoming intimately intertwined with our daily life and professional activities, raising scientific challenges that go beyond the boundaries of single field of expertise.

2.2. A Multi-Disciplinary Approach

We focus our attention on the domain of applications that orchestrate networked objects, whether populating smart spaces or worn by individuals on-the-go. Because such applications are intimately intertwined with the users' daily life and professional activities, they can improve users' efficiency in performing tasks or compensate for the users' deficiencies and disabilities, promoting autonomy. However, this emerging domain of *assistive computing* raises scientific challenges that go beyond the boundaries of Computer Science. To address these challenges, the Phoenix group has been conducting interdisciplinary research that combines

- Cognitive Science to study user needs and make a rigorous assessment of the services provided to users;
- Sensing and actuating expertise to support users, based on accurate and rich interactions with their environment;
- Design-driven software engineering to support and guide all the development process of the services provided to users.

2.3. Research Avenues

The activities of the Phoenix group revolve around three main avenues of research.

Design-driven software development. We further the study of design-driven software development, exploring the integration of both functional and non-functional concerns in the design phase, as well as the human-computer interaction dimension. We also expand the scope of our approach by scaling it up to the orchestration of masses of sensors and actuators.

Assistive computing in the home. This line of work leverages DiaSuite to develop an assisted living platform, named HomeAssist, which exploits the capabilities of smart spaces to provide services that compensate or remediate cognitive difficulties of users, drawn from needs analyses. This work is validated in the context of two research projects: HomeAssist for older adults, and ANDDI for adults with Intellectual Disabilities (ID). This platform is currently deployed in the homes of older adults where a variety of applications assist them with their daily activities.

Assistive computing on-the-go. We develop mobile assistive computing support based on tablets. In particular, we have developed a cognitive assistive technology for the inclusion of children with Autism in mainstreamed environments, named School+.

3. Research Program

3.1. Design-Driven Software Development

Raising the level of abstraction beyond programming is a very active research topic involving a range of areas, including software engineering, programming languages and formal verification. The challenge is to allow design dimensions of a software system, both functional and non-functional, to be expressed in a high-level way, instead of being encoded with a programming language. Such design dimensions can then be leveraged to verify conformance properties and to generate programming support.

Our research on this topic is to take up this challenge with an approach inspired by programming languages, introducing a full-fledged language for designing software systems and processing design descriptions both for verification and code generation purposes. Our approach is also DSL-inspired in that it defines a conceptual framework to guide software development. Lastly, to make our approach practical to software developers, we introduce a methodology and a suite of tools covering the development life-cycle.

To raise the level of abstraction beyond programming, the key approaches are model-driven engineering and architecture description languages. A number of *architecture description languages* have been proposed; they are either (1) coupled with a programming language (e.g., [37]), providing some level of abstraction above programming, or (2) integrated into a programming language (e.g., [33], [38]), mixing levels of abstraction. Furthermore, these approaches poorly leverage architecture descriptions to support programming, they are crudely integrated into existing development environments, or they are solely used for verification purposes. *Model-driven software development* is another actively researched area. This approach often lacks code generation and verification support. Finally, most (if not all) approaches related to our research goal are *general purpose*; their universal nature provides little, if any, guidance to design a software system. This situation is a major impediment to both reasoning about a design artifact and generating programming support.

3.2. Integrating Non-Functional Concerns into Software Design

Most existing design approaches do not address non-functional concerns. When they do, they do not provide an approach to non-functional concerns that covers the entire development life-cycle. Furthermore, they usually are general purpose, impeding the use of non-functional declarations for verification and code generation. For example, the Architecture Analysis & Design Language (AADL) is a standard dedicated to real-time embedded systems [34]. AADL provides language constructs for the specification of software systems (e.g., component, port) and their deployment on execution platforms (e.g., thread, process, memory). Using AADL,

designers specify non-functional aspects by adding properties on language constructs (*e.g.*, the period of a thread) or using language extensions such as the Error Model Annex.⁰ The software design concepts of AADL are still rather general purpose and give little guidance to the designer.

Beyond offering a conceptual framework, our language-based approach provides an ideal setting to address non-functional properties (*e.g.*, performance, reliability, security, ...). Specifically, a design language can be enriched with non-functional declarations to pursue three goals: (1) expanding further the type of conformance that can be checked between the design of a software system and its implementation or execution infrastructure, (2) enabling additional programming support and guidance, and (3) leveraging the design declarations to optimize the generated implementation.

We are investigating this idea by extending our design language with non-functional declarations. For example, we have addressed error handling [9], access conflicts to resources [36], quality of service constraints [35], and more recently, data delivery models and parallel computation models for masses of sensors citekaba:hal-01319730.

Following our approach to paradigm-oriented software development, non-functional declarations are verified at design time, they generate support that guides and constrains programming, they produce a runtime system that preserves invariants and performs efficiently.

3.3. Human-Driven Software Design

Knowledge of the human characteristics (individual, social and organizational) allow the design of complex system and artifacts for increasing their efficacy. In our approach of assistive computing, a main challenge is the integration of facets of Human Factors in order to design technology support adapted to user needs in term of ergonomic properties (acceptability, usability, utility etc) and delivered functionalities (oriented task under user abilities constraints).

We adapt this approach to improve the independent living and self-determination of users with cognitive impairments by developing a variety of orchestration scenarios of networked objects (hardware/software) to provide a pervasive support to their activities. Human factors methodologies are adopted in our approach with the direct purpose the reliability and efficiency of the performance of digital support systems in respect of objectives of health and well-being of the person (monitoring, evaluation, and rehabilitation).

Precisely, our methodologies are based on a closed iterative loop, as described in the figure below :

- Identifying the person needs in a natural situation (*i.e.*, desired but problematic activities) according to Human Factors Models of activity (*i.e.*, environmental constraints; social support networks - caregivers and family; person's abilities)
- Designing environmental support that will assist the users to bypass their cognitive impairment (according to environmental models of cognitive compensatory mechanisms); and then implement this support in terms of technological solutions (scenarios of networked objects, hardware interface, software interface, interaction style, *etc*)
- Empirically evaluating the assistive solution based on human experimentations that includes ergonomic assessments (acceptability, usability, usefulness, *etc*) as well as longitudinal evaluations of use's efficacy in terms of activities performed by the individual, of satisfaction and well-being provided to the individual but also to his/her entourage (family and caregivers).

4. Application Domains

4.1. Internet of Things

The Internet of Things (IoT) has become a reality with the emergence of Smart Cities, populated with large amounts of smart objects which are used to deliver a range of citizen services (*e.g.*, security, well being, *etc.*) The IoT paradigm relies on the pervasive presence of smart objects or "things", which raises a number of new challenges in the software engineering domain.

⁰The Error Model Annex is a standardized AADL extension for the description of errors [39].

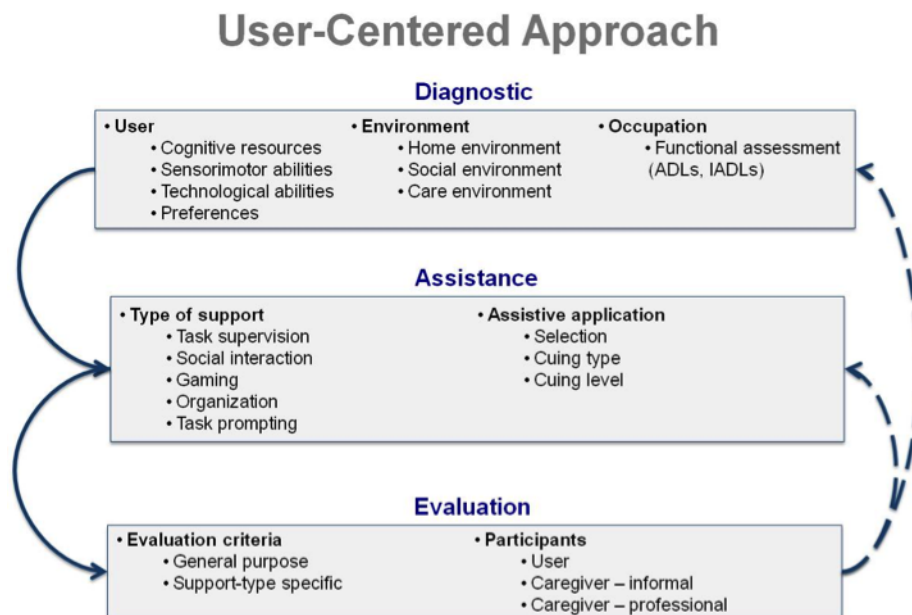


Figure 1. User-Centered Approach

We introduce a design-driven development approach that is dedicated to the domain of orchestration of masses of sensors. The developer declares what an application does using a domain-specific language (DSL), named DiaSwarm. Our compiler processes domain-specific declarations to generate a customized programming framework that guides and supports the programming phase.

DiaSwarm addresses the main phases of an application orchestrating masses of sensors.

Service discovery Standard service discovery at the individual object level does not address the needs of applications orchestrating large numbers of smart objects. Instead, a high-level approach which provides constructs to specifying subsets of interest is needed. Our approach allows developers to introduce application-specific concepts (e.g., regrouping parking spaces into lots or districts) at the design time and then these can be used to express discovery operations. Following our design-driven development approach, these concepts are used to generate code to support and guide the programming phase.

Data gathering Applications need to acquire data from a large number of objects through a variety of delivery models. For instance, air pollution sensors across a city may only push data to the relevant applications when pollution levels exceed tolerated levels. Tracking sensors, however, might determine the location of vehicles and send the acquired measurements to applications periodically (e.g., 10 min. intervals). Data delivery models need to be introduced at design time since they have a direct impact on the application's program structure. In doing so, the delivery models used by an application can be checked against sensor features early in the development process.

Data processing Data that is generated from hundreds of thousands of objects and accumulated over a period of time calls for efficient processing strategies to ensure the required performance is attained. Our approach allows for an efficient implementation of the data processing stage by providing the developer with a framework based on the MapReduce [34] programming model which is intended for the processing of large data sets.

4.2. Assistive computing in the home

In this avenue of research, we have been developing a systemic approach to introducing an assisted living platform for the home of older adults. To do so, we formed an interdisciplinary team that allows (1) to identify the user needs from a gerontological and psychological viewpoint; (2) to propose assistive applications designed by human factors and HCI experts, in collaboration with caregivers and users; (3) to develop and test applications designed and developed by software engineers; (4) to conduct a field study to assess the benefits of the platform and assistive applications, in collaboration with caregivers, by deploying the system at the actual homes.

Our research activities for assistive computing in the home are conducted under the *HomeAssist* project. This work takes the form of a platform offering an online catalog of assistive applications that orchestrate an open-ended set of networked objects. Our platform leverages DiaSuite to quickly and safely develop applications at a high level.

Our scientific achievements include the design principles of our platform, its key features to effectively assist individuals in their home, field studies to validate HomeAssist, the expansion of HomeAssist to serve individuals with ID, and the technology transfer of HomeAssist. Note that a complete presentation of this work, from a Cognitive Science perspective, is given in the doctoral thesis of Lucile Dupuy published this year.

4.2.1. Project-team positioning

There is a range of platforms for assisted living aimed at older adults that have been developed for more than a decade. Most of these platforms are used in a setting where participants come to a research apartment to perform certain tasks. This setting makes it difficult to assess user acceptance and satisfaction of the proposed approaches because the user does not interact with the technology on a daily basis, over a period of time. Furthermore, older adults adopt routines to optimize their daily functioning at home. This situation calls for field studies in a naturalistic setting to strengthen the evaluation of assisted living platforms.

HomeAssist innovates in that it supports independent living across the activities of daily living and is validated by field studies in naturalistic setting.

4.3. Assistive computing on-the-go

We conduct research on assistive computing supported by mobile devices such as smart phones and tablets. Both research projects presented in this section are supported by tablets and leverage their functionalities to guide users with cognitive challenges performing activities and tasks, whether in mainstream schools to support inclusion or in residential settings to support their autonomy. The mobile nature of tablets allows to envision such devices as supporting users with cognitive challenges across a range of environments.

Many research projects bring cognitive-support applications to users based on tablets and smartphones. However, few projects equip users with such devices in actual mainstream environments, including stakeholders in the design process and targeting an autonomous usage of assistive applications. An additional originality of our approach is our interdisciplinary approach that allows us to integrate key psychological dimensions in our design, such as self-determination.

5. Highlights of the Year

5.1. Highlights of the Year

5.1.1. Awards

- The paper “Designing Parallel Data Processing for Large-Scale Sensor Orchestration” by Milan Kabac and Charles Consel received a Best Paper award at UIC 2016, the 13th IEEE International Conference on Ubiquitous Intelligence and Computing, held in July 2016 in Toulouse, France.
- The web application “It’s my life. I choose it!”, developed by the Phoenix team in collaboration with the University of Bordeaux (Laboratoire handicap action cognition santé), the University of Mons (Service d’ortho-pédagogie clinique), and the association Trisomie 21 France, received the Universal Accessibility Prize at APAJH 2016, held on November 14th, 2016, in Paris. The web application is available at <http://www.monprojetdevie.trisomie21-france.org/>.
- The pitch for a startup based on technology from the HomeAssist project received a prize at the “Journée Horizon Startup”, held on December, 1st, 2016, in Paris.

BEST PAPERS AWARDS :

[26] **13th IEEE International Conference on Ubiquitous Intelligence and Computing (UIC 2016)**. M. KABÁČ, C. CONSEL.

6. New Software and Platforms

6.1. College +

KEYWORDS: Neurosciences - Health - Autism - Mobile application

School+ (or College+ in french) is a package of 7 applications. Three applications are assistive applications, guiding the child doing specific tasks. Three others are training applications made as serious games, addressing specific skills. The last application is a meta-application, comprising a link to the three training applications, with an access to statistics of their usage. For each application, data are separated from the design, meaning that every element of each application (pictures, texts, settings, etc.) can be changed at any time. Each application records a log file containing all the interactions performed by the child.

6.1.1. Assistive applications

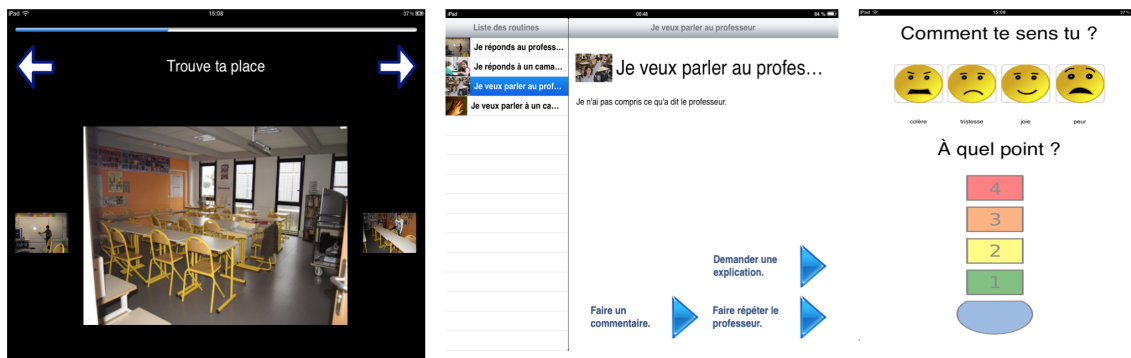


Figure 2. Assistive applications

6.1.1.1. Routines application

This application shows a list of tasks, with a short description. After clicking the starting button, a specific slideshow is shown; it decomposes a task into steps. For each step, a text and a picture can be displayed. Thumbnail of previous and next steps are also displayed. This application guides the child through classroom situations: entering classroom, taking school materials out of a backpack, writing notes, handling agenda, leaving the classroom.

6.1.1.2. Communication application

With the same design, the assistance provided by this application targets to communicating situations inside the classroom. The application covers four scenarios addressing two interaction situations (initiating and answering the interaction) and two types of interlocutors (professor and classmate). For each scenario, different slideshows guide the child, depending on the goal of the interaction.

6.1.1.3. Emotion Regulation application

This application aims to assist the child to self-regulate his/her emotions. Four simplified emoticons are proposed to the child to choose from: anger, sadness, joy and fear. Then, (s)he selects a level of intensity via a thermometer with a scale from 1 to 4. In response, the application delivers different multimedia contents according to the level selected to help the child regulate his/her emotions. Typically, a text (breathing instructions) are shown at level 1, pictures at level 2, a video at level 3 and another text at level 4.

6.1.2. Training applications

These three applications are serious games with increasing levels of difficulties, reachable after a ratio of good answers has been attained.

6.1.2.1. Emotion Recognition application with pictures

In this application, the child is instructed to identify a specific emotion among 4 pictures showing different people exhibiting an emotion. Seven emotions are involved in this application: joy, sadness, fear, anger, surprise, disgust and neutral. The emotion to be recognized is displayed together with its simplified emoticon. The type of pictures changes with the difficulty level: level 1 contains pictures of unfamiliar people and level 2 contains pictures of friends and relatives of the child.

6.1.2.2. Emotion Recognition application with videos

In this application, the child is presented with a fragment of an animated cartoon. At some point, the video stops and the child is asked to identify the emotion of the character. Four emotions are involved in this application: joy, sadness, fear and anger. Videos are slowed down, with a speed percentage that can be changed at each

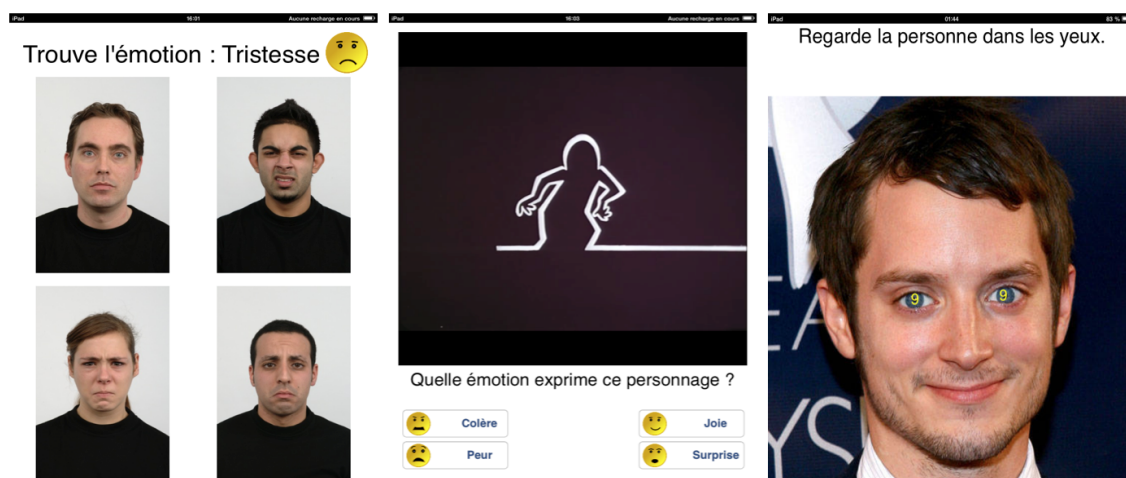


Figure 3. Training applications

level. Videos change with difficulty level: level 1 contains videos of a very basic cartoon (only one cartoon character drawn by basic form un-textured), level 2 contains a video of more sophisticated cartoons and level 3 contains movies with actors.

6.1.2.3. Attention Training

In this application, the child is presented a picture of a face and asked to make eye contact with it. Second, a symbol appears briefly in the eyes of the character. Third, the child is asked to identify the symbol shown in the previously displayed picture, to make sure he kept eye contact. The speed at which the symbol appears and disappears is changed according to the difficulty level. Types of pictures also change with the level : level 1 contains pictures of faces and level 2 contains pictures of classroom situations.

- Participants: Damien Martin Guillerez, Charles Fage, Helene Sauzeon and Alexandre Spriet
- Contact: Charles Consel

6.2. DiaSuite

SCIENTIFIC DESCRIPTION

DiaSuite is a suite of tools covering the development life-cycle of a pervasive computing application:

6.2.1. Defining an application area

First, an expert defines a catalog of entities, whether hardware or software, that are specific to a target area. These entities serve as building blocks to develop applications in this area. They are gathered in a taxonomy definition, written in the taxonomy layer of the DiaSpec language.

6.2.2. Designing an application

Given a taxonomy, the architect can design and structure applications. To do so, the DiaSpec language provides an application design layer. This layer is dedicated to an architectural pattern commonly used in the pervasive computing domain. Describing the architecture application allows to further model a pervasive computing system, making explicit its functional decomposition.

6.2.3. Implementing an application

We leverage the taxonomy definition and the architecture description to provide dedicated support to both the entity and the application developers. This support takes the form of a Java programming framework, generated by the DiaGen compiler. The generated programming framework precisely guides the developer with respect to the taxonomy definition and the architecture description. It consists of high-level operations to discover entities and interact with both entities and application components. In doing so, it abstracts away from the underlying distributed technologies, providing further separation of concerns.

6.2.4. Testing an application

DiaGen generates a simulation support to test pervasive computing applications before their actual deployment. An application is simulated in the DiaSim tool, without requiring any code modification. DiaSim provides an editor to define simulation scenarios and a 2D-renderer to monitor the simulated application. Furthermore, simulated and actual entities can be mixed. This hybrid simulation enables an application to migrate incrementally to an actual environment.

6.2.5. Deploying a system

Finally, the system administrator deploys the pervasive computing system. To this end, a distributed systems technology is selected. We have developed a back-end that currently targets the following technologies: Web Services, RMI, SIP and OSGI. This targeting is transparent for the application code. The variety of these target technologies demonstrates that our development approach separates concerns into well-defined layers. This development cycle is summarized in the Figure 2 .

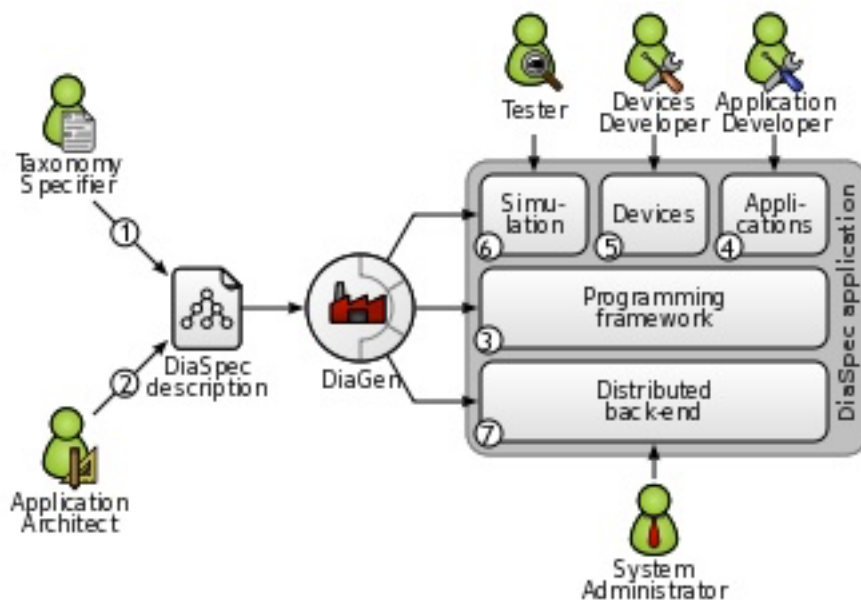


Figure 4. DiaSuite Development Cycle

FUNCTIONAL DESCRIPTION

DiaSuite is developed as a research project by the Inria/LaBRI Phoenix research group. The DiaSuite approach covers the development life-cycle of a pervasive computing application. It takes the form of a methodology, supported by (1) a high-level design language and (2) a suite of tools covering the development life-cycle of a pervasive computing application. Specifically, we have developed a design language dedicated to describing pervasive computing systems and a suite of tools providing customized support for each development stage of a pervasive computing system, namely, implementation (e.g., programming support), testing (e.g., unit test, 2D simulator), and deployment (e.g., distribution platforms like SIP and Web Services).

- Participants: Charles Consel, Milan Kabac, Paul Van Der Walt, Adrien Carteron and Alexandre Spriet
- Contact: Charles Consel

6.3. DiaSuiteBOX

KEYWORDS: Health - Smart home - Open application store - Development tool suite - Application certification - Home care

FUNCTIONAL DESCRIPTION

DiaSuiteBOX proposes an application store that gathers the devices deployed at home. This store is open and available online such as an application store for Smartphone.

- Participants: Bertran Benjamin, Bruneau Julien, Consel Charles, Quentin Enard, Milan Kabac, Damien Martin Guillerez, Emilie Balland, Damien Cassou, Amelie Marzin, Julien Durand, Quentin Barlas, Ludovic Fornasari, Joan Rieu, Adrien Carteron, Eugene Volanschi and Helene Sauzeon
- Partners: CNRS - IPB - Université de Bordeaux
- Contact: Charles Consel
- URL: <https://diasuitebox.inria.fr/>

6.4. DomAssist

KEYWORDS: Health - Mobile application - Persons attendant - Home care

The HomeAssist platform (or DomAssist in french) proposes a systemic approach to introducing an assistive technological platform for older people. To do so, we formed a trans-disciplinary team that allows (1) to identify the user needs from a gerontological and psychological viewpoint; (2) to propose assistive applications designed by human factors and HCI experts, in collaboration with caregivers and users; (3) to develop and test applications by software engineers; (4) to conduct a field study for assessing the benefits of the platform and assistive applications, in collaboration with caregivers, by deploying the system at the actual home of older adults.

The HomeAssist platform is implemented on top of the DiaSuiteBox platform, using a suite of tools, namely DiaSuite, that have been designed, developed and tested by our research group at Inria. The DiaSuite tools include a dedicated integrated development environment that enables applications to be developed quickly and safely. This technology has been successfully applied to a variety of domains where environments consist of networked objects that need to be orchestrated.

6.4.1. Applications

HomeAssist offers an online catalog of applications. Using this catalog, the user and the caregiver determine what and how activities should be assisted by selecting the appropriate assistive applications and configuring them with respect to the user's requirements and preferences. The resulting set of applications forms a personalized assistive support. Additionally, to respond to evolving needs, our platform allows to stop/remove applications easily and to install new ones from the online catalog.

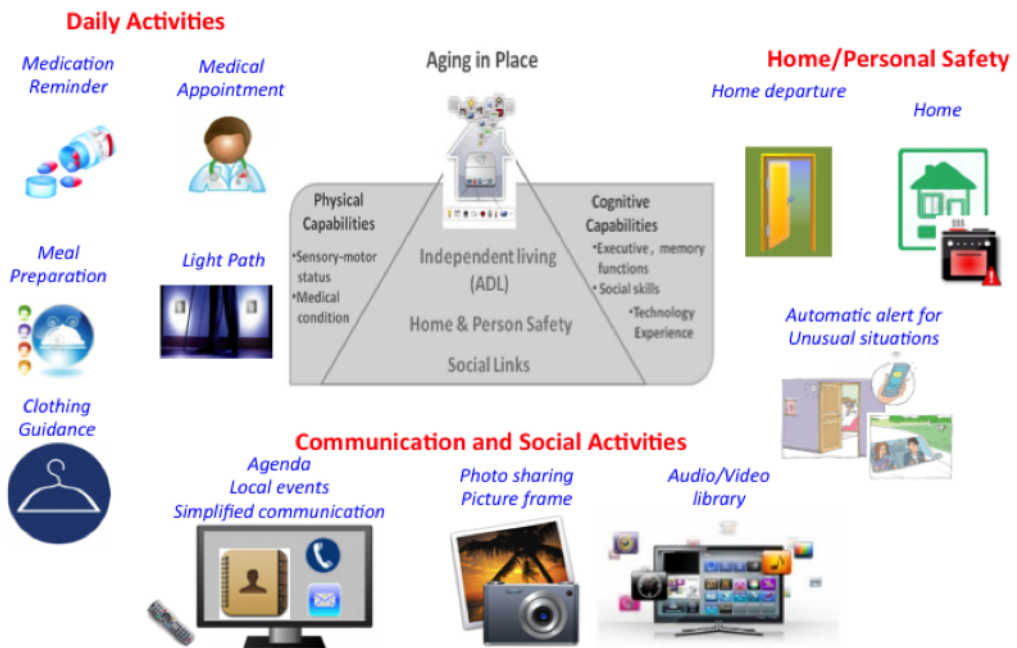


Figure 5. The HomeAssist platform and applications

This platform proposes many applications in three domains of everyday life.

Daily activities: including activity monitoring, light path, and a reminder.

Home or personal safety: including entrance monitoring, stove monitoring, and warning if no movements are detected after a certain amount of time.

Communications and social activities: including collaborative games, videoconference, information about local events, TV programming, etc.

For video presentations of HomeAssist, see the following:

- <http://videotheque.inria.fr/videotheque/media/23705>. Title: “DiaSuiteBox”, 2013.
- <http://videotheque.inria.fr/videotheque/media/29998>. Title: “DomAssist : L’assistance numérique à la personne”, 2014.

6.4.2. Devices

Several entities have been identified to deliver an assistive support. These entities include (1) technological devices: wireless sensors (motion detectors, contact sensors and smart electric switches), and two tablets, and (2) software services (agenda, address book, mail agent, and photo agent) to monitor everyday activities and propose assistive applications. Sensors are placed in relevant rooms in the house: kitchen, bedroom, bathroom, and around the entrance.



Figure 6. HomeAssist devices

FUNCTIONAL DESCRIPTION

3 mobile applications for assistive living : (1) DiAndroid : Interface for the main tablet with the DiaSuiteBox applications including those for the daily activities, the meetings scheduling, etc. and for home and personal safety; (2) Accueil : home screen restraining the use of a secondary tablet and offering communications and social activities applications with simplified communication means (ie. eMail), collaborative games, etc.; (3) eMail : mail client made for older people.

- Participants: Alexandre Spriet, Charles Consel, Helene Sauzeon and Julien Durand
- Partners: CNRS - IPB - Université de Bordeaux
- Contact: Charles Consel
- URL: <http://phoenix.inria.fr/research-projects/homeassist>

7. New Results

7.1. Tablet-Based Activity Schedule in Mainstream Environment for Children with Autism and Children with ID

Including children with autism spectrum disorders (ASD) in mainstream environments creates a need for new interventions whose efficacy must be assessed in situ. This article presents a tablet-based application for activity schedules that has been designed following a participatory design approach involving mainstream teachers, special education teachers, and school aides. This application addresses two domains of activities: classroom routines and verbal communications. We assessed the efficiency of our application with two overlapping user studies in mainstream inclusion, sharing a group of children with ASD. The first experiment involved 10 children with ASD, where five children were equipped with our tabled-based application and five were not equipped. We show that (1) the use of the application is rapidly self-initiated (after 2 months for almost all the participants) and (2) the tablet-supported routines are better performed after 3 months of intervention. The second experiment involved 10 children equipped with our application; it shared the data collected for the five children with ASD and compared them with data collected for five children with intellectual disability (ID). We show that (1) children with ID are not autonomous in the use of the application at the end of the intervention, (2) both groups exhibited the same benefits on classroom routines, and (3) children with ID improve significantly less their performance on verbal communication routines. These results are discussed in relation with our design principles. Importantly, the inclusion of a group with another neurodevelopmental condition provided insights about the applicability of these principles beyond the target population of children with ASD.

7.2. Self Determination-Based Design To Achieve Acceptance of Assisted Living Technologies For Older Adults

Providing technological support to assist older adults in their daily activities is a promising approach to aging in place. However, acceptance is critical when technologies are embedded in the user's life. Recently, Lee et al. established a connection between acceptance and motivation. They approached motivation via the Self-Determination Theory (SDT): the capacity to make choices and to take decisions. This paper leverages SDT to promote a new design style for gerontechnologies that consists of principles and requirements. We applied our approach to develop an assisted living platform, which was used to conduct a six-month field study with 34 older adults. We show that self-determination is a determining factor of technology acceptance. Furthermore, our platform improved the self-determination of equipped participants, compared to the control group, suggesting that our approach is effective. As such, SDT opens up new opportunities for improving the design process of gerontechnologies.

7.3. Frameworks compiled from declarations: a language-independent approach

Programming frameworks are an accepted fixture in the object-oriented world, motivated by the need for code reuse, developer guidance, and restriction. A new trend is emerging where frameworks require domain experts to provide declarations using a domain-specific language (DSL), influencing the structure and behaviour of the resulting application. These mechanisms address concerns such as user privacy. Although many popular open platforms such as Android are based on declaration-driven frameworks, current implementations provide ad hoc and narrow solutions to concerns raised by their openness to non-certified developers. Most widely used frameworks fail to address serious privacy leaks, and provide the user with little insight into application behaviour. To address these shortcomings, we show that declaration-driven frameworks can limit privacy leaks, as well as guide developers, independently from the underlying programming paradigm. To do so, we identify concepts that underlie declaration-driven frameworks, and apply them systematically to both an object-oriented language, Java, and a dynamic functional language, Racket. The resulting programming framework generators are used to develop a prototype mobile application, illustrating how we mitigate a common class of privacy leaks. Finally, we explore the possible design choices and propose development principles for developing domain-specific language compilers to produce frameworks, applicable across a spectrum of programming paradigms.

7.4. Analysis of How People with Intellectual Disabilities Organize Information Using Computerized Guidance

Access to residential settings for people with intellectual disabilities (ID) contributes to their social participation, but presents particular challenges. Assistive technologies can help people perform activities of daily living. However, the majority of the computerized solutions offered use guidance modes with a fixed, unchanging sequencing that leaves little room for self-determination to emerge. The objective of the project was to develop a flexible guidance mode and to test it with participants, to describe their information organization methods. This research used a descriptive exploratory design and conducted a comparison between five participants with ID and five participants with no ID. The results showed a difference in the information organization methods for both categories of participants. The people with ID used more diversified organization methods (categorical, schematic, action-directed) than the neurotypical participants (visual, action-directed). These organization methods varied depending on the people, but also on the characteristics of the requested task. Furthermore, several people with ID presented difficulties when switching from virtual to real mode. These results demonstrate the importance of developing flexible guidance modes adapted to the users' cognitive strategies, to maximize their benefits. Studies using experimental designs will have to be conducted to determine the impacts of more-flexible guidance modes.

7.5. Leveraging Declarations over the Lifecycle of Large-Scale Sensor Applications

Masses of sensors and actuators are being deployed in our daily environments to provide innovative services for such spaces as parking lots, buildings, and railway networks. Yet, to realize the full potentials of these sensor network infrastructures, services need to be developed. Service development raises a number of challenges due to existing approaches that are often low level and network/hardware-centric. This paper proposes a high-level approach to the development of large-scale orchestrating applications. It revolves around a declaration language that allows to express the sensor-network dimensions of an application (sensor discovery, delivery models, actuation process). These declarations define the behavior of an application with respect to the sensor network infrastructure. We demonstrate the key relevance of these declarations at every stage of an application lifecycle, from design to runtime. In doing so, declarations allow to match the sensor-network behavior of an application to the target infrastructure. Our approach summarizes and puts in perspective our development of industrial case studies and our experience in using a commercially-operated sensor infrastructure.

7.6. Improving the Reliability of Pervasive Computing Applications By Continuous Checking of Sensor Readings

This paper shows that context-aware applications commonly make implicit assumptions about a sensor infrastructure. Because context-awareness critically relies on these assumptions, the developer typically need to ensure their validity by encoding them in the application code, polluting it with non-functional concerns. This defensive programming approach can be avoided by formulating these assumptions aside from the application, thus factorizing them as an explicit model of the sensor infrastructure. This model can be expressed as a set of rules and can be checked automatically and continuously to ensure the reliability of a sensor infrastructure, both at installation time and during normal functioning. The usefulness of our approach is demonstrated in the domain of assisted living for seniors. We applied it to sensor data collected in the context of a 9-month field study of an assisted living platform, deployed at the home of 24 seniors. We show that several kinds of sensor malfunctions could have been identified upon their occurrence, thanks for our continuous checking, and resolved.

7.7. Designing Parallel Data Processing for Large-Scale Sensor Orchestration

Masses of sensors are being deployed at the scale of cities to manage parking spaces, transportation infrastructures to monitor traffic, and campuses of buildings to reduce energy consumption. These large-scale infrastructures become a reality for citizens via applications that orchestrate sensors to deliver high-value, innovative services. These applications critically rely on the processing of large amounts of data to analyze situations, inform users, and control devices. This paper proposes a design-driven approach to developing orchestrating applications for masses of sensors that integrates parallel processing of large amounts of data. Specifically, an application design exposes declarations that are used to generate a programming framework based on the MapReduce programming model. We have developed a prototype of our approach, using Apache Hadoop. We applied it to a case study and obtained significant speedups by parallelizing computations over twelve nodes. In doing so, we demonstrate that our design-driven approach allows to abstract over implementation details, while exposing architectural properties used to generate high-performance code for processing large datasets.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Grants with Industry

Funding for the DomAssist500 project was obtained from the following industrial partner: AG2R La Mondiale.

9. Partnerships and Cooperations

9.1. Regional Initiatives

9.1.1. *Independent living with intellectual disabilities – ANDDI – 2014 - 2017*

ANDDI leverages the abilities of individuals with ID and the recent technological advances to develop a variety of assistive services addressing their daily needs. These services draw on our expertise in cognitive science and computer science, dedicated to assisting users with technologies. In particular, we use our platform, named HomeAssist, dedicated to the independently living of older adults. This project is funded by the Region of Aquitaine.

9.1.2. Platform for Assisted Living – HomeAssist 24 – 2013 – 2016

The objective of this project is to provide an open platform of digital assistance dedicated to aging in place. This project is in collaboration with researchers in Cognitive Science (University of Bordeaux) and the UDCCAS Gironde (Union Départementale des Centres Communaux d'Action Sociale) managing elderly care. This project includes a need analysis, the development of assistive applications and their experimental validation. To validate HomeAssist 24 homes of older adults are equipped during 9 months, and matched with 24 control, non-equipped participants. This work is funded by CARSAT, the Region of Aquitaine, and the District of Gironde.

9.1.3. Populational Study of HomeAssist – HomeAssist 500 – 2015 - 2017

We conduct a Randomized Controlled Trial (RCT) of HomeAssist with older adults, ranging from autonomous to mildly cognitively impaired (e.g., Alzheimer disease (AD) in its early stage). The RCT is considered as the gold standard of a true experimental design. Furthermore, it provides strong evidence for causal relationships, as well as the ability to generalize the results to people outside the study's sample. The study design will thus be a single-blinded RCT. It will include up to 500 participants, matched with non-equipped participants. The HomeAssist intervention will involve monitoring as well as compensation services to support independent living in place. The duration of the HomeAssist intervention is of 12 months. This project is funded by the Region of Aquitaine, the Districts of Gironde and Pyrénées Atlantique, CARSAT Aquitaine, UDCCAS, and CNSA.

9.2. National Initiatives

9.2.1. School Inclusion for Children with Autism

The objective of this project is to provide children with assistive technologies dedicated to the school routines. This project is in collaboration with the “Handicap et Système Nerveux” research group (EA 4136, Bordeaux University), the PsyCLÉ research center (EA 3273, Provence Aix-Marseille University) and the “Parole et Langage” research laboratory (CNRS, Provence Aix-Marseille University).

This work is funded by the French Ministry of National Education and Orange Foundation.

9.3. International Initiatives

9.3.1. Participation in Other International Programs

- Cooperation program with UB-University of Waterloo-Canada — Aging (2015-16), Coordinated by M. Fernandes and H. Sauzéron.
- International exchange program IDEX (2016-17) — Pr. Luc Noreau, Centre Interdisciplinaire de Recherche en réadaptation et intégration sociale-University of Laval, Canada. Coordinated by P. Dehail.
- Mobility program IDEX UB-University of Waterloo, Canada — Aging (2016-17), Coordinated by M. Fernandes and H. Sauzéron.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

10.1.1.1. Member of the Organizing Committees

Hélène Sauzéron was member of the organizing committee of the workshop “Journées d'étude du vieillissement cognitif”, Bordeaux, 2016.

10.1.2. Scientific Events Selection

10.1.2.1. Member of the Conference Program Committees

Charles Consel was member in the PC of the IEEE 2nd International Conference on Collaboration and Internet Computing (CIC 2016).

Hélène Sauzéron was member in the PC of the workshop “Journées d’étude du vieillissement cognitif”, Bordeaux, 2016.

10.1.3. Journal

10.1.3.1. Reviewer - Reviewing Activities

Hélène Sauzéron was solicited as a reviewer for the Journal of Cognitive Psychology and the British Journal of Psychology.

10.1.4. Invited Talks

Charles Consel gave the following invited talks:

- Invited talk on HomeAssist at ORCATECH, Oregon Health and Science University, Portland, USA. August 2016.
- Invited talk on “DiaSwarm – Orchestration of Masses of Sensors at the International Conference on Software & Systems Engineering and their Applications”, Paris, France. May 2016.
- Invited talk on “DiaSwarm – Orchestration of Masses of Sensors” at Northeastern University, Boston, USA. May 2016.
- Invited talk on “DiaSwarm – Orchestration of Masses of Sensors” at Galois Inc., Portland, USA. August 2016.
- Invited talk on HomeAssist at “Journées Inria Industries” entitled “Interaction avec les objets et services numériques”, Tourcoing, France. Nov 2016.

Hélène Sauzéron gave the following invited talks:

- “Assistance numérique pour la cognition sociale pour favoriser l’inclusion scolaire d’enfants avec troubles du développement” at 43èmes Entretiens de Médecine Physique et de Réadaptation (EMPR), held on March 25th 2015 in Montpellier, France.
- “La cognition sociale au-delà du cerveau : une cognition inclusive” at 43èmes Entretiens de Médecine Physique et de Réadaptation (EMPR), held on March 25th 2015 in Montpellier, France.
- “HomeAssist : An Assisted Living Platform for Aging in Place Based on an Interdisciplinary Approach”, at WORRKSHOP ACCEPT16- Deuxièmes rencontres interdisciplinaires autour des aides techniques, du handicap cognitif et de la perte d’autonomie, held on October 6-7, in Nîmes, France.
- “Everyday cognition, Aging and Cognitive disorders: insights and opportunities provided by Information and Communication Technologies”, at Scientific seminar of Dpt. of Psychology, University of Waterloo, on 18th Jul., 2016, Waterloo, Canada.

10.1.5. Research Administration

Hélène Sauzéron is associate director of the lab “Activité, handicap, cognition et système nerveux”, since 2015, where she leads the Cognitive Handicap research axis.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

Licence: H  l  ne Sauz  on, “General Cognitive Psychology”, 18h, L2/L3, University of Bordeaux, France

Licence: H  l  ne Sauz  on, “Cognitive Neuropsychology”, 7h, DU, University of Bordeaux, France

Master: H  l  ne Sauz  on, “Cognitive Fonctions in Context”, “Technologies for Handicap and Autonomy”, “Virtual Reality and Health Applications”, 60h, M1/M2, University of Bordeaux, France

Master: Charles Consel, “Telephony Over IP”, 43h, M2, Bordeaux INP, France.

Master: Charles Consel, “Software Engineering for Smart Spaces”, 10h, M2, Bordeaux INP, France.

Master: Charles Consel, “Ubiquitous Computing”, 10h, M2, Bordeaux INP, France.

10.2.2. Supervision

Charles FAGES, “Design and Experimental Validation of a Technological Assistant for School Inclusion of Children with Autism Spectrum Disorders in Mainstream Classrooms”, University of Bordeaux, defended on May 30th 2016, co-directed by H  l  ne Sauz  on and Charles Consel.

Lucile DUPUY, “Design and validation of a home-based digital assistant for seniors with slight autonomy decline”, University of Bordeaux, defended on November 30th 2016, co-directed by H  l  ne Sauz  on and Charles Consel.

C  cile MAZON, “Personalization and evaluation of a digital assistant for school inclusion of college students with autism and/or intellectual disability”, University of Bordeaux, started in September 2016, co-directed by H  l  ne Sauz  on and Charles Consel.

P.A. CINQUIN, “Design and validation of a reader accessible to persons with cognitive troubles for a e-learning system”, University of Bordeaux, started in September 2016, co-directed by H  l  ne Sauz  on and Pascal Guitton.

10.2.3. Juries

H  l  ne Sauz  on was member of the thesis committee for:

- Lucile Burger, for her thesis in Psychology called “Effect of training executive functions on appropriate usage of memory strategies during ageing : a behavioural and electrophysiological study”, University of Tours, on December 9 2016.
- Caroline Pigeon, for her thesis in Neuropsychology called “Mobilisation attentionnelle des pi  tons aveugles : Effets de l’  ge, de l’ant  riorit   de la c  cit   et de l’aide    la mobilit   utilis  e”, University of Lyon 2, on December 6th 2016.

Nic Volanschki was member of the thesis committee for Milan Kabac for his thesis in Computer Science called “A Design-Driven Methodology for the Development of Large-Scale Orchestrating Applications”, University of Bordeaux, on September 26th 2016.

10.3. Popularization

H  l  ne Sauz  on gave talks to the following events for professional or general audiences:

- “Handicaps et technologies d’assistance pour les personnes avec d  ficiences cognitives” at “Les outils num  riques au service des personnes avec autisme”, on October 7th, at H  pital de Niort, France.
- “Pr  sentation de la solution DomAssist et ses effets sur le fonctionnement quotidien de la personne et ses aidant professionnel” at “Territoire et solidarit   entre les   ges : accompagnement du bien vieillir”, organised by Union R  gionale des F  d  rations des Centres Sociaux d’Aquitaine, on November 14th, in Lormont, France.
- “Coll  ge + : un nouvel outil d’apprentissage”, at Semaine de la m  moire, organised by Observatoire B2V, on September 21st, at Mus  e CapScience, Bordeaux, France.

Nic Volanschi participated on October 13th to the “Science fest” at Inria Bordeaux, where he gave 4 workshop sessions on “Manual digital sciences” for children aged 11 to 15. These workshop sessions are aimed to communicate basic notions of computer science to young students by using manual games.

11. Bibliography

Major publications by the team in recent years

- [1] E. BALLAND, C. CONSEL, H. SAUZÉON, B. N’KAOUA. *A Case for Human-Driven Software Development*, in "ICSE'13: Proceedings of the 35th International Conference on Software Engineering (NIER track)", San Francisco, United States, May 2013, <http://hal.inria.fr/hal-00814296>.
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Team PLEIADE

From patterns to models in computational biodiversity and biotechnology

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
Computational Biology

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Team PLEIADE

Creation of the Team: 2015 January 01

Keywords:

Computer Science and Digital Science:

- 3.1. - Data
- 3.2. - Knowledge
- 3.3.2. - Data mining
- 3.3.3. - Big data analysis
- 3.4. - Machine learning and statistics
- 6.1.4. - Multiscale modeling
- 6.2.8. - Computational geometry and meshes

Other Research Topics and Application Domains:

- 1.1.6. - Genomics
- 1.1.9. - Bioinformatics
- 1.1.11. - Systems biology
- 1.1.12. - Synthetic biology
- 1.2. - Ecology
- 3. - Environment and planet

PLEIADE is located in two sites: Inria Bordeaux Sud-Ouest on the Talence campus of the Université de Bordeaux and INRA Pierroton.

1. Members

Research Scientists

David Sherman [Team leader, Inria, Senior Researcher, HDR]
Pascal Durrens [CNRS, Researcher, HDR]
Alain Franc [INRA, Senior Researcher]
Stephanie Mariette [INRA, Researcher, until Aug 2016]

Technical Staff

Redouane Bouchouirbat [INRA]
Philippe Chaumeil [INRA]
Jean-Marc Frigerio [INRA]
Franck Salin [INRA]

Administrative Assistants

Cecile Boutros [Inria]
Anne-Laure Gautier [Inria, until Feb 2016]

Others

Arthur Demene [Univ. Bordeaux, from Mar 2016]
Christian Dutech [INRA, Researcher, from Feb 2016]
Razanne Issa [Univ. Bordeaux]
Adrien Lopez [Min. de l'Éducation Nationale, Feb 2016]
Remi Pellerin [Inria, from Jun 2016 until Jul 2016]
Anna Zhukova [Institut Pasteur, until Jun 2016]

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 [35] 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 exploiting diversity data are still not adapted to high throughput data production. A better connection is 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.

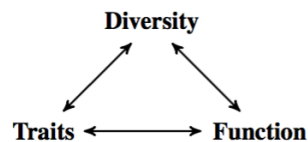


Figure 1. Diversity informs both the study of traits, and the study of biological functions. The double challenge is to measure these links quickly and precisely with pattern recognition, and to explore the relations between diversity in traits and diversity in function through modeling.

PLEIADE links pattern recognition with modeling 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.

3. Research Program

3.1. Distances and pattern recognition

Diversity may be understood as a set of dissimilarities between objects. The underlying mathematical construction is the notion of distance. Knowing a set of objects, on the condition that pairwise distances can be measured, it is possible to build a Euclidan 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. It is still true that the reference for recognizing patterns or shapes is the human eye. One objective of our project is to narrow the gap between the story that a human eye can read, and the story that an algorithm can tell. Several directions will be explored. First, it is necessary to master dimension reduction, mainly classical algebraic tools (PCA, NGS, Isomap, eigenmaps, etc ...), and collaborate with experts in efficient methods in spectral methods. Second, a neighborhood in a point cloud naturally leads to graphs describing the neighborhood networks. There is a natural link between modular structures in distance arrays and communities on graphs. Third, points defined by DNA sequences

(for example) are samples of diversity. Dimension reduction may show that they live on a given manifold. This leads to geometry (differential or Riemannian geometry). Knowing some properties of the manifold can inform us about the constraints on the space where the measured individuals live. The connection between Riemannian geometry and graphs, where weighted graphs are seen as meshes embedded in a manifold, is currently an active field of research [33], [32].

To resolve these objectives computationally will require investment in research directions in computational geometry (such as convex hulls of high-dimension sets of points), on circumventing the curse of dimensionality, and on linking distance geometry with convex optimization procedures through matrix completion. None of these questions is trivial: most recent work has focused on two or three dimensions, for example for image analysis or for reconstruction of protein conformation from local distances between atoms. The methodological goal is to extend these approaches to higher dimension spaces.

3.2. Modeling by successive refinement

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 [17]. 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* [14] 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 certain kinds of systems in biotechnology [2], [18] and medicine [16]. 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 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 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).

4.2. 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 Eukaryotes) 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 grapevine, 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 disassemble 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 [22]. About one decade ago, some works [30] 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 developing graph-based models of co-occurrence 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 addressed 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 [28]. 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 [25]. Several approaches were proposed to correct for paralogy, either by working directly on the sequences issued from mapped reads [25] 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 [15]. 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. Biotechnology

In collaboration with MIAT INRA and UMR 5234 CNRS/Université de Bordeaux, PLEIADE assembled and analyzed *Clavispora lusitaniae*, an ubiquitous environmental ascomycetous yeast that can be pathogenic and is responsible for invasive candidiasis in pediatric and onco-haematology patients [24].

In collaboration with UMR 5200 CNRS/Université de Bordeaux, PLEIADE assembled and analyzed transcriptomes from three tissues of the oil palm tree *Elaeis guineensis* Jacq., whose mesocarp contains oil up to 90% of its dry weight. Our goal is to increase, by synthetic biology approaches, the yield in oil for crops grown in Europe. The yield and the composition of oil measured from wild-type palm tree specimens varies dramatically, indicating a high level of bio-diversity.

5.1.2. Biodiversity

PLEIADE and the HIEPACS team developed connections between random projection methods and multi-dimensional scaling, in order to compute eigenvectors and eigenvalues in space of reasonable dimension. The method for MDS developed by Pierre Blanchard has proved to be surprisingly efficient and precise. It was presented at PASC 2016 Lausanne. This work improves the analysis of microbial communities, where the shape of the point cloud built from pairwise distances between a large set of NGS reads is used to describe the diversity of the community.

6. New Software and Platforms

6.1. Magus

KEYWORDS: Bioinformatics - Genomic sequence - Knowledge database

FUNCTIONAL DESCRIPTION

Comparative genomics requires efficient and scalable tools for managing knowledge about genomes, genes, and the high-dimensional relations between them.

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.

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.

- Participants: David Sherman, Pascal Durrens
- Partners: CNRS - INRA - Université de Bordeaux
- Contact: David James Sherman
- URL: <http://magus.gforge.inria.fr>

6.2. 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. The software creates a 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 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. The resulting map can be explored on-line, or downloaded in a COMBINE archive.

- Participants: Anna Zhukova and David James Sherman
- Contact: David James Sherman
- URL: <http://mimoza.bordeaux.inria.fr/>

6.3. Pantograph

KEYWORDS: Systems Biology - Bioinformatics - Genomics - Gene regulatory networks

FUNCTIONAL DESCRIPTION

Pantograph is a software toolbox to reconstruct, curate and validate genome-scale metabolic models. It uses existing metabolic models as templates, to start its reconstructions process, to which new, species-specific reactions are added. Pantograph uses an iterative approach to improve reconstructed models, facilitating manual curation and comparisons between reconstructed model's predictions and experimental evidence.

Pantograph uses a consensus procedure to infer relationships between metabolic models, based on several sources of orthology between genomes. This allows for a very detailed rewriting of reaction's genome associations between template models and the model you want to reconstruct.

- Participants: Nicolas Loira, Anna Zhukova, David James Sherman and Pascal Durrens
- Partner: University of Chile
- Contact: Nicolas Loira
- URL: <http://pathtastic.gforge.inria.fr/>

6.4. BioRica

KEYWORDS: Systems Biology - Bioinformatics - Hierarchical models - Hybrid models - Stochastic models

FUNCTIONAL DESCRIPTION

BioRica is used to mathematically describe the behavior of complex biological systems.

It is a software platform that permits simulation of biological systems on the basis of their description. It allows one to reuse existing biological models and to combine them into more complex models.

- Partner: University of Chile
- Contact: David Sherman
- URL: <http://biorica.gforge.inria.fr/>

6.5. Declic

Metabarcoding relies on mapping large sets of reads on reliable databases, with taxonomically annotated sequences. Declic facilitates data analyses for metabarcoding.

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

6.6. Platforms

6.6.1. Plafrim

Plafrim (<http://plafrim.fr>) is an essential instrument for PLEIADE. We use it for developing software data analysis methods and evaluating them at real world scale. The platform combines considerable computing power with excellent support, both in terms of the quality of the interactions with the local staff and of the ease of large-scale data transfer between Plafrim and PLEIADE's data storage infrastructure. Plafrim facilitates collaboration between team members who are not in the Bordeaux Sud-Ouest building, and furthermore allows us to share best practices and tools with other teams from the Center.

6.6.2. Inria forge and Inria continuous integration

The Inria forge (<http://gforge.inria.fr>) provides a secure collaboration platform for software project administration and source code management, and Inria's continuous integration platform (<http://ci.inria.fr>) provides a cloud-based service for automatic compilation and testing of software systems. PLEIADE uses these two services extensively for agile software development. The continuous integration platform allows us to verify the correct operation of our methods in different operating system and deployment environments.

6.6.3. Team Platform

PLEIADE maintains a dedicated computing platform for software development and experimentation by the team, comprised of a private cloud, storage, and a Project Atomic cluster for hosting Docker containers

7. New Results

7.1. *Clavispora lusitaniae* genome

Clavispora lusitaniae is an ubiquitous environmental ascomycetous yeast, with no known specific ecological niche. It can be isolated from different substrates, such as soils, waters, plants, and gastrointestinal tracts of many animals including birds, mammals and humans. In immunocompromised hosts, *C. lusitaniae* can be pathogenic and is responsible for about 1% of invasive candidiasis, particularly in pediatric and onco-haematology patients [24].

So far, two strains have had their genomes sequenced: ATCC 42720, isolated from the blood of a patient with myeloid leukemia [29], and MTCC 1001, a self-fertile strain isolated from citrus [27]. We performed the genome assembly of the *C. lusitaniae* type strain CBS 6936 [37], isolated from citrus peel juice.

Illumina sequences were obtained by our collaborator (T. Noel, UMR 5234 CNRS Université Bordeaux) and we ran the assemblies using several assemblers, e.g. MINIA [21], MIRA [20] and SPAdes [19]. Each assembly gave sequence scaffolds colinear with the already sequence genome of ATCC 42720. However the number of scaffolds varied dramatically in assemblies. SPAdes gave the best results by an order of magnitude (MINIA: 2913, MIRA: 930, SPAdes: 53). This last assembly will serve as a basis for further experiments and SNP detections in mutants strains derived from CBS 6936.

This work is a collaboration between Pleiade team, UMR 5234 CNRS/Université de Bordeaux, and MIAT INRA.

7.2. *Elaeis guineensis* transcriptome

The mesocarp of the oil palm tree (*Elaeis guineensis* Jacq.) contains oil up to 90% of its dry weight and is the oil richest known vegetal tissue [23]. Our goal is to understand how this tissue achieves this result, in order to increase, by synthetic biology approaches, the yield in oil for crops grown in Europe. In a first milestone, oil palm tree genes relevant for oil synthesis from fatty acids will be transiently expressed in tobacco leaves.

In order to select relevant gene candidates, we performed transcriptome assemblies on high quality Illumina sequences. As an annotated genome is available [34], we performed genome-guided assemblies with TRINITY assembler [26]. The sequence reads (total 300 millions) came from 5 RNA independent isolates from 3 tissues: leaf (2 isolates), kernel (1 isolate) and mesocarp (2 isolates). Transcriptomes coming from duplicate isolates show a good level of overlap as regards the predicted transcripts.

Using expression specificity, abundance and transcript annotation from the genome, we selected genes or transcript isoforms candidates, as well as transcription factors. A set of 19 sequences has been retained for expression in tobacco leaves and is under genetic engineering processing.

The 5 transcriptomes were fused into a pan-transcriptome which will be used in another angle of the project. The yield and the composition of oil measured from wild-type palm tree specimens varies dramatically, indicating a high level of bio-diversity. We are currently doing a sampling campaign in Africa, RNA extracts will be sequenced and compared to our pan-genome to serve in variant detection (SNPs) and association genetics studies.

This work is a collaboration between Pleiade team and UMR 5200 CNRS/Université de Bordeaux.

7.3. A Geometric View of Diversity

Diversity may be understood as a set of dissimilarities between objects. The underlying mathematical construction is the notion of distance. Knowing a set of objects, on which pairwise distances can be measured, it is possible to build a Euclidean image of it as a point cloud in a space of relevant dimension. The objects under study are microbial communities, given as a set of reads produced by NGS technologies. Distances between specimen are computed as genetic distances between associated reads (so called amplicon approach). Then, the diversity of a community can be associated with the shape of the point cloud built from such distances. Such an embedding is classically implemented by MDS (Multidimensional Scaling). Such an approach triggers two methodological questions, addressed in 2016:

- the numerical solution is through finding the eigenvectors and eigenvalues of a large, full, symmetric matrix. Current algorithm, parallelized or not, are in complexity $\mathcal{O}(n^3)$ if n is the number of specimen on which to study patterns of diversity, i.e. the size of the matrix. This is not feasible for dataset produced by NGS technologies, which can assemble 10^5 to 10^6 sequences. We have set up a collaboration with a PhD student in HIEPACS Team (Inria Bordeaux SO), Pierre Blanchard, to develop a connection between random projection methods and MDS. Random Projection Methods are methods relying on Johnson-Lindenstrauss Lemma, which states that the likelihood that the

distances are very well conserved is very high when projecting a point cloud in a space of very large dimension (say n) to a random space of large dimension (say, proportional to $\text{Log } n$). This permits to compute eigenvectors and eigenvalues in space of reasonable dimension. The method for MDS has been studied by Pierre Blanchard, under supervision by Olivier Coulaud and Alain Franc, and proved to be surprisingly efficient and precise. This work builds one chapter of the PhD thesis of P. B. to be defended by early 2017. This collaboration has led to a joint poster at Platform for Advanced Scientific Computing (PASC), June 2016, Lausanne, Switzerland.

- The eigenvalues of the matrix under study can be positive or negative. Positive eigenvalues lead to Euclidean structure behind MDS. Classically, negative eigenvalues are ignored. We have begun a study on the role of negative eigenvalues in the discrepancy between Euclidean distances computed between points in MDS, and genetic distances between reads produced by NGS, which adds to the well understood discrepancy in MDS due to dimension reduction. This has led to three seminars or presentations:
 - a seminar at MIAT research Unit, Toulouse, on February 19
 - a seminar at LABRI on April, 28
 - a presentation at the days of mathematics and computing sciences organized by MIA INRA division (INRA global meeting), on October, 5

These three events have permitted to “polish” the analysis of the problem through several exchanges, and to orientate its study towards quadratic embedding, or isometry into pseudo-euclidean spaces.

7.4. Topological Data Analysis

Leyla Mirvakhabova has defended and obtained her BSc memoir on "Distance geometry and biodiversity patterns" at the Department of Mathematics of the National Research University - Higher School of Economics, Moscow. Here is the abstract: In this work, we study the biodiversity of the tree species in French Guiana. We consider the matrix of the pairwise genetic distances between the 1501 species. The distances are measured by using the Smith-Waterman algorithm applied to the trnH regions - the chloroplasts of trees. The aim of the project is to analyze the shape of a point cloud in a Euclidean space built from the pairwise distances. To study the structure of the point cloud built from the given distances, we have considered the following methods: Hierarchical Clustering, Multidimensional Scaling (MDS), Nonlinear Mapping (NLM), t-Distributed Stochastic Neighbor Embedding (t-SNE), and Topological Data Analysis (TDA). For the first four methods, we used the Python package scikit-learn 0.17.1 implementations and have written the program for the TDA algorithm. All of these methods were tested on the given dataset. This work has been performed as part of a collaborative research project of the PLEIADE team in the Inria Bordeaux – Sud-Ouest (supervisor Alain Franc) with the Laboratory of System Biology and Computational Genetics in the Vavilov Institute of General Genetics (supervisor Ivan Kulakovskiy).

7.5. Bespoke tools for comparative genomics

Large-scale comparison of strains of cell factory species is an indispensable tool for understanding the genetic origin of phenotypic variability, and can considerably optimize the selection and construction of high-performing industrial strains. For example, in oenological applications new strains may be selected based on their influence on aroma, their adaptation to grape musts, or their robustness during fermentation. In oil production applications, new strains may be selected based on their yield, or on the saturation degree of the lipids, or on their growth characteristics. Comparative genomics has proven quite effective in understanding cell factory diversity [1], [6], [5], [36], [31]. A typical project will involve 500 segregants and 50 genomes. Accurate and rapid analysis of the concomitant data volumes requires efficient tool sets that must be adapted to the real use cases of the industrial application.

PLEIADE addresses this problem through the definition of bespoke software systems that associate integrated sets of tools, including its Magus software platform (section 6.1). A key challenge in defining this kind of integrated system is the need to connect the components. We develop configuration formalisms whose solutions are orchestrations of weakly-coupled microservices running in independent containers. These services may be data banks, genome browser and visualization software, workflow tools like Galaxy, machine learning algorithms for classification, or shared workbooks like Jupyter or Zeppelin. By formalizing the connections between services, we can simplify deployment, and also create an opportunity for *continuous deployment*.

8. Partnerships and Cooperations

8.1. National Initiatives

8.1.1. ANTICOR – Biocontamination in aircraft reservoirs

ANTICOR is an industrial-academic research and development working group coordinated by Dassault Aviation, investigating the causes of microbial contamination in aircraft reservoirs and aimed at developing mitigating procedures and equipment. Previous results have shown that this contamination forms biofilms at the fuel-water interface and is comprised of complex communities of hundreds of bacterial and fungal species. PLEIADE is particularly interested in measuring and modeling these communities, especially as concerns understanding how they change based on environmental conditions and on reservoir geometry.

8.1.2. CAER – Alternative Fuels for Aeronautics

CAER is a 6 M-Euro contract with the Civil Aviation Directorate (Direction Générale de l'Aviation Civile, DGAC), coordinated by the French Petroleum Institute (Institut français de pétrole-énergies nouvelles, IFPEN) on behalf of a large consortium of industrial (EADS, Dassault, Snecma, Turbomeca, Airbus, Air France, Total) and academic (CNRS, INRA, Inria) partners to explore different technologies for alternative fuels for aviation. PLEIADE's role concerns the genomics of highly-performant oleaginous microorganisms.

8.2. International Initiatives

8.2.1. Supervised clustering

One way to build an inventory in a community on a molecular basis is to map unknown reads onto a taxonomically annotated reference database. We (AF, PC, JMF, FS) have developed a cooperation with UMR Carrel (A. Bouchez, F. Rimet) and SLU at Uppsala (Sweden, M. Kahlert) for industrializing molecular based inventories from data production (NGS facilities, PGTB, Pierroton) to data analysis. Molecular based inventories of about 200 samples have been done, for diatoms Mayotte rivers, and the same number for diatoms in Fennoscandian rivers. The method has been published in [13]. As far as those tools and metagenomics are concerned, a complementary partnership has been established with UMR BioGER (V. Laval) on metabarcoding of fungal communities.

8.2.2. Metagenomics for zoonoses

In the framework of CEBA Cluster of Excellence (Centre d'Etude de la Biodiversité Amazonienne), Pleiade team has been successful in an application for being part of a so called long term strategic project (2017-2019) called microbiome, chaired by Institut Pasteur in Cayenne and UMR MIVEGEC (CNRS-IRD) at Montpellier. The role of the team is twofold: (i) develop methods for metabarcoding of viral and bacterial communities in some hosts (bats, birds, ...) and (ii) run some data analysis for scaling up from microbiomes to landscape ecology, having in mind the dilution effect, i.e. pristine forest offer a better protection against disease spread than disturbed ones. The project starts on January 1, 2017.

8.2.3. Historical biogeography of plant families

In the framework of CEBA too, AF and David Sherman have worked in providing some tools for mapping paleoclimatic conditions on the Earth over geological times, elaborating on datasets of paleoclimates produced by running General Circulation Models (work done by UMR LSCE, Orsay, in a previous ANR project lead by AF). These maps will be part of a collaboration established with The Royal Botanical Gardens at Kew (UK) and several Brazilian Universities in a joint project on historical biogeography of Myrtaceae, a large family of trees and shrubs, well developed in the Neotropics. A. Franc has been visiting E. Lucas, at Kew Botanical gardens, in March 2016 for setting up a cooperation. A first workshop has been organized by F. Salgeiro and AF at Rio in May 2016. The next one will be held in August 2017, organized by E. Lucas and coll. An open access paper on historical biogeography of the genus *Quercus*, in collaboration with University of Padova and Museum of Natural History of Stockholm, is [11].

8.2.4. Informal International Partners

PLEIADE collaborates with Rodrigo Assar of the Universidad Andrés Bello, and Nicolás Loira and Alessandro Maass of the Center for Genomic Regulation, in Santiago de Chile (Chile). Our focus is inference of metabolic and regulatory models by comparative genomics, and their description using stochastic transition systems.

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.

9.1.1.2. Reviewer - Reviewing Activities

Alain Franc has been reviewing in 2016 manuscripts for BMC Evolutionary Biology, Nature reports, Methods in Ecology and Evolution, Research in Microbiology, Molecular Ecology.

9.2. Teaching - Supervision - Juries

9.2.1. Juries

A. Franc has been supervisor of PhD Thesis of François Keck, UMR Carrel, Thonon, Grenoble University, with Agnès Bouchez and Frédéric Rimet as co-supervisors. The PhD has been defended on April, 26, 2016. Reference: <https://www.theses.fr/196768691>. The topic is the use of phylogenetic signal for improving the assessment of water quality from inventories of diatoms. Three papers have been published by François Keck [7], [8], [9].

A. Franc has been

- member of the committee of the PhD of Cyril Noël at IPREM, University of Pau and Pays de l'Adour (PhD advisor: Cristiana Cravo-Laureau)
- reviewer of the HdR of Jean-Daniel Bontemps on large scale forest growth models, University of Nancy
- reviewer of the HdR of Benoit de Thoisy, University of Cayenne, on “from Pleistocene to likely to the dawn of the sixth extinction crisis: the tormented history of Amazonian mammals”.
- member of the jury for PhD defense of Arielle Salmier, University of Cayenne, on the response of chiroptera to changing environment: viral diversity and adaptation, at Cayenne on December, 13, 2016.

D. Sherman was president of the jury for Claire Capdevielle in the University of Bordeaux on Novembre 3, 2016.

D. Sherman was president of a first-year jury for the Mathematics and Computer Science Doctoral School at the University of Bordeaux.

9.2.2. Internships

Rémi Pellerin of the ENS Lyon was an intern in PLEIADE during June–July 2016, and contributed to Declic, a software package written in Python by A. Franc that provides several tools for data analysis, in the domains of multivariate data analysis, machine learning, and graph based methods. It permits users to study in depth the accuracy of the dictionary between molecular based and morphological based taxonomy.

Adrien Lopez of the Collège Henri Brisson in Talence spent a week in PLEIADE for his “stage du troisième”.

9.3. Popularization

David Sherman participated in popularization activities based on Thymio-II mobile robots for education, coordinated by the Mobsya association and EPFL (Switzerland). He helped organize a team in the R2T2 event (<http://r2t2.org>) on November 2, 2016. He contributed code to the Aseba project for piloting Thymio-IIs from the Scratch programming language, and with Thibault Lainé of Inria Bordeaux Sud-Ouest helped improve a photo-realistic simulator for multiple robots.

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Team POSET

Modèles pour la Programmation Structurée de l'Espace et du Temps

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
Embedded and Real-time Systems

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Team POSET

Creation of the Team: 2015 January 01, end of the Team: 2016 December 31

Keywords:

Computer Science and Digital Science:

- 1.2.5. - Internet of things
- 1.3. - Distributed Systems
- 1.5.2. - Communicating systems
- 2.1. - Programming Languages
- 2.1.1. - Semantics of programming languages
- 2.1.10. - Domain-specific languages
- 2.2.1. - Static analysis
- 2.3.3. - Real-time systems
- 2.5. - Software engineering
- 2.5.1. - Software Architecture & Design
- 2.5.2. - Component-based Design
- 5.1.1. - Engineering of interactive systems
- 5.1.7. - Multimodal interfaces
- 5.2. - Data visualization
- 5.4.4. - 3D and spatio-temporal reconstruction
- 5.5.1. - Geometrical modeling
- 5.5.4. - Animation
- 5.7.2. - Music
- 5.7.4. - Analysis
- 5.7.5. - Synthesis
- 6.1.3. - Discrete Modeling (multi-agent, people centered)
- 7.4. - Logic in Computer Science
- 7.5. - Geometry, Topology
- 7.6. - Computer Algebra
- 7.14. - Game Theory

Other Research Topics and Application Domains:

- 6.1.1. - Software engineering
- 6.4. - Internet of things
- 6.6. - Embedded systems
- 9.1.1. - E-learning, MOOC
- 9.2.1. - Music, sound
- 9.4.1. - Computer science
- 9.4.2. - Mathematics
- 9.5.10. - Digital humanities
- 9.6. - Reproducibility
- 9.7. - Knowledge dissemination
- 9.7.1. - Open access

1. Members

Faculty Members

David Janin [Team leader, Bordeaux INP, Associate Professor, HDR]
Myriam Desainte-Catherine [Bordeaux INP, Professor, HDR]
Anne Dicky [Univ. Bordeaux, Associate Professor]
Sylvain Salvati [Univ. Lille I, Professor, HDR]

Technical Staff

Jaime Eduardo Arias Almeida [Inria]

PhD Students

Simon Archipoff [Univ. Bordeaux]
Jean-Michaël Celerier [CIFFRE, Blue Yeti]
Etienne Dubourg [Univ. Bordeaux, until Aug 2016]
Pauline Mouawad [Univ. Bordeaux]

Administrative Assistants

Sabine Delarboulas Cusin [INRA]
Anne-Laure Gautier [Inria]

Other

Edwin Buger [Intermittent du spectacle]

2. Overall Objectives

2.1. Overall Objectives

How to capture, analyse, mix, combine or transform temporal media streams as varied as sounds, animations, melodies, videos, control gestures? Modern technologies make it possible to produce complex multimodal artistic computerized systems, but require the support of specially trained technicians to turn artistic intentions into technical realizations. Since modern system designers are more often artists than software developers, we aim at developing system design tools directly accessible to the artists.

In this project, we try to offer simple, uniform formalisms and tools for the representation and the manipulation of temporal media streams. This is achieved by developing new models for the hierarchical and modular design of interactive timed systems, and applying these models to the realization of artistic interactive applications. Our concrete experiments, guided by formal models challenged by experimental needs, ensure the adequacy and the robustness of our proposals.

The resulting software methodologies and design tools for the creation of interactive pieces of art should be user-friendly and robust. In particular, the resulting technical constraints should no longer hide the inadequacy of ad hoc and immature interfaces, but address critical issues such as the coherence and compatibility of design objectives .

Remark: the PoSET Inria team was created on the first of January 2015 in the Inria research center of Bordeaux with members of the UMR CNRS LaBRI. The project has eventually been ended of the 31th of December 2016.

3. Research Program

3.1. Research Program

Our research programs is structured into three complementary research axis : models, languages and systems, allowing us to develop our multi-disciplinary approach while validating each progress in the related specific fields of computer science ranging among computer music, multi-modal system design, reactive and real-time programming, typed functional programming, formal languages, graph representation theory, applied algebra, logic in computer science, etc.

3.1.1. Models

Inverse semigroup theory has recently been shown [13], [7], [12] [20] to unify most string-based, tree-based or even graph-based modeling approaches. It thus provides a consistent and robust mathematical framework to model the sequential, parallel and reactive aspects of temporal media. Developing the mathematical foundations of our proposal amounts to:

- studying the combinatorial and algorithmic properties of the emerging algebra-based model of structured temporal media,
- developing formal techniques and tools for expressing and verifying properties of temporal media programs especially with a view towards capturing temporal media programming by constraint satisfaction approaches,
- deriving from the known generators of these models adequate sets of application-oriented modeling functions.

3.1.2. Languages

Functional programming is the key link between well-defined mathematical structures and their computerized realizations. Based on functional programming frameworks such as Haskell⁰, we are prototyping a Domain Specific Language (DSL) [10] [15] dedicated to the programming of interactive temporal media programming. In this research axis, we aim more specifically at

- designing a robust and modular software architecture that allows to reuse existing pieces of software as well as simply combining them together with new ones,
- defining and implementing a DSL for programming interactive multimedia systems via a simple algebra-based high-level and multi-scale control and combination layer,
- finding the right balance between generic views of temporal media when seen as abstract temporal frames and their specializations when representing concrete gestures, sound, audio, videos, animations, etc.

3.1.3. Systems

Multi-modal interactive systems gather various techniques to capture and analyze gestures, and to combine, transform and produce temporal media. Through regular experiments in collaboration with artists, we also aim at assessing, refining and extending the applicability of our proposal by:

- developing a robust and mathematically well-founded representation of systems and of their behaviors, both programmatic and visual,
- developing and evaluating the adequacy of the GUI induced by this representation when used by artists,
- relating the new models with more classical models of music formalisms and, beyond, other temporal media such as animations, videos, etc.

4. Application Domains

4.1. Application Domains

4.1.1. Temporal media analysis and creation

Our first application domain concerns temporal media analysis and creation. Of course, many existing tools allow to create, combine and transform temporal media such as sounds, music, videos, animations. Strictly speaking, we do not aim at offering new possibilities. However, with an approach based on modern development theory and software technologies, we shall offer more reliable tools, that enjoy much higher productivity and reusability. As an immediate application, the fruit of our research may increase the quality of the technological assistance provided by Art & Science studios such as the SCRIME⁰. In this view, we shall concentrate our application perspectives on temporal media analysis (e.g. structure inference algorithms and learning tools) and on temporal media combination and synthesis (e.g. tools for music composition).

⁰See [31] for an historical presentation of the Haskell programming language.

⁰Studio de Création et de Recherche en Informatique et Musiques Expérimentales

4.1.2. Interactive and distributed interfaces

Our second application domain lays in the field of interaction. New technologies already used in artistic installations are connected and interactive. But there is still a whole world to be discovered and equipped with adequate technologies to design tomorrow's interactive and distributed pieces of digital arts. In this perspective, we shall concentrate on developing techniques for the capture and the on-the-fly analysis of input streams, together with techniques to combine them and turn them into new media types.

5. Highlights of the Year

5.1. Highlights of the Year

An α -version of the T-calculus [21] have been released ⁰.

It has been experimented in an Art & Science project ⁰ that have illustrated its expressiveness and simplicity for describing reactive music [19], [23]. This Art & Science project will be "on stage" in february 2017 via a "Duo solo for piano and computer".

The software *i-score* have also been further experimented [24], [16] especially during the visit of Shlomo Dubnov (UCSD) in 2016.

6. New Software and Platforms

6.1. T-calculus

Sketched in [10], the *T-calculus* is a Domain Specific Language ⁰ to provide simple and robust high-level description mechanisms of reactive systems. It will offer a programmatic view of the tile modeling paradigm [3], [9]. Its definition has been refined a number of times (see e.g. [10], [8]). A prototype implementation of its reactive kernel has eventually been achieved in Haskell on top of the Euterpea libraries during the spring 2016 [15], [21], [19], [23]

7. New Results

7.1. Alpha release of the *T*-calculus

One of the main achievement of the PoSET project in 2016 is the alpha release of the *T*-calculus [15] that not only implements the tiled front-end programing interface that was proposed earlier [10], [8], but also an original mid-end programing interface for implementing interactive behavior and the related categorical combinators that allows for effectively running these high level constructs.

7.2. A new collaboration with Bernard Serpette

A new collaboration with Bernard Serpette also aim at developing a formal models for the T-calculus semantics [27], [25]. Though at its birth, such an approach eventually reveals rather deep connection with Matsikoudis and Lee works on causal functions semantics [33], opening new perspectives towards higher-order timed programing.

⁰see [the T-calculus url](#)

⁰see [the Interpolation project](#)

⁰See [30] for an early note by Hudak about the notion of Domain Specific Language, and see [29], [32] for application of this notion is computer music.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

- PhD Grant CIFFRE, 2015-2018, for Jean-Michael Célérier, in partnership with **Blue Yeti** (Royan),

9. Partnerships and Cooperations

9.1. Regional Initiatives

9.1.1. SCRIME

The **Studio de Création et de Recherche en Informatique et Musiques Expérimentales (SCRIME)** located on Bordeaux University Campus, is a *Groupement d'Intérêt Scientifique et Artistique (GIS&A)* gathering Université de Bordeaux, CNRS, Bordeaux INP, Ministère de la Culture et de la Communication, Ville de Bordeaux and Région Aquitaine. It is a privileged partner of the PoSET project. Most PoSET artistic projects are organized in cooperation with the SCRIME.

9.1.2. IDEX Bordeaux

- 2 *Arts & Science* projects of Bordeaux eventually granted in 2016 by the Initiative of Excellence (IDEX) of Bordeaux,

9.2. International Initiatives

9.2.1. Inria International Partners

9.2.1.1. Informal International Partners

In 2016, PoSET members had active collaboration with

- Shlomo Dubnov, UCSD, USA,
- Mark Lawson, Herriot-Watt University, Edimbourg, UK,
- Camillo Rueda, Universidad Javeriana, Cali, Colombia,

9.3. International Research Visitors

9.3.1. Visits of International Scientists

Shlomo Dubnov, Professor at UCSD (USA), was member of the PoSET project for nine months, thanks to an Bordeaux IDEX fellowship in 2016.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

10.1.1.1. General Chair, Scientific Chair

- D. Janin, General Chair of **ACM Workshop on Functional Art, Music, Modeling and Design (FARM)**, Nara (Japan), associated with ICFP,

10.1.2. Scientific Events Selection

10.1.2.1. Chair of Conference Program Committees

- D. Janin, PC Chair of **Journées d'Informatique Musicale (JIM 2015)**, Albi (France),

10.1.2.2. Member of the Conference Program Committees

- M. Desainte-Catherine, PC member of **Journées d'Informatique Musicale (JIM 2015)**, Albi (France),

10.1.2.3. Reviewer

Members of the project are yearly reviewers for a number of international conferences including LICS, ICALP, STACS, MFCS, FST&TCS, in theoretical computer science, and ICMC, SMC, NIME, FARM, TENOR, JIM in computer music.

10.1.3. Journal

10.1.3.1. Member of the editorial boards

- S. Salvati is editor of the **Journal of Logic Language and Information (JoLLI)**; since the end of 2015, he has been promoted as Editor in Chief,
- M. Desainte-Catherine is editor of the **Revue francophone d'informatique musicale (RFIM)**.

10.1.3.2. Reviewer - Reviewing activities

Members of the project are regular reviewers for a number of international journal including **ACM Computers In Entertainment (CIE)**, **Journal of New Music Research (JNMR)**, **Journal of Logic Language and Information (JoLLI)**, **Revue francophone d'informatique musicale (RFIM)**, **Discrete Mathematics & Theoretical Computer Science (DMTCS)**, **International Journal of Foundations of Computer Science (IJFCS)**, **Information & Computation (I&C)** ...

10.1.4. Leadership within the Scientific Community

- M. Desainte-Catherine is president of the **Association Française d'Informatique Musicale (AFIM)**
- S. Salvati is the secretary of the **Foundation for Logic Language and Information (FoLLI)**.

10.1.5. Research Administration

- M. Desainte-Catherine, directrice adjointe du LaBRI,
- M. Desainte-Catherine, directrice scientifique et administrative du SCRIME,
- M. Desainte-Catherine, responsable du thème SI de l'équipe image et son du LaBRI,
- D. Janin, membre commission recherche Bordeaux INP/ENSEIRB-MATMECA.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

Licence: Myriam Desainte-Catherine, *Programmation fonctionnelle*, 44 h, L3, Software Engineering department, Bordeaux INP, France,

Licence: Myriam Desainte-Catherine, *Projet d'algorithmique et de programmation*, 25 h, L3, Software Engineering department, Bordeaux INP, France,

Licence: Anne Dicky, *Algorithmique des graphes*, 30 h, L3, Computer Science Departement, Paris VI University, Vietnam,

Licence: Anne Dicky, *Probabilités et combinatoire*, 75 h, L3, Computer Science Departement, Bordeaux University, France,

Licence: Anne Dicky, *Algorithmique et structures de données*, 50h, L2, Computer Science Departement, Bordeaux University, France,

Licence: Anne Dicky, *Fondamentaux pour les mathématiques et l'informatique*, 35 h, L1, Computer Science Departement, Bordeaux University, France,

Master: Sylvain Salvati, *Logique*, 12h, M1, Computer Science Departement, Bordeaux University, France,

Licence: David Janin, *Projet d'algorithmique et de programmation*, 25 h, L3, Software Engineering department, Bordeaux INP, France,

Licence: Sylvain Salvati, *Analyse syntaxique et projet de programmation 3*, 37,5 h, niveau L3, Computer Science Departement, Bordeaux University, France,

Master: Myriam Desainte-Catherine, *Compilation*, 14 h, M1, Software Engineering department, Bordeaux INP, France,

Master: Myriam Desainte-Catherine, *Projet de Génie Logiciel*, 25 h, M1, Software Engineering department, Bordeaux INP, France,

Master: Myriam Desainte-Catherine, *Informatique musicale contrôle et composition*, 25 h, M2, Software Engineering department, Bordeaux INP, France,

Master: Anne Dicky, *Recherche operationelle*, 70 h, M1, Computer Science Departement, Bordeaux University, France,

Master: David Janin, *Projet de Génie Logiciel*, 25 h, M1, Software Engineering department, Bordeaux INP, France,

Master: David Janin, *Compilation*, 20 h, M1, Network and System Engineering department (RSI), Bordeaux INP, France,

Master: David Janin, *Tutorat*, 15 h, M1, M2, Network and System Engineering department (RSI), Bordeaux INP, France,

Doctorat: Sylvain Salvati, *Initiation à CoQ*, 12 h, Ecole Doctorale Mathématique et Informatique, Bordeaux University, France.

10.2.2. Supervision

PhD : Etienne Dubourg, “Contribution à la théorie des langages de tuiles”, defended in July 2016, supervised by D. Janin

PhD in progress : Pauline Mouawad, “Analyse et modélisation de l’émotion musicale”, started in september 2012, supervised by M. Desainte-Catherine,

PhD in progress : Jean-Michaël Célérier, “Outils d’écriture spatiale pour les partitions interactives”, started in january 2015, supervised by M. Desainte-Catherine,

PhD in progress : Simon Archipoff, “Modélisation et programmation tuilée réactive”, started in september 2015, supervised by D. Janin,

10.2.3. Juries

- D. Janin, member of the PhD jury of Clément Poncelet, “Model-Based Testing Real-Time and Interactive Music Systems”, Université Paris VI / IRCAM, November 2016,

10.3. Popularization

The development of the T-calculus has eventually led us to a piano & computer performance that is going to be performed on stage in February 2017 with the pianist Edwin Bugger, associate member of the PoSET project.

11. Bibliography

Major publications by the team in recent years

- [1] A. ALLOMBERT, M. DESAINTE-CATHERINE. *Interactive scores : A model for specifying temporal relations between interactive and static events*, in "Journal of New Music Research (JNMR)", 2005, vol. 34, n^o 4, p. 361–374.
- [2] J. ARIAS, M. DESAINTE-CATHERINE, C. RUEDA. *Modelling Data Processing for Interactive Scores Using Coloured Petri Nets*, in "14th International Conference on Application of Concurrency to System Design", Tunis, Tunisia, June 2014 [DOI : 10.1109/ACSD.2014.23], <https://hal.archives-ouvertes.fr/hal-01095176>.
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- [10] D. JANIN, F. BERTHAUT, M. DESAINTE-CATHERINE, Y. ORLAREY, S. SALVATI. *The T-Calculus : towards a structured programming of (musical) time and space*, in "Work. on Functional Art, Music, Modeling and Design (FARM)", ACM Press, 2013, p. 23-34 [DOI : 10.1145/2505341.2505347], <http://hal.archives-ouvertes.fr/hal-00789189>.
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Publications of the year

Articles in International Peer-Reviewed Journal

- [14] J. ARIAS, J.-M. CELERIER, M. DESAINTE-CATHERINE. *Authoring and automatic verification of interactive multimedia scores*, in "Journal of New Music Research", November 2016, p. 1 - 19 [DOI : 10.1080/09298215.2016.1248444], <https://hal.archives-ouvertes.fr/hal-01399925>.

International Conferences with Proceedings

- [15] S. ARCHIPOFF, D. JANIN. *Structured reactive programming with polymorphic temporal tiles*, in "ACM International Workshop on Functional Art, Music, Modelling, and Design (FARM)", Nara, Japan, 2016 [DOI : 10.1145/2975980.2975984], <https://hal.archives-ouvertes.fr/hal-01350525>.
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Scientific Books (or Scientific Book chapters)

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Project-Team POTIOC

Popular interaction

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

Keywords:

Computer Science and Digital Science:

- 3.2.2. - Knowledge extraction, cleaning
- 3.4.1. - Supervised learning
- 5.1. - Human-Computer Interaction
 - 5.1.1. - Engineering of interactive systems
 - 5.1.2. - Evaluation of interactive systems
 - 5.1.4. - Brain-computer interfaces, physiological computing
 - 5.1.5. - Body-based interfaces
 - 5.1.6. - Tangible interfaces
 - 5.1.7. - Multimodal interfaces
 - 5.1.8. - 3D User Interfaces
- 5.6. - Virtual reality, augmented reality
- 5.9. - Signal processing
 - 5.9.2. - Estimation, modeling
- 8.2. - Machine learning
- 8.3. - Signal analysis

Other Research Topics and Application Domains:

- 1.3. - Neuroscience and cognitive science
- 2.1. - Well being
- 2.5.1. - Sensorimotor disabilities
- 2.5.2. - Cognitive disabilities
- 2.6.1. - Brain imaging
- 5.2.4. - Aerospace
- 9.1. - Education
 - 9.1.1. - E-learning, MOOC
- 9.2. - Art
 - 9.2.1. - Music, sound
- 9.4.3. - Physics
- 9.5.1. - Psychology
- 9.5.7. - Geography

1. Members

Research Scientists

Martin Hachet [Team leader, Inria, Researcher, HDR]
Fabien Lotte [Inria, Researcher, HDR]
Anke Brock [Inria, Researcher]

Faculty Member

Pascal Guitton [Univ. Bordeaux, Professor, HDR]

Technical Staff

Jeremy Laviolle [Inria, until Aug 2016]
Renaud Gervais [Inria, until Nov 2016]
Benoit Coulais [Inria]
Robin Gourdel [SATT Nancy Grand-Est, until May 2016]
Boris Mansencal [Bordeaux INP, From January to May 2016]

PhD Students

Camille Jeunet [Univ. Bordeaux, defence on Dec. 2nd]
Joan Sol Roo [Inria]
Damien Clergeaud [Inria]
Julia Chatain [Univ. Bordeaux]
Jelena Mladenovic [Inria]
Pierre-Antoine Cinquin [Univ. Bordeaux, from September 2016]
Lea Pillette [Inria, from October 2016]

Post-Doctoral Fellows

David Furio [Univ. Bordeaux]
Jeremy Frey [Univ. Bordeaux, ATER, until July 2016]

Administrative Assistants

Cecile Boutros [Inria]
Catherine Cattaert Megrat [Inria]

Others

Suzy Teillet [ENSC, Internship M2, from Feb 2016 until Jul 2016]
Hugo Germain [CentraleSupélec, Internship M1, from Jun 2016 until Aug 2016]
Benjamin Muzart [Univ. Bordeaux, Internship M1, from Apr 2016 until Jun 2016]
Juliette Pelletier [ENSC, Internship 1st Year, from May 2016 until Jul 2016]

2. Overall Objectives

2.1. Overall Objectives

The overall objective of Potioc is **to design, to develop, and to evaluate** new approaches that provide **rich interaction experiences between users and the digital world**. Thus, we aim at stimulating motivation, curiosity, engagement, or pleasure of use. In other words, we are interested in **popular interaction**, mainly targeted at the general public.

We believe that such popular interaction may enhance **learning, creation, entertainment or popularization of science** that are the main application areas targeted by our project-team. To this end, we explore input and output modalities that go beyond standard interaction approaches which are based on mice/keyboards and (touch)screens. Similarly, we are interested in 3D content that offers new opportunities compared to traditional 2D contexts. More precisely, Potioc explores interaction approaches that rely notably on interactive 3D graphics, augmented and virtual reality (AR/VR), tangible interaction, brain-computer interfaces (BCI) and physiological computing.

Such approaches hold great promises in a number of fields. For example, interactive 3D graphics have become ubiquitous in the industry, where they have revolutionized usages, notably by improving work cycles for conception or simulation tasks. However, except for video games, we believe that such approaches are still far from being exploited to their full extent outside such industrial contexts despite having a huge potential for the masses in the areas targeted by our project.

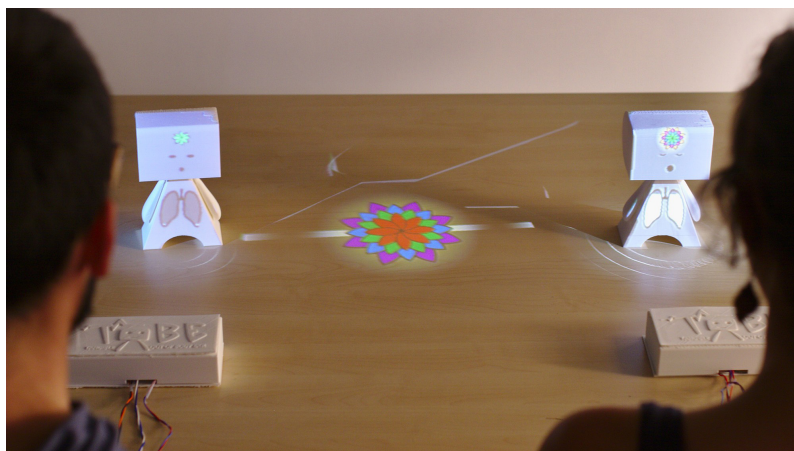


Figure 1. Tobe combines tangible interaction, spatial augmented reality, and physiological computing. It allows users to feel and explore their inner states.

In order to design interactive systems that can be beneficial to many people, and not only expert users, we propose to change the usual design approaches that are generally driven by criteria such as speed, efficiency or precision. Instead, we give more credit to the user experience, in particular criteria such as interface appeal and enjoyment arising from the interface use. Indeed, these criteria have been often neglected in academic research whereas we believe they are crucial for users who are novices with 3D interaction, multisensory spaces, or brain-computer interfaces. An interface with a strong appeal and enjoyment factor will motivate users to use and benefit from the system.

In the Potioc team, we follow a multidisciplinary approach in order to tackle the problem as a whole, from the most fundamental works on human sensori-motor and cognitive abilities and preferences, to the aspects that are linked to the usage and applications, passing through the technical aspects of the interaction, both at a hardware and software level.

3. Research Program

3.1. Introduction

The project of team potioc is oriented along three axes:

- Understanding humans interacting with the digital world
- Creating interactive systems
- Exploring new applications and usages

These axes are depicted in Figure 2.

Objective 1 is centered on the human sensori-motor and cognitive abilities, as well as user strategies and preferences, for completing interaction tasks. Our target contribution for this objective are a better understanding of humans interacting with interactive systems. The impact of this objective is mainly at a fundamental level.

In objective 2, our goal is to create interactive systems. This may include hardware parts where new input and output modalities are explored. This also includes software parts, that are strongly linked to the underlying hardware components. Our target contribution in objective 2 is to develop (hardware/software) interaction techniques allowing humans to perform interaction tasks.

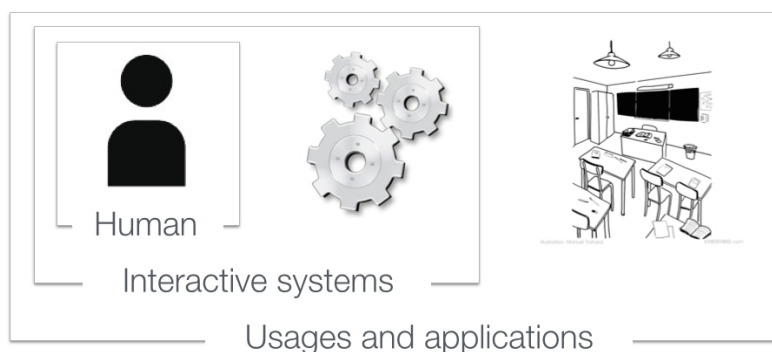


Figure 2. The three axes of the potioc team objectives.

Finally, in objective 3, we consider interaction at a higher level, taking into account factors that are linked to specific application domains and usages. Our target contribution in this area is the exploration and the emergence of new applications and usages that take benefit from the results of the project. With this objective, we target mainly a societal impact.

Of course, strong links exist between the three objectives of the project. For example, the results obtained in objective 1 guide the development of objective 2. Conversely, new systems developed in objective 2 may feed research questions of objective 1. There are similar links with objective 3.

3.2. Objective 1: Understanding humans interacting with the digital world

Our first objective is centered on the human side. Our finality is not to enhance the general knowledge about the human being as a research team in psychology would do. Instead, we focus on human skills and behaviors during interaction processes. To this end, we conduct experiments that allow us to better understand what users like, where and why they have difficulties. Thanks to these investigations, we are able to design interaction techniques and systems (described in Objective 2) that are well suited to the targeted users. We believe that this fundamental piece of work is the first step that is required for the design of usable popular interactions. We are particularly interested in 3D interaction tasks for which we design dedicated experiments. We also explore a new approach based on physiological and brain (ElectroEncephaloGraphy - EEG) signals for the evaluation of these interactions.

3.2.1. Interacting with physical and virtual environments

Interacting with digital content displayed on 2D screens has been extensively studied in HCI. On the other hand, less conventional contexts have been studied less. This is the case of 3D environments, immersive virtual environments, augmented reality, and tangible objects. With the final goal of making interaction in such contexts user-friendly, we conduct experiments to better understand user strategies and performance. This allows us to propose guidelines to help designers creating of tools that are accessible to non-expert users.

3.2.2. Evaluating (3D) interaction with physiological signals

Recently, physiological computing has been shown to be a promising complement to Human-Computer Interfaces (HCI) in general, and to 3D User Interfaces (3DUI) in particular, in several directions. Within this research area, we are interested in using various physiological signals, and notably EEG signals, as a new tool to assess objectively the ergonomic quality of a given (3D) UI, to identify where and when are the pros and cons of this interface, based on the user's mental state during interaction. For instance, estimating the user's mental workload during interaction can give insights about where and when the interface is cognitively

difficult to use. This could be useful for 2D HCI in general, and even more for 3DUI. Indeed, in a 3DUI, the user perception of the 3D scene – part of which could potentially be measured in EEG - is essential. Moreover, the usual need for a mapping between the user inputs and the corresponding actions on 3D objects make 3DUI and interaction techniques more difficult to assess and to design.

3.2.3. Interacting with Brain-Computer Interfaces

Although very promising for numerous applications, BCIs mostly remain prototypes not used outside laboratories, due to their low reliability. Poor BCI performances are partly due to imperfect EEG signal processing algorithms but also to the user who may not be able to produce reliable EEG patterns. Indeed, BCI use is a skill, requiring the user to be properly trained to achieve BCI control. If he/she cannot perform the desired mental commands, no signal processing algorithm can identify them. Therefore, rather than improving EEG signal processing alone, an interesting research direction is to also guide users to learn BCI control mastery. We aim at addressing this objective. We are notably exploring theoretical models and guidelines from educational sciences to improve BCI training protocols. We also study which users' profiles (personality and cognitive profile) fail or succeed at learning BCI control. Finally, we explore new feedback types and new EEG visualization techniques in order to help users gain BCI control skills more efficiently. These new feedback and visualizations notably aim at providing BCI users with more information about their EEG patterns, in order to identify more easily relevant BCI control strategies, as well as motivating and engaging them in the learning task.

3.2.4. Interaction for people with special needs

Interaction capabilities and needs largely depend on the target user group. In the Potioc project-team, we work with people having special needs. As an example, we work with children in the context of education, which requires us to design interfaces that are usable, engaging and support learning for this target group. Furthermore, we work with people with cognitive or perceptive disabilities, which requires us to consider accessibility, while at the same time designing interfaces that are learnable and enjoyable to use. In order to meet the needs of the different target groups, we apply participative and user-centred design methods.

3.3. Objective 2: Creating interactive systems

Our objective here is to create interactive systems and design interaction techniques dedicated to the completion of interaction tasks. We divide our work into three main categories:

- Interaction techniques based on existing Input/Output (IO) devices.
- New IO and related techniques.
- BCI and physiological computing.

3.3.1. Interaction techniques based on existing Input/Output (IO) devices

When using desktop IOs (i.e., based on mice/keyboards/monitors), a big challenge is to design interaction techniques that allow users to complete 3D interaction tasks. Indeed, the desktop IO space that is mainly dedicated to the completion of 2D interaction task is not well suited to 3D content and, consequently, 3D user interfaces need to be designed with a great care. In the past few years, we have been particularly interested in the problem of interaction when the 3D content is displayed on a touchscreen. Indeed, standard (2D) HCI has evolved from mouse to touch input, and numerous research projects have been conducted. On the contrary, in 3D, very little work has been proposed. We are contributing to moving desktop 3D UIs from the mouse to the touch paradigm; what we used to do with mice in front of a screen does not work well on touch devices anymore. In the future, we will continue designing new interaction techniques that are based on standard IOs (eg. pointing devices and webcams) and that target the main objectives of Potioc which are to enhance the interaction bandwidth for non expert users.

3.3.2. *New IO and related techniques*

Beyond standard IOs, we are interested in exploring new IO modalities that may make interaction easier, more engaging and motivating. In Potioc, we design new interactive systems that exploit unconventional IO modalities such as stereoscopy, 3D spatial input, augmented reality and so on. In particular, tangible interaction and spatial augmented reality are major subjects of interest for us. Indeed, we believe that manipulating directly physical objects for interacting with the digital world has a great potential, in particular when the general public is targeted. With such approaches, the computer disappears, and the user interacts with the digital content as he or she would do with physical content, which reduces the distance to the manipulated content. As an example, we recently designed Teegi, a new system based on a unique combination of spatial augmented reality, tangible interaction and real-time neurotechnologies. With Teegi, a user can visualize and analyze his or her own brain activity in real-time, on a tangible character that can be easily manipulated, and with which it is possible to interact. Such unconventional user interfaces that are based on rich sensing modalities hold great promises in the field of popular interaction.

We are also interested in designing systems that combine different sensory modalities, such as vision, touch and audition. Concrete examples include the design of tangible user interfaces or interfaces for visually impaired people. It has been shown that multimodality can provide rich interaction that can efficiently support learning, and it is also important in the context of accessibility.

3.3.3. *BCI and physiological computing*

Although Brain-Computer Interfaces (BCI) have demonstrated their tremendous potential in numerous applications, they are still mostly prototypes, not used outside laboratories. This is mainly due to the following limitations:

- **Performances:** the poor classification accuracies of BCIs make them inconvenient to use or simply useless compared to available alternatives
- **Stability and robustness:** the sensibility of ElectroEncephaloGraphic (EEG) signals to noise and their inherent non-stationarity make the already poor initial performances difficult to maintain over time
- **Calibration time:** the need to tune current BCIs to each user's EEG signals makes their calibration times too long.

As part of our research on EEG-based BCIs, we notably aim at addressing these limitations by designing robust EEG signal processing tools with minimal calibration times, in order to design practical BCI systems, usable and useful outside laboratories. To do so we explore the design of alternative features and robust spatial filtering algorithms to make BCIs more robust to noise and non-stationarities, as well as more accurate. We also explore artificial EEG data generation and user-to-user data transfer to reduce calibration times.

3.4. **Objective 3: Exploring new applications and usages**

Objective 3 is centered on the applications and usages. Beyond the human sensori-motor and cognitive skills (Objective 1), and the hardware and software components (Objective 2), Objectives 3 takes into account broader criteria for the emergence of new usages and applications in various areas, and in particular in the scope of education, art, popularization of science and entertainment. Our goal here is not to develop full-fledged end-user applications. Instead, our contribution is to stimulate the evolution of current applications with new engaging interactive systems.

3.4.1. *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 are also working with special education centres for the blind on accessible augmented reality prototypes. In the future, we will continue exploring new interactive approaches dedicated to education, in various fields.

3.4.2. Popularization of science

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. In particular, we have built a strong partnership with Cap Sciences, which is a center dedicated to the popularization of science in Bordeaux that is visited by thousands of visitors every month. This was initiated with the ANR national project InSTInCT, whose goal was to study the benefits of 3D touch-based interaction in public exhibitions. This project has led to the creation of a Living Lab where several systems developed by Potioc have been tested and will be tested by the visitors. This provides us with very interesting observations that go beyond the feedback we can obtain in our controlled lab-experiments.

3.4.3. 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 are working with colleagues who are specialists in digital music, and with musicians. We are also working with jugglers and mockup builders with the goal of enhancing interactivity and user experience.

3.4.4. 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. Application Domains

4.1. Education, popularization of science, art, entertainment

Our project aims at providing rich interaction experiences between users and the digital world, in particular for non-expert users. The final goal is to stimulate understanding, learning, communication and creation. Our scope of applications encompasses

- education
- popularization of science
- art
- entertainment

See "Objective 3: Exploring new applications and usages" (3.4) for a detailed description.

5. Highlights of the Year

5.1. Highlights of the Year

- ERC Grant "BrainConquest : Boosting Brain-Computer Communication with high Quality User Training" (Fabien Lotte)
- EFRAN project e-tac "Tangible and augmented interface for collaborative learning" (Martin Hachet)
- First book in French about BCI [50] [51] (Fabien Lotte)
- First accessible MOOC on "Accessibilité numérique" <https://www.fun-mooc.fr/courses/inria/41012/session01/about> (Pascal Guitton)

6. New Software and Platforms

6.1. PapARt

PapARt is a software development kit (SDK) that enables the creation of interactive projection mapping (See <https://project.inria.fr/papart>). This year, we focused on making this toolkit widely available. We created a set of examples and created tutorials. The PapARt code is now Open Source, our objective being to favor a wide appropriation by artists, teachers, or students.

Participants: Jeremy Laviolle, Martin Hachet

URL: <https://github.com/poqudrof/Papart-examples/wiki>

6.2. Helios

Helios is a software tool (Unity3D) we have developed in collaboration with Stéphanie Fleck from Université de Lorraine. It is dedicated to the learning of astronomy at school. It bases on augmented reality and tangible interaction. See Section 7.4.

Participants: Robin Gourdel, Jérémy Laviolle, Benoit Coulais, Martin Hachet.

Partners: Université de Lorraine - SATT Nancy Grand-Est.

6.3. Aïana

We have developed Aïana, a MOOC player, with the support of the Inria MOOC Lab. Aïana offers original interaction features in order to enable a wide spectrum of users including persons with disabilities. The first version of Aïana has been used by the 3700 participants of the Digital Accessibility MOOC we have produced on the national MOOC platform FUN. See Section 7.9.

Participants: Pierre-Antoine Cinquin, Pascal Guitton

Partners: LearningLab Inria

6.4. HOBIT

Along with the project HOBIT (see Section 7.1), we continue enhancing the platform that is dedicated to the simulation and augmentation of optics experiments. In particular, this year, we did a major evolution that consists in making the system reconfigurable. Various optical components be plugged in, and the simulation and augmentations are updated accordingly.

Participants: Benoit Coulais, David Furio, Martin Hachet.

Partners: Université de Bordeaux - IUT de Bordeaux, LaBRI, IMS, CELIA

<https://project.inria.fr/hobit>

7. New Results

7.1. HOBIT

Participants: David Furio, Benoit Coulais, Martin Hachet

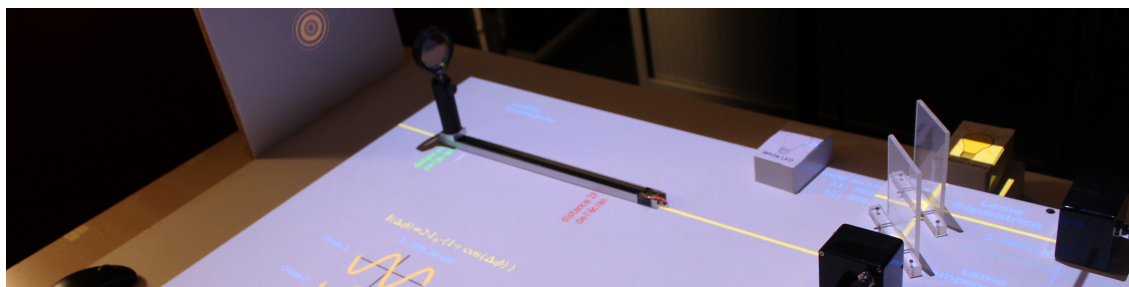


Figure 3. HOBIT: Hybrid Optical Bench for Innovative Teaching

Practical work in optics learning allows supporting the construction of knowledge, in particular when the concept to be learned remains diffuse. To overcome the limitations of the current experimental setups, we have designed a hybrid system that combines physical interaction and numerical simulation. This system relies on 3D-printed replicas of optical elements, which are augmented with pedagogical information (see Figure 3). In a first step, we have focused on the well-known Michelson interferometer experiment, widely studied in under graduate programs of Science. A 3-months user study with 101 students and 6 teachers showed that, beyond the practical aspects offered by this system, such an approach enhances the technical and scientific learning compared to a standard Michelson interferometer experiment. A second version of HOBIT is currently being developed. This new version will let us simulate and augment multiple experiments related with optics, like polarization or Young's interferometer.

A paper presenting HOBIT has been (conditionally) accepted at ACM CHI 2017.

7.2. Inner Garden

Participants: Joan Sol Roo, Renaud Gervais, Jeremy Frey, Martin Hachet

Digital technology has completely integrated our daily lives; we use it for entertainment, productivity and our social lives. However, the potential of leveraging technology to improve its users' overall happiness and life satisfaction is still largely untapped. Mindfulness, the act of paying a deliberate and non-judgmental attention to the present moment, has been shown to have a positive impact on a person's subjective well-being. With this in mind we created Inner Garden, an ambient mixed reality installation, inspired by a zen garden, comprised of an augmented sandbox along with a virtual reality modality to support mindful experiences (Figure 4). By shaping the sand, the user creates a living miniature world that is projected back onto the sand. Moreover, using a VR headset, she can take a moment to herself by actually going inside her own garden to meditate. The natural elements of the garden are connected to real-time physiological measurements, such as breathing, helping staying focused on the body. We evaluated the system through a first user study and consulted meditation teachers, who envisioned the use of the garden in their teaching, especially for novice practitioners. The reception of the system seems to indicate that technology can, when designed carefully, both engage the users and foster well-being.

A paper presenting Inner Garden has been (conditionally) accepted at ACM CHI 2017.

7.3. Hybridation of Spatial Augmented Reality and Virtual Reality

Participants: Joan Sol Roo and Martin Hachet



Figure 4. Inner Garden, an ambient mixed reality installation to support mindful experiences

Spatial Augmented Reality (SAR) allows a user, or a group of users, to benefit from digital augmentations embedded directly into the physical world. This enables co-located information and unobstructed interaction. On the other hand, SAR suffers from limitations that are inherently linked to its physical dependency, which is not the case for see-through or immersive displays. In this work, we explore how to facilitate the transition from SAR to VR, and vice versa, integrating both into a unified experience (Figure 5). We developed a set of interaction techniques and obtained first feedback from informal interviews.

A technote presenting this work has been (conditionally) accepted at IEEE 3DUI 2017.

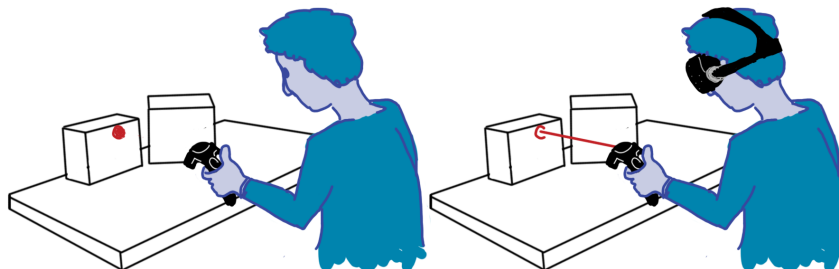


Figure 5. Transition from Spatial Augmented Reality to Virtual Reality

7.4. Augmented Reality and Tangible User Interfaces for Understanding Astronomy

Participants: Robin Gourdel, Benoit Coulais, Jeremy Laviolle, Martin Hachet

We have worked with Stephanie Fleck (Université de Lorraine) to improve the learning environment AIBLE she had imagined (see <http://stefleck4.wixsite.com/aible/-propos2-cw4c>). We have designed Helios, an augmented reality platform that aims at enhancing the understanding of abstract concepts in astronomy, specifically for primary schools' curriculum with children aged from 8 to 11. In order to provide physical evidence

for the influence of sunlight on the Earth and the Moon, and of the consequences of their relative positions, the learning tasks are designed on inquiry-based learning principles. Children have to test their own hypotheses by using tangible props and a set of cards that trigger dedicated pedagogical activities (e.g. seasons and the Earth revolution around the Sun, lunation origin, Earth rotation and time measurement).

Helios basically consists of a standard laptop computer, a webcam, printable AR markers placed on tangible props and on dedicated pedagogical cards (See Figure 6). The (virtual) celestial bodies are displayed on the screen, and many visual feedback help understanding various phenomena (e.g. shadow cones, time zones, and so on). In [13], we discuss how such an approach allows learners to better understand abstract phenomena.

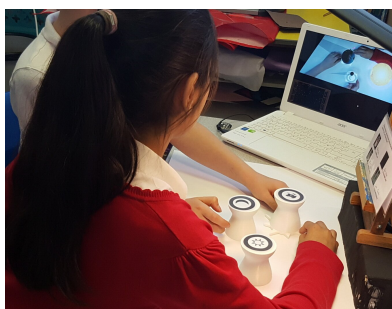


Figure 6. Helios: Manipulation of tangible objects and visualization of an augmented scene to learn astronomy.

7.5. Collaboration in VR

Participants: Damien Clergeaud and Pascal Guitton

The Airbus company regularly uses virtual reality for design, manufacturing and maintenance. We work with them on collaborative interaction in order to enable an efficient collaboration between operators immersed in the same virtual environment from remote locations and with heterogeneous equipment (large displays, CAVE, HMD). More precisely, we have developed tools to point and manipulate 3D objects, to remotely visualize the virtual environment, to be aware of remote manipulations and to describe tools and components trajectories (Figure 7). These tools have been validated by Airbus experts and the next step is to integrate them in their global process.

We are also working on Through-The-Lens Interaction techniques to ease the collaboration in some asymmetric tasks that requires a guide and an operator. Through-The-Lens techniques enable the guide to interact with the surroundings of the operator in order to help him in the task he has to perform. A paper presenting such a technique has been (conditionally) accepted at IEEE 3DUI 2017.

7.6. Interactive 3D Environments for Immersive Musical Performances

Participants: Martin Hachet

Together with Florent Berthaut (Univeristé Lille 3), we presented a set of works that attempts to extend the frontiers of music creation as well as the experience of audiences attending digital performances. Indeed, the power of interactive 3D graphics, immersive displays, and spatial interfaces is still under-explored in domains where the main target is to enhance creativity and emotional experiences. The goal of our work is to connect sounds to interactive 3D graphics that musicians can interact with and the audience can observe [11].

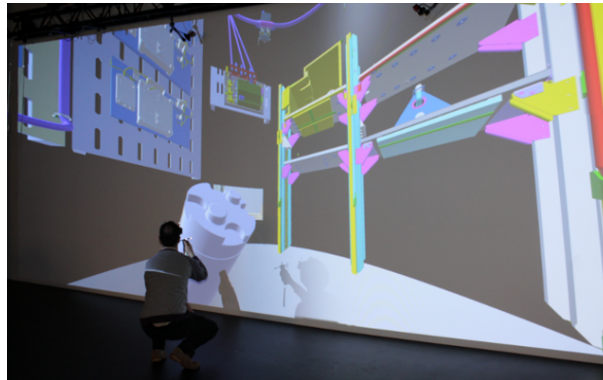


Figure 7. An immersed user has to perform a virtual task in a complex environment. In order to help the user to be fully aware of the VE, another immersed operator may guide him using a Through-The-Lens metaphor.

7.7. Multisensory Maps and 3D Printed Interactive Maps for Visually Impaired People

Participant: Anke Brock

Visually impaired people face important challenges related to orientation and mobility. Accessible geographic maps are helpful for acquiring knowledge of an urban environment. Historically, raised-line paper maps with braille text have been used, but these maps possess significant limitations. For instance, only a small percentage of the visually impaired population reads braille. Recent technological advances have enabled the design of accessible interactive maps with the aim to overcome these limitations. We designed Mappie, an accessible interactive map prototype based on the use of a multi-touch screen with a raised-line map overlay and speech output (Figure 8). Then, we deployed Mappie in a class of seven children and one caretaker during three months. Our formative study showed promising results and allowed insights in the design of accessible interactive maps, such as using olfactory and gustatory modalities to foster reflective learning, and using tangible objects to support storytelling. Following this first study, we designed MapSense as an extension of Mappie. MapSense uses the same hardware and interaction techniques as Mappie, but additionally provides fourteen "Do-It-Yourself" conductive tangibles. Some tangibles could be filled with scented material, such as olive oil, smashed raisins or honey, thus creating a real multi-sensory experience. The map was explored during two classes of three hours separated by a week, taught conjointly by a locomotion trainer and a specialized teacher. We observed that the map and tangible objects triggered strong positive emotions and stimulated spatial learning as well as creativity of the visually impaired students. This work has been conducted as part of the PhD thesis of Emeline Brulé under the supervision of Gilles Bailly and Annie Gentes, and in collaboration with the IRIT research lab in Toulouse. It has been published at CHI'16 [20].

As part of the postdoc of Stephanie Giraud at IRIT Toulouse under the supervision of Christophe Jouffrais, we have investigated how to print entire interactive maps in 3D, allowing users to construct a city like using a puzzle. We have conducted a user study comparing an interactive map that has been entirely 3D printed to a raised-line map with braille text (Figure 8 left). Our results suggest that the interactive map is significantly more effective for providing spatial knowledge than a tactile paper map with braille.

7.8. Navidrone

Participants: Julia Chatain, Anke Brock, Martin Hachet

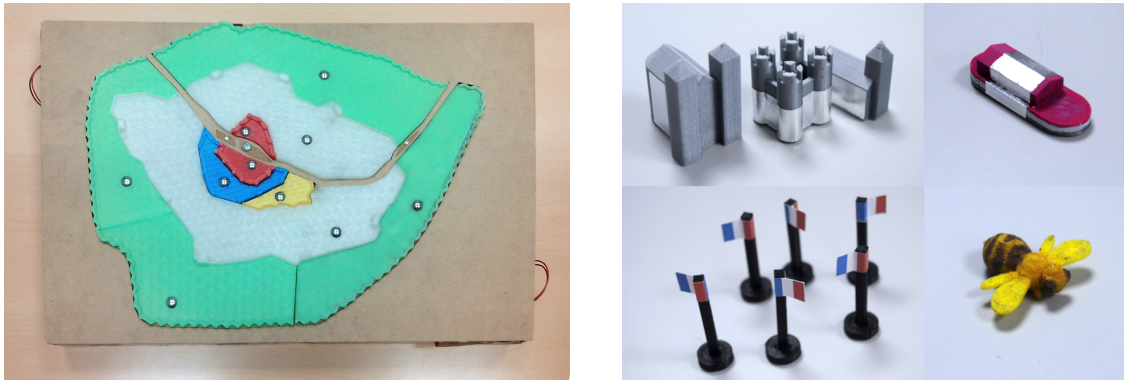


Figure 8. (Left) 3D printed interactive map, (Right) 3D printed tangibles for multisensory maps

With recent technological advances, the shapes of mobile devices are evolving. For example, we now see the emergence of new types of devices in form of autonomous aerial vehicles (drones) that become available in our everyday environment. As drones are becoming increasingly autonomous, it is crucial to understand how interaction with such devices will happen. These new devices, allow us to imagine new contexts of map usage, as for instance drone-based autonomous tour guides ((Figure 9). In order for those scenarios to happen, many problems need to be investigated. From a perspective in Human-Computer Interaction (HCI), the first questions to study are related to suitable input and output techniques. We iteratively designed interaction techniques for Navidrone, a drone-based autonomous tour guide. This work has been done in collaboration with the Prof. James Landay and Dr. Jessica Cauchard from the Stanford HCI Group.



Figure 9. Sketch showing the Navidrone concept: users interact with maps projected from drones by using their phones.

7.9. Accessibility of e-learning systems

Participants: Pierre-Antoine Cinquin and Pascal Guitton

E-learning systems, such as MOOC or serious games, are increasingly taking part in training process. Unfortunately, like most digital systems, they suffer from a lack of accessibility, in particular for people with cognitive disabilities (e.g. who have limited attention and memory). In this project, we develop a framework based on various disciplinary fields (education, cognitive sciences, human factors) but also participatory design research with students with disabilities to design interfaces promoting e-learning accessibility. From this 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. We are currently working on the analysis of this first play in order to enhance Aïana by designing new interaction modalities.

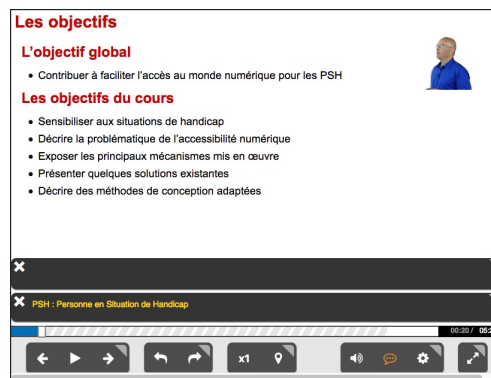


Figure 10. The Aïana MOOC player.

7.10. Teegi, a tangible EEG interface for scientific outreach

Participants : Thibault Lainé, Renaud Gervais, Jérémy Frey, Hugo Germain, Fabien Lotte, Martin Hachet

Teegi is an interactive systems that combines electroencephalographic (EEG) recordings and tangible interaction in order to let novices learn about how their brain works. By displaying EEG activity in real time on a support that is easy to manipulate and to comprehend, Teegi is a good tool for scientific outreach, that raises public interest.

While last year we developed a semi-spherical display based on LEDs, we push the project further during 2016 and built a complete autonomous puppet (Figure 11). The robot can move its two hands independently or its feet, and it can close its eyes. Beside the display of EEG activity, Teegi can react accordingly to the brain patterns recorded in real time from the user.

We demonstrated this new prototype in various occasions over the year, during public events such as “Fête de la Science” in La Cité des Sciences in Paris, a manifestation that gathered thousands of visitors (See Section 10.3 "Popularization").

7.11. Neuroergonomy

Participants : Jérémy Frey, Martin Hachet, Fabien Lotte

3D user interfaces are increasingly used in a number of applications, spanning from entertainment to industrial design. However, 3D interaction tasks are generally more complex for users since interacting with a 3D environment is more cognitively demanding than perceiving and interacting with a 2D one. As such, it is essential that we could finely evaluate user experience, in order to propose seamless interfaces. To do

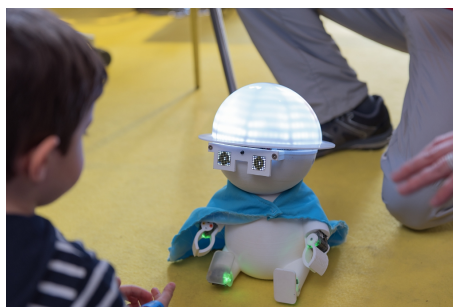


Figure 11. Teegi is a “Tangible EEG interface” that displays cerebral activity in real time by the mean of electroencephalography. A new robotized version can move and react accordingly to the brain patterns of the user, helping to explain to novices how the brain works.

so, a promising research direction is to measure users’ inner states based on brain signals acquired during interaction, by following a neuroergonomics approach. Combined with existing methods, such tool can be used to strengthen the understanding of user experience.

In [15][26], we reviewed the related work in this area. We summarized what has been achieved and the new challenges that arise. We described how a mobile brain imaging technique such as electroencephalography (EEG) brings continuous and non-disruptive measures. EEG-based evaluation of users can give insights about multiple dimensions of the user experience, with realistic interaction tasks or novel interfaces. We investigate four constructs: workload, attention, error recognition and visual comfort. Ultimately, these metrics could help to alleviate users when they interact with computers.

Such advance in the understanding of the users will eventually come forward thanks to the increasing dissemination of non-invasive brain imaging devices that record electrical activity onto the scalp. In [24][23] we compared side by side two EEG amplifiers, the consumer grade OpenBCI and the medical grade g.tec g.USBamp. We suggested how an affordable and open-hardware device could facilitate, beside neuroergonomics, the appearance of various brain-computer interfaces applications.

7.12. Physiological computing

7.12.1. Physiological computing

Participants : Jérémy Frey

While physiological sensors enter the mass market and reach the general public, they are still mainly employed to monitor health. Over the course of a thesis that explored the new possibilities offered by physiological computing in terms of communication and social presence, we described several use-cases involving the externalization of inner states through novel user interfaces.

For example, we created an application that uses heart rate feedback as an incentive for social interactions. A traditional board game was “augmented” through remote physiological sensing (Figure 12), using webcams to account for the subtle changes in blood flow that occur with each heartbeat. Projection helped to conceal the technological aspects from users and merged the biofeedback with the physical environment. We detailed how players reacted – stressful situations could emerge when users are deprived from their own signals – and we gave directions for game designers to integrate physiological sensors.

We envisioned a second application, that merges virtual reality, interactive fiction and physiological computing in order to craft *truly* immersive stories; narratives that evolve depending both on the actions and on the inner states of the user/reader, stretching a medium that shaped for ages humanity (Figure 13) [32].



Figure 12. We augmented a traditional board game with remote physiological monitoring and projection to demonstrate how physiological computing could be used to foster new interactions between people and increase social presence.

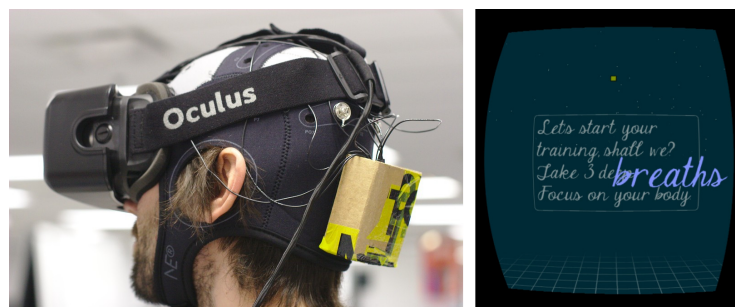


Figure 13. A combination of physiological sensors and head-mounted display (left) is used to immerse the reader in a narrative that reacts to gaze and to bodily activity (right).

7.13. EEG signal classification for BCI based on Riemannian geometry

Participants : Fabien Lotte

Although promising from numerous applications, current Brain-Computer Interfaces (BCIs) still suffer from a number of limitations. In particular, they are sensitive to noise, outliers and the non-stationarity of ElectroEncephaloGraphic (EEG) signals, they require long calibration times and are not reliable. Thus, new approaches and tools, notably at the EEG signal processing and classification level, are necessary to address these limitations. Riemannian approaches, spearheaded by the use of covariance matrices, are such a very promising tool slowly adopted by a growing number of researchers. We proposed a review of how these approaches have been used for EEG-based BCI, in particular for feature representation and learning, classifier design and calibration time reduction. Finally, we also identified relevant challenges and promising research directions for EEG signal classification in BCIs, such as feature tracking on manifold or multi-task learning [18].

7.14. Understanding Mental Imagery-based Brain-Computer Interface user-training

Participants : Camille Jeunet, Fabien Lotte

Mental Imagery-based Brain-Computer Interface (MI-BCI) enable their users to send commands to computer by imagining mental tasks (i.e., by performing MI) that are recognized in their brain signals. This type of BCI requires user training, and this training is currently poorly understood, and we basically do not know, who can learn MI-BCI control, what is to learn and how to learn it efficiently. Moreover, we have shown that current MI-BCI training protocols were both theoretically and practically inappropriate, and that there is a lack of fundamental knowledge on BCI user training, which prevents us from designing better user training approach [12].

In order to address these points, we first proposed a review and classification of cognitive and psychological predictors of MI-BCI performance. Three categories were defined: the user-technology relationship, attention and spatial abilities. The user-technology relationship refers to personality traits and states that influence users' perception of the technology and consequently impact the way they will interact with the technology (i.e., their feeling of being in control, their self-efficacy, etc.). The attention category gathers, among others, users' attentional abilities, motivation and engagement towards the task. These elements are essential to learn, whatever the skill targeted. They are also closely related to the user-technology relationship (for instance, feeling in control will increase users' engagement towards the task, thus they will allocate more attentional resources to the task). Finally, spatial abilities are the ability to produce, manipulate and transform mental images, which is closely related to the ability to control an MI-BCI. The description of these categories and of their neurophysiological correlates enabled us to submit ideas to improve MI-BCI user-training. For instance, we explained how to reduce computer-anxiety and increase the sense of agency, notably through the use of a positively biased feedback for novice users. Also, we proposed solutions to raise and improve attention, e.g., using neurofeedback or meditation. Finally, we argued that spatial abilities could be trained to improve users' capacity to perform mental imagery and consequently, potentially improve their MI-BCI performance [17].

We also did a review of the literature of current training protocols (published as a book chapter in [41]) which suggests that these protocols are, at least theoretically, inappropriate to acquire a skill and thus that they could be one of the factors responsible for inefficient MI-BCI user-training. In particular, participants are most of the time provided with uni-modal and evaluative feedback while literature recommends multi-modal, informative and supporting feedback. Although instructive, these insights only provide theoretical considerations about the flaws associated with the feedback approaches used in MI-BCI. It was therefore necessary to *concretely* assess whether standard MI-BCI feedback is appropriate to train a skill, and to what extent the feedback impacts BCI performance and skill acquisition. In order to experimentally evaluate the extent to which such a feedback has an impact on their ability to acquire a skill, we used it to teach users to perform simple motor tasks. Results (N=53 participants) revealed that with this feedback, 17% did not manage to learn the skill. This suggests that current BCI feedback is most probably suboptimal to teach a skill. A sub-group of our participants (N=20) then took part in a motor-imagery based BCI experiment. Results showed that those who struggled during the

first experiment improved in performance during the second, while the others did not. We hypothesised that these results are linked to the considerable cognitive resources required to process this feedback [16].

It should be noted that there are many connections between BCI user training, and neurofeedback training for clinical applications, both field aiming at training their users to perform self regulation of their brain activity. We have therefore shown how these two field share fundamental research questions on BCI user training, and how they can both benefit from each other [10].

7.15. Improving Mental Imagery BCI user-training & feedback

7.15.1. Spatial Ability Training Protocol

Participants : Suzy Teillet, Camille Jeunet, Fabien Lotte

The results of one of our previous studies suggested that users' MI-BCI performance correlates with their spatial abilities [34], which is consistent with the literature. This result was replicated in a second study in a pure motor-imagery based BCI [16]. We thus decided to explore the potential causal relationship between both: would an improvement of spatial abilities lead to better MI-BCI performances? To try to answer this question, we designed and implemented a spatial ability (SA) training procedure (see Figure 14). Then, we performed two user studies to validate the SA training procedure: results suggest that it efficiently improves participants' SA [29]. Consequently, we included this SA training procedure in an MI-BCI protocol. Results (N=24) showed no difference in classification accuracy between participants performing 6 MI-BCI sessions and those performing 3 SA and 3 MI-BCI sessions. Nonetheless, SA training intensity impacted users' progression, and neurophysiological analyses provided us with valuable insights into brain pattern evolution throughout the training process.



Figure 14. One item per exercise included in the Spatial Ability training: the shape on top is the target, and the participant must identify the two shapes that are identical to the target among the four below. From the left to the right are displayed the shapes, matrices, cubes, arms exercises.

7.15.2. PEANUT: Personalised Emotional Agent for Neurotechnology User-Training

Participants : Léa Pillette, Camille Jeunet, Boris Mansencal, Fabien Lotte

Mental-Imagery based Brain-Computer Interfaces (MI-BCI) are neurotechnologies enabling users to control applications using their brain activity alone. These neurotechnologies are very promising. However, existing training protocols do not enable every user to acquire the skills needed to use them. Indeed, those protocols are not consonant with psychological field recommendations. In particular, the current protocols do not provide social presence and emotional support to the user. Therefore, we designed and tested PEANUT, the first Learning Companion dedicated to the improvement of MI-BCI user-training. PEANUT has been designed throughout a combination of recommendations from the literature, the analysis of data from previous experiments and user-studies. He provides emotional support using spoken sentences, such as "C'est avec la pratique que l'on progresse", and facial expressions. Experiments were conducted in order to assess his influence on user's performance and experience. The first results indicate that PEANUT improves the user experience. Indeed, people who trained with PEANUT found it was easier to learn and memorize how to use the MI-BCI system and rated themselves more efficient and effective than participants who had no learning

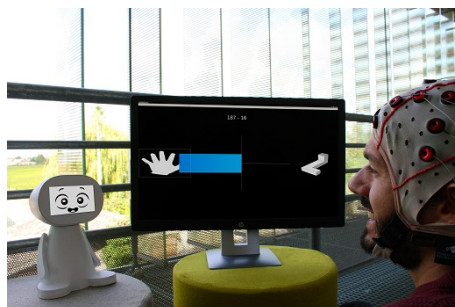


Figure 15. A participant taking part in a Brain-Computer Interface training process during which he learns to perform different mental imagery tasks (here, imagining a left-hand movement) to control the system. Along the training, PEANUT (on the left) provides the user with social presence and emotional support adapted to his performance and progression.

companion. These results indicate that using PEANUT does benefit MI-BCI user training. Future research will keep focusing on how to provide adapted cognitive and emotional feedback to MI-BCI users thanks to the use of learning companions.

7.16. Adaptive BCI training and operation

Participants : Jelena Mladenović, Jérémy Frey, Fabien Lotte

7.16.1. A generic framework for adaptive EEG-based BCI training and operation

There are two main approaches engaged in improving BCI systems: (i) improving the machine learning techniques, and the newly introduced (ii) improving human learning, by using the knowledge from instructional design and positive psychology. Both agree that the system needs to be adapted to the user but rely on different sources of adaptation: the machine for the former and the brain for the latter. In particular, machine learning algorithms should adapt to non-stationary brain signals, while human learning approaches should adapt the system to the various users' skills and profiles. Including both aspects of adaptation would give rise to a system ready to be used in real life conditions. However, a major obstacle lies in the large spectrum of sources of variability during BCI use, ranging from (i) imperfect recording conditions (e.g., environmental noise, humidity, static electricity etc. to (ii) the fluctuations in the user's psychophysiological states, due to e.g., fatigue, motivation or attention. For these reasons a BCI has not yet proved to be reliable enough to be used outside the laboratory. Particularly, it is still almost impossible to create one BCI design effective for every user, due to large inter subject variability. Therefore, the main concerns are to create a more robust system with the same high level of success for everyone, at all times, and to improve the current usability of the system. This calls for adaptive BCI training and operation.

We propose a conceptual framework which encompasses most important approaches to fit them in such a way that a reader can clearly visualize which elements can be adapted and for what reason. In the interest of having a clear review of the existing adaptive BCIs, this framework considers adaptation approaches for both the user and the machine, i.e., referring to instructional design observations as well as the usual machine learning techniques. It provides not only a coherent review of the extensive literature but also enables the reader to perceive gaps and flaws in current BCI systems, which would, hopefully, bring novel solutions for an overall improvement.

The framework (see Figure 16) has a hierarchical structure, from the lowest level elements which endure rapid changes, to the highest level elements which change at a much slower rate. It is comprised of: (i) one or several BCI systems/pipelines; (ii) a user model, whose elements are arranged according to different time scales ; (iii) a task model, enabling the system adaptation with respect to the user model; (iv) the conductor, an intelligent agent which implements the adaptive control of the whole system. A book chapter on this framework was submitted to a handbook on BCI.

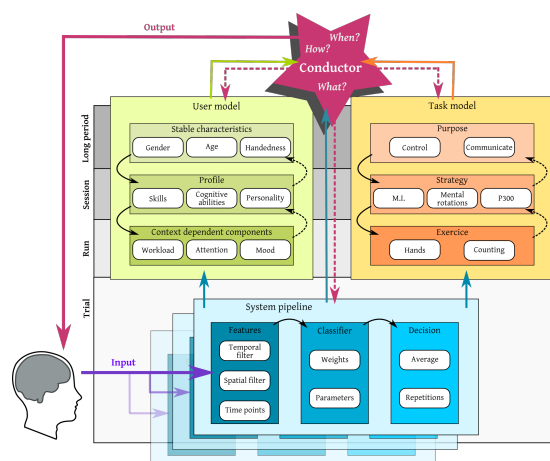


Figure 16. Multiple signals (input) maybe observed and processed in parallel in order to infer complementary states or intents, at the trial wise time scale. All the information extracted from these parallel pipelines may trigger the up-dating of the user or task model, which in turn might yield a decision from the conductor to take action, such as adapting one of the systems or the output, or modifying the task or the user model.

7.16.2. Adapting BCI Feedback based on Flow Theory

Using BCI systems can be very frustrating for people because it is not trivial and so it takes time to master. Differently from other learning procedures, BCIs do not have enough, if any explanatory feedback in assisting the learning of users. Also, as the feedback is not engaging the user's mind might easily wander off, which highly affects the system's accuracy as well as the person's learning pace. For this reason it takes more time to train a user to understand the procedure and have control over the system. Hence, we want to create an immersive and playful environment to attract the user's attention and help them learn with less effort and frustration.

We rely on the theory of Flow, introduced by Csikszentmihalyi in the 1970s. Flow is a state of enjoyment while effortlessly focused on a task so immersive that one loses the perception of time. In order to fulfil these requirements, we choose the users to be involved in an open-source video game called Tux Racer. Also, to ensure the maximal attention of the users, the game difficulty adapts according to users performance in real-time.

7.17. Brain-Computer Interfaces 1 and 2: foundations, methods, practice and applications

Participants : Jérémy Frey, Camille Jeunet, Fabien Lotte



Figure 17. A subject using motor imagery, i.e., imagining left or right hand movements to manipulate Tux to catch fish.

Together with Maureen Clerc (Inria Sophia) and Laurent Bougrain (Inria Nancy), we co-edited the first book on Brain-Computer Interfaces in French [50], [51], this book being also translated into English [48], [49]. It is published in two volumes, and co-written with researchers from all over France from many disciplines related to BCI. It covers both theoretical and practical aspects, as well as the neuroscience, mathematics, psychology, computer science, engineering, and ethical aspects of BCI. It is aimed at being a key resource for anyone who wants to start BCI research or want to deepen their knowledge in the many aspects of this exciting discipline.



Figure 18. The two volumes of the French version of the BCI book we edited.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

Interactive Collaboration in Virtual Reality for Aerospace Scenarios:

Duration: 2014-2017

PhD Thesis of Damien Clergeaud

Partners: Airbus Group

The Airbus company regularly uses virtual reality for design, manufacturing and maintenance. We work with them on collaborative interaction in order to enable an efficient collaboration between operators immersed in the virtual environment from remote locations and with heterogeneous equipment. More precisely, we have developed tools to point and manipulate objects, to remotely visualize the virtual environment, to be aware of remote manipulations and to describe tools and components trajectories (see Section 7.5).

9. Partnerships and Cooperations

9.1. Regional Initiatives

HOBIT: Hybrid Optical Bench for Innovative Teaching:

Duration: 2015-2017

Funding: Idex CPU & LAPHIA, and Inria ADT

Partners: Université de Bordeaux (IUT mesures physiques) & Université de Lorraine

The goal of the Hobit project (Hybrid Optical Bench for Innovative Teaching) is to design a hybrid optical bench that benefits from both the physical and the virtual worlds to enhance teaching and training in the field of optics and photonics (See Section 7.1).

website: <https://project.inria.fr/hobit>

OpenStreetMap

Collaboration with Marina Duféal (Assistant Professor in Geography at PASSAGES, UMR 5319, Univ. Bordeaux Montaigne) and Vincent Bergeot (Num&Lib) regarding contribution to OpenStreetMap. We have jointly organized a cartopartie for “Fête de la Science2016” at Inria Bordeaux.

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.

ANR Rebel:

Duration: 2016-2019

Coordinator: Fabien Lotte

Funding: ANR Jeune Chercheur Jeune Chercheuse Project

Partners: Disabilities and Nervous Systems Laboratory Bordeaux

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.

ANR Project ISAR:

Duration: 2014-2017

Coordinator: Martin Hachet

Partners: LIG-CNRS (Grenoble), Diotasoft (Paris)

Acronym: Interaction en Réalité Augmentée Spatiale / Interacting with Spatial Augmented Reality

The ISAR project (Interaction with Spatial Augmented Reality) focuses on the design, implementation, and evaluation of new paradigms to improve interaction with the digital world when digital content is directly projected onto physical objects. It opens new perspectives for exciting tomorrow's applications, beyond traditional screen-based applications.

website: <https://team.inria.fr/potioc/scientific-subjects/papart/>

Inria ADT Artik:

Duration: 2014-2016

Coordinator: Jérémy Laviolle & Martin Hachet

The Artik projet is focused on the development of Papart (Paper Augmented Reality Toolkit). Papart is a toolkit that enables projector/cameras (ProCam) and depth camera to work together to create interactive surfaces. It works with consumer-available hardware and enables tabletop interactions, although high-end cameras and projectors are also well supported. Here are the major advances of the developments of 2015: The hardware is now managed with a dedicated application, each Papart application is now hardware agnostic. Extrinsic calibration of projector / color and depth cameras can be done with any application running, the calibration processing is now below 2 minutes. The touch detection can be tweaked to fit any surface: it has been tested on a table, wall, and floor with respectively finger, hand, and foot interaction. This project relies on open source software, we also maintain the support of Maven distribution for the Processing project.

website: <https://project.inria.fr/papart/>

Inria ADT OpenViBE-X:

Duration: 2014-2016

Partners: Inria teams Hybrid and Athena

Coordinator: Maureen Clerc (Inria Sophia Antipolis)

This is the follow-up project of OpenViBE-NT

website: <http://openvibe.inria.fr>

Inria Project Lab BCI-LIFT:

Duration: 2015-2018

Partners: Inria team Athena (Inria Sophia-Antipolis), Inria team Hybrid (Inria Rennes), Inria team Neurosys (Inria Nancy), LITIS (Université de Rouen), Inria team DEMAR (Inria Sophia-Antipolis), Inria team MINT (Inria Lille), DyCOG (INSERM Lyon)

Coordinator: Maureen Clerc (Inria Sophia Antipolis)

The aim is to reach a next generation of non-invasive Brain-Computer Interfaces (BCI), more specifically BCI that are easier to appropriate, more efficient, and suit a larger number of people. With this concern of usability as our driving objective, we will build non-invasive systems that benefit from advanced signal processing and machine learning methods, from smart interface design, and where the user immediately receives supportive feedback. What drives this project is the concern that a substantial proportion of human participants is currently categorized "BCI-illiterate" because of their apparent inability to communicate through BCI. Through this project we aim at making it easier for people to learn to use the BCI, by implementing appropriate machine learning methods and developing user training scenarios.

website: <http://bci-lift.inria.fr/>

Helios:

Duration: 2015-2016

Partners: Université de Lorraine

Funding: SATT Nancy Grand Est

Coordinator: Stéphanie Fleck (Université de Lorraine)

The Helios project aims to provide a methodology and innovative media for the improvement of learning of basic astronomical phenomena for school groups (8-11 years). As part of this project, Potioc has focused on the development of the final application for augmented reality based and 3D manipulation, for providing a high-fidelity prototype.

9.3. European Initiatives

9.3.1. FP7 & H2020 Projects

Program: ERC Starting Grant

Project acronym: BrainConquest

Project title: Boosting Brain-Computer Communication with High Quality User Training

Duration: 2017-2021

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%. 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

Program: ERASMUS+

Project acronym: VISTE

Project title: Empowering spatial thinking of students with visual impairment

Duration: 2016-2019

Coordinator: National Technical University of Athens (Greece)

Other partners: Intrasoft International SA (Greece), Casa Corpului Didactic Cluj (Romania), Liceul Special pentru Deficienti de Vedere Cluj-Napoca (Romania), Eidiko Dimotiko Sxolio Tiflon Kallithreas (Greece)

Abstract: VISTE addresses inclusion and diversity through an innovative, integrated approach for enhancing spatial thinking focusing on the unique needs of students with blindness or visual impairment. However, since spatial thinking is a critical competence for all students, the VISTE framework and associated resources and tools will focus on cultivating this competence through collaborative learning of spatial concepts and skills both for sighted and visually impaired students to foster inclusion within mainstream education. The VISTE project will introduce innovative educational practices for empowering students with blindness or visual impairment with spatial skills through specially designed educational scenarios and learning activities as well as through a spatial augmented reality prototype to support collaborative learning of spatial skills both for sighted and visually impaired students.

9.4. International Initiatives

9.4.1. Inria International Partners

9.4.1.1. Informal International Partners

Prof. James Landay and Dr. Jessica Cauchard at the Stanford HCI Group (USA) on interaction with maps projected from drones

Prof. Niels Henze (University Stuttgart, Germany) and Prof. Katrin Wolf (Hamburg University of Applied Science, Germany) on mobile applications for visually impaired people

Prof. Pierre Dillenbourg (EPFL, Switzerland) on HCI for Education

9.4.2. Participation in Other International Programs

DGA-DSTL Project with UK, "Assessing and Optimising Human-Machine Symbiosis through Neural signals for Big Data Analytics", 2014-2018

9.5. International Research Visitors

9.5.1. Visits of International Scientists

Andreas Meinel, University of Freiburg, Germany, Apr. and Dec. 2016

Katrin Wolf, University of Art and Design, Berlin, Germany, Jul. 2016

9.5.2. Visits to International Teams

9.5.2.1. Research Stays Abroad

Fabien Lotte - Visiting scientist At RIKEN Brain Science Institute, Cichocki's advanced Brain Signal Processing Laboratory, Wakoshi, Japan, October-November 2016

Camille Jeunet - University of Sussex (Brighton - UK) 01/11/2015 - 30/01/2016

Camille Jeunet - UQAM (Montréal - CA) 10/06/2016 - 10/07/2016

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

10.1.1.1. General Chair, Scientific Chair

“2nd International OpenViBE workshop”, International BCI meeting 2016, Asilomar, CA, USA, 2016 (Fabien Lotte)

10.1.1.2. Member of the Organizing Committees

”IHM et Education”, workshop at IHM conference, Fribourg, Switzerland, Nov. 2016 (Martin Hachet, Anke Brock)

“2nd International OpenViBE workshop”, International BCI meeting 2016, Asilomar, CA, USA, 2016 (Fabien Lotte, Camille Jeunet, Jérémy Frey)

“What’s wrong with us? Roadblocks and pitfalls in designing BCI applications”, International BCI meeting, Asilomar, CA, USA, 2016 (Fabien Lotte)

Special session “Human Factors and performance metrics for BMI Training and Operation”, IEEE SMC 2016, Budapest, Hungary, (Fabien Lotte, Camille Jeunet)

Diversity Co-Chair at the ACM CHI’16 conference, San José, USA, 05/2016 (Anke Brock)

Microsoft Student Research Competition at the ACM ASSETS’16 conference, Reno, USA, 10/2016 (Anke Brock)

10.1.2. Scientific Events Selection

10.1.2.1. Member of the Conference Program Committees

IEEE VR 2017 (Martin Hachet)

Eurographics STAR 2017 (Martin Hachet)

IHM 2016 (Martin Hachet)

Mobile and Ubiquitous Multimedia MUM 2016 (Anke Brock)

Mobile and Ubiquitous Multimedia MUM 2016 Poster Committee (David Furió, Anke Brock)

1st International Neuroadaptive Technology Conference 2017 (Fabien Lotte)

7th International Brain-Computer Interface Conference, 2017 (Fabien Lotte)

International Conference on Systems, Man and Cybernetics, Brain-Machine Interface Workshop (IEEE SMC) 2016 (Fabien Lotte, Camille Jeunet)

International workshop on Pattern Recognition in NeuroImaging (PRNI) 2016 (Fabien Lotte)

International Brain-Computer Interface Meeting 2016 (publicity committee+ review committee) (Fabien Lotte)

7th Augmented Human International Conference, 2016 (Fabien Lotte)

8th Augmented Human International Conference, 2017 (Fabien Lotte)

ACM ASSETS 2016 (Anke Brock)

Computer Applications and Quantitative Methods in Archaeology 2016 (CAA) (Pascal Guitton)

8th Augmented Human International Conference, 2017 (Fabien Lotte)

7th International Brain-Computer Interface Conference, 2017 (Camille Jeunet)

10.1.2.2. Reviewer

ACM SIGGRAPH 2016 (Martin Hachet)

IEEE 3DUI 2017 (Martin Hachet)

ACM ISS 2016 (Joan Sol Roo)

ACM CHI 2016 (Fabien Lotte, Anke Brock, Camille Jeunet, Jérémy Frey)

ACM CHI 2017 (Fabien Lotte, Camille Jeunet, Anke Brock, David Furió, Camille Jeunet, Jérémy Frey)

Augmented Humans 2016 (Fabien Lotte)

International BCI Meeting 2016 (Fabien Lotte)

EICS 2016 (Fabien Lotte)
IJCNN 2016 (Fabien Lotte)
PRNI 2016 (Fabien Lotte)
IEEE SMC 2016 (Fabien Lotte, Camille Jeunet)
Eurohaptics 2016 (Anke Brock)
Handicap 2016 (Anke Brock)
HapticsSymposium 2016 (Anke Brock)
ACM IHM 2016 (Anke Brock)
ACM MobileHCI 2016 (Anke Brock)
ACM NordiCHI 2016 (Anke Brock)
ACM TEI 2016 (Anke Brock)
ACM Ubicomp 2016 (Anke Brock)
ACM UIST 2016 (Anke Brock)

10.1.3. Journal

10.1.3.1. Member of the Editorial Boards

Associate Editor in Brain Computer Interfaces (Fabien Lotte)
Associate Editor in Journal of Neural Engineering (Fabien Lotte)
Review Editor for Frontiers in Robotics and AI (Martin Hachet)
Review Editor for Frontiers in Neuroprosthetics (Fabien Lotte)
Review Editor for Frontiers in Human-Media Interaction (Fabien Lotte)
Guest Associate Editor, Frontiers in Robotics and AI, with D. Friedman, on “Brain-Computer Interfaces Technologies for Robotics and Virtual Reality”, 2016 (Fabien Lotte)
TACCESS Special Issue for ASSETS’17 conference (Anke Brock)

10.1.3.2. Reviewer - Reviewing Activities

Computer and Graphics (Martin Hachet)
Computers and Education (David Furió)
Computational Intelligence and Neurosciences (Fabien Lotte)
Journal of Neural Engineering (Fabien Lotte)
Frontiers in Neurosciences / Frontiers in ICT (Fabien Lotte)
IEEE Transactions on Biomedical Engineering (Fabien Lotte)
IEEE Transactions on Neural Systems and Rehabilitation Engineering (Fabien Lotte)
Le Travail Humain (Fabien Lotte)
ACM TOCHI (Fabien Lotte)
Nature Scientific Reports (Fabien Lotte)
ACM TACCESS (Anke Brock)
Journal of Psychophysiology (Camille Jeunet)
PLOS One (Camille Jeunet)
Progress in Brain Research (Camille Jeunet)
Transaction in Human Machine Systems (Camille Jeunet)
Brain Science (Camille Jeunet)

10.1.4. Invited Talks

- "Tangible Interaction and Spatial Augmented Reality for Education", University of Sussex, Jan. 2016 (Martin Hachet).
- "Vers des interfaces cerveau-ordinateur populaires", Conférence What's Up In Your Mind, Paris, Jun 2016 (Jérémy Frey)
- "Interaction Homme-Machine pour l'Education : au-delà de la souris et de l'écran", Colloque Robotique et Education, Bordeaux, Juin 2016 (Martin Hachet).
- "Human Learning and Alternative Applications Towards Usable Electroencephalography-based Brain-Computer Interfaces", Max Planck Institute, Tuebingen, Germany, December 2016 (Fabien Lotte)
- "The birth and scope of the BrainConquest ERC starting grant project", European Research Day 2016, Tokyo, Japan, November 2016 (Fabien Lotte)
- "Towards Usable EEG-based Brain-Computer Interfaces", Tokyo University of Agriculture and Technology, Tokyo, Japan, November 2016 (Fabien Lotte)
- "Principles and promises of EEG-based Brain-Computer Interface technologies", 1st Iranian IBRO/APRC School of Cognitive Neuroscience, Tehran, Iran, September 2016 (Fabien Lotte)
- "When Brain-Computer Interaction meets Educational Sciences", LaBRI general assembly, Bordeaux, France, July 2016 (Fabien Lotte)
- "Toward Usable Mental Imagery-based Brain-Computer Interfaces", Brain and Spine Institute, Paris, France, July 2016 (Fabien Lotte)
- « From Neurofeedback to Brain-Computer Interfaces », Neurofeedback workshop in Bordeaux, France, July 2016 (Fabien Lotte)
- "Brain-Computer Interaction and Spatial Augmented Reality Research in Potioc team", Concordia University, Montreal, Canada, June 2016 (Fabien Lotte, Camille Jeunet)
- "Latest research results in Brain-Computer Interfaces and Augmented Reality", Brain and Computers Digital Media Conference, Center for Digital Media, Vancouver, Canada, June 2016 (Fabien Lotte)
- « Educational Science Principles for Brain-Computer Interface Design », Inserm Lyon, France, April 2016 (Fabien Lotte)
- "Considering User Training and Alternative Applications to Design Usable EEG-based BCI Technologies", EPFL, Center for Neuroprosthetics, Geneva, Switzerland, March 2016 (Fabien Lotte)
- "Traitement des signaux cérébraux et classification des états mentaux", Journée scientifique de l'IFRATH "Interfaces Cerveau-Ordinateur", Paris, France, February 2016 (Fabien Lotte)
- "Reciprocal learning between machines and humans for neurofeedback and BCI", Première Journée Nationale sur le Neurofeedback, Paris, France, January 2016 (Fabien Lotte)
- "Interacting with spatial information" , Stanford HCI Group, Stanford University, USA, May 2016 (Anke Brock)
- "Interacting with spatial information" , HERE, Berkeley, USA , May 2016 (Anke Brock)
- "Interaction avec des cartes géographiques pour tous", Immersion, Bordeaux, France, April 2016 (Anke Brock, Julia Chatain)
- "Interacting with spatial information" , University of Sussex, UK, February 2016 (Anke Brock)
- Animation table ronde, Journée URFIST « Vers de nouveaux paradigmes pour l'édition scientifique », Bordeaux, March 2016 (Pascal Guitton)
- "L'éthique en Sciences du numérique", Ecole du Management Inria, Paris, September 2016 (Pascal Guitton)
- "Physiological computing and spatial augmented reality: reflecting on inner state", Paris Open Source Summit, Paris, November 2016 (Jérémy Frey)

"Transparence algorithmique et éthique", Journée nouveaux arrivants Inria, Saclay, December 2016 (Pascal Guitton)

"Interfaces cerveau-ordinateur : quoi, pourquoi et comment ?", ENSCBP - Media Sciences, Bordeaux, Février 2016 (Camille Jeunet)

"How Cognitive Sciences Can Contribute to Research in Brain-Computer Interaction", National Cognitive Science Conference 2016, San Diego (Camille Jeunet)

"Understanding and Improving Mental-Imagery based Brain-Computer Interface User Training: Towards Efficient, Reliable and Accessible BCIs", University of Oldenburg, October 2016 (Camille Jeunet)

"Understanding and Improving MI-BCI User-Training", University of Freiburg, Germany, November 2016 (Camille Jeunet)

10.1.5. Leadership within the Scientific Community

IEEE 3DUI Steering committee - Leader (Martin Hachet)

10.1.6. Scientific Expertise

Member of Jury for recruitment of Researcher (CR2-CR1) Inria Bordeaux (Martin Hachet)

Expert for the Millennium Science Initiative research group evaluation, Chile (Fabien Lotte)

Expert for the « Sapienza », University of Rome, research projects, Italy (Fabien Lotte)

Expert for the Partenariats Hubert-Curien (PHC) Germaine deStaël, France-Switzerland research projects (Fabien Lotte)

Etude "Panorama du cyberspace dans 3 à 5 ans" - Workshop "Evolutions technologiques", CEIS, CREC (Fabien Lotte)

Member of Inria Cellule de veille et de prospective (Pascal Guitton)

Expert for Credit Impot Recherche (Martin Hachet)

Member of the scientific committee of SCRIME (Martin Hachet)

10.1.7. Research Administration

Member of Inria Bordeaux Sustainable Development Committee (Martin Hachet)

Member of Inria Ethical Committee (COERLE) (Pascal Guitton)

Member of Inria International Chairs Committee (Pascal Guitton)

Responsable of Inria RA2020 Committee (new annual Activity Report) (Pascal Guitton)

Member of Comité de Pilotage de Software Heritage (Pascal Guitton)

Member of Comité de Pilotage Responsabilité Sociétale de l'Université, Université de Bordeaux (Pascal Guitton)

Member of Conseil d'administration Institut d'Optique Graduate School (Pascal Guitton)

Member of Commission de recrutement des Inspecteurs Généraux de l'Education Nationale (IGEN) (Pascal Guitton)

Member of Inria Bordeaux Committee for Technological Development (Fabien Lotte)

Member of Inria Bordeaux Young Researchers Committee (Anke Brock)

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

Licence : Jérémy Frey, Unix and Programming, CM-TD, 74.67h eqtd, L1 Computer Science, University of Bordeaux, France

Licence : Damien Clergeaud, Algorithmes et Programmation, TD et TP, 32h eqtd, L1 Computer Science, University of Bordeaux, France

Licence : Damien Clergeaud, Algorithmique des structures de données, TD et TP, 32h eqtd, L2 Computer Science, University of Bordeaux, France

Licence : Camille Jeunet, Sciences humaines et méthodes, CM-TD, 18h eqtd, Licence MIASHS, University of Bordeaux, France

Master : Jérémy Frey, Programming projects, TD, 18h eqtd, M1 Computer Science, University of Bordeaux, France

Master : Pascal Guitton, Virtual and Augmented Realities, CM, 36h eqtd, M2 Computer Science, University of Bordeaux, France

Master : Pascal Guitton, Digital accessibility, CM, 12h eqtd, M1 Cognitive Science, University of Bordeaux, France

Master : Jérémy Frey, Programming projects, TD, 10h eqtd, M2 Computer Science, University of Bordeaux, France

Master : Pascal Guitton, Assistive technologies, CM, 30h eqtd, M2 Cognitive Science, University of Bordeaux, France

Master : Anke Brock, Virtual Reality and 3D Interaction, CM-TD, 7,5h eqtd, M2 Cognitive Science, University of Bordeaux, France

Master : Martin Hachet, Virtual Reality and 3D Interaction, CM, 12h eqtd, M2 Cognitive Science, University of Bordeaux, France

Master : Fabien Lotte, Virtual Reality and 3D Interaction, CM, 4h eqtd, M2 Cognitive Science, University of Bordeaux, France

Master : Anke Brock, Interaction and Ergonomics, CM-TD, 10h eqtd, 3rd year (M2), Enseirb, Bordeaux, France

Master : Martin Hachet, Interaction and Ergonomics, CM-TD, 8h eqtd, 3rd year (M2), Enseirb, Bordeaux, France

Master: Fabien Lotte, Virtual Reality, Accesibility and Brain-Computer Interfaces, 4h eqtd, 3rd year (M2), ENSSAT, Lannion, France

Master: Fabien Lotte, Brain Computer Interfaces, 6h eqtd, 3rd year (M2), ESIEA, Laval, France

Master : Anke Brock, Human-Computer Interaction, CM-TD, 12h eqtd, M2 SRI, Upsitech Toulouse, France

Master: Fabien Lotte, Human-Computer Interactions, CM-TD, 7.5 eqtd, M1 Cognitive Sciences and Ergonomy, University of Bordeaux, France

Master : Anke Brock, Accessibility of interactive systems, CM-TD, 6h eqtd, M2 IHM, ENAC and University Toulouse, France

Master : Anke Brock, Accessibility of interactive systems, CM-TD, 6h eqtd, M2 Systèmes Mobiles Autonomes Communicants / Internet des Objets (Mobiles), University Bordeaux, France

Master : Camille Jeunet, HCI and Human factors, CM-TD, 18h eqtd, M1 Sciences Cognitives and Ergonomie, University of Bordeaux, France

MOOC : Pascal Guitton and H el ene Sauz eon, "Comment favoriser l'accessibilit e num erique", 5 weeks, Plate-forme France Universit  Num erique (FUN), large audience, initial and continuous training, about 4000 registered people.

10.2.2. Supervision

PhD: Camille Jeunet, "Improving User training approaches for Brain-Computer Interface", University of Bordeaux, Defense on December 2nd, 2016 (Martin Hachet, Fabien Lotte, co-supervision with Bernard N'Kaoua, and Sriram Subramanian)

PhD in progress: Julia Chatain, "Design and evaluation of augmented geographic maps", University of Bordeaux, since September 2015 (Anke Brock and Martin Hachet)

PhD in progress: Damien Clergeaud, "Collaborative interaction for aerospace scenarios", University of Bordeaux, since November 2014 (Pascal Guitton)

PhD in progress: Joan Sol Roo, "Interaction with Spatial Augmented Reality", University of Bordeaux, since December 2014 (Martin Hachet)

PhD in progress: Jelena Mladenovic, "User Modeling for Adaptive BCI training and operation", University of Bordeaux, since December 2015 (Fabien Lotte, co-supervised with Jérémie Mattout)

PhD in progress: Pierre-Antoine Cinquin, "Design and Experimental Validation of Accessible E-learning systems for people with cognitive disabilities", University of Bordeaux, since September 2016 (Hélène Sauzéon, Pascal Guitton)

PhD in progress: Léa Pillette, "Redefining Formative Feedback in Brain-Computer Interface User Training", University of Bordeaux, since September 2016 (Fabien Lotte, Bernard N'Kaoua)

PhD in progress: Lorraine Perronnet, "Neurofeedback and Brain Rehabilitation based on EEG and fMRI", Rennes University, since January 2014 (Fabien Lotte, co-supervision with Anatole Lécuyer, Christian Barillot, Inria Rennes and Maureen Clerc, Inria Sophia Antipolis)

PhD in progress: Stephanie Lees, "Assessing and Optimising Human-Machine Symbiosis through Neural signals for Big Data Analytics", Ulster University, since February 2014 (Fabien Lotte, co-supervision with Damien Coyle, Paul McCullagh and Liam Maguire, Ulster University)

10.2.3. *Juries*

PhD (Rapporteur): Elizabeth Rousset, INP Grenoble, February 2016 (Pascal Guitton)

PhD (Rapporteur): Sareh Saeedi, Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland, March 2016 (Fabien Lotte)

PhD (Rapporteur): Hind Gacem, Telecom ParisTech, April 2016 (Martin Hachet)

PhD (Rapporteur): Honyun Cho, Gwangju Institute of Science and Technology, South Korea, June 2016 (Fabien Lotte)

PhD (Rapporteur): Sebastien Pelurson, Université Grenoble Alpes, August 2016 (Martin Hachet)

PhD (Président): Brett Ridell, Université de Bordeaux, October 2016 (Pascal Guitton)

PhD (Président): Carlos Zubiaga, Université de Bordeaux, November 2016 (Pascal Guitton)

PhD (Examinateur): Emeric Baldisser, Université de Bordeaux, March 2016 (Pascal Guitton)

PhD (Examinateur): Guillaume Claude, INSA Rennes, July 2016 (Pascal Guitton)

PhD (Examinateur): Benoit Bossavit, Universidad de Navarra, Nov. 2016 (Martin Hachet)

PhD (Examinateur): Liming Yang, Ecole Centrale de Nantes, December 2016 (Pascal Guitton)

Thesis Advisory Committee: Lonni Besançon, Université Paris Saclay, June 2016 (Martin Hachet)

Thesis Advisory Committee: Sarah Buchanan, University Central Florida, July 2016 (Martin Hachet)

10.3. Popularization

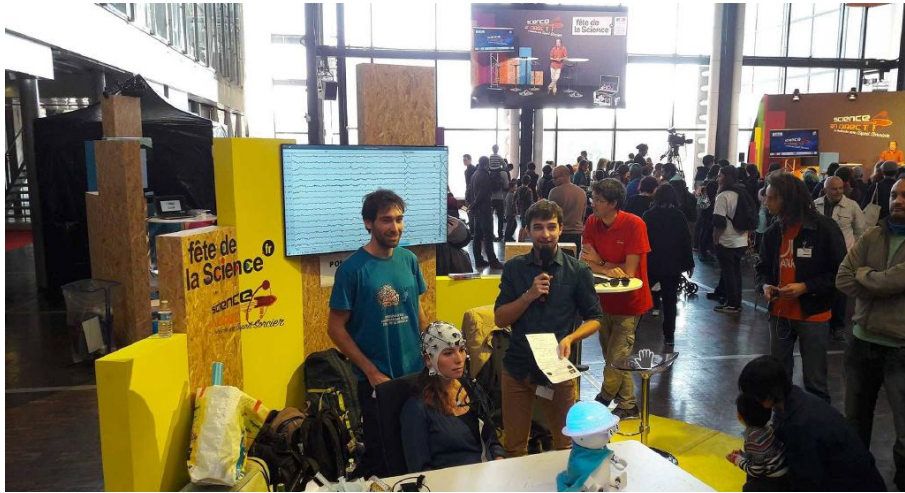


Figure 19. Teegi was demonstrated during several public events over the year, including “Fête de la Science” in La Cité des Sciences in Paris.

10.3.1. Science Festivals

Science Agora, Miraikan, Tokyo, Japan, November 2016 (Fabien Lotte)

Cartopartie, Fête de la Science, Bordeaux, October 2016 (Anke Brock)

Démonstration de Teegi, Cité des Sciences, Paris, retransmission en direct sur l’Esprit Sorcier, October 2016 (Jérémy Frey, Jelena Mladenovic, Thibault Lainé)

"Contrôler par la pensée: Apprenez comment fonctionne une interface cerveau-ordinateur en jouant à Tux Race et découvrez Teegi", Cap science, October 2016 (Jelena Mladenovic, Jérémy Frey, Thibault Lainé)

10.3.2. Popularization Talks

“Les Interfaces Cerveau-Ordinateur”, CogTalk, Bordeaux, October 2016 (Fabien Lotte)

TEDx UTC (Compiègne, France, 01/2016): ”Toucher et entendre les cartes géographiques” https://www.youtube.com/watch?v=sr2l8PQg_2E&feature=youtu.be, (Anke Brock)

"Comment le numérique nous aide à changer", Séminaire Science et développement durable, Bordeaux, June 2016 (Pascal Guitton)

"Réalité virtuelle et réalité augmentée : quelles réalités et quels futurs ?", Séminaire Photonique et réalité virtuelle, Bordeaux, November 2016 (Pascal Guitton)

"Le numérique et ses sciences dans le réel", Séminaire national « Enseigner l’option Informatique et création numérique au cycle terminal », ISENER (Futuroscope), November 2016 (Pascal Guitton)

Pint of Science, "Interfaces cerveau-ordinateur : Entre mythes et réalité", Bordeaux, May 2016 (Camille Jeunet)

10.3.3. Popularization Articles

"Mythes et réalités sur l’interaction cerveau-ordinateur", Livre "5 jeunes chercheurs d’avenir" (Prix de Thèse le Monde), Editions Le Pommier (Fabien Lotte)

10.3.4. Demonstrations

Inner Garden, Bordeaux Geek Festival (BGF), May 2016 (Joan Sol Roo, Julia Chatain).
 Augmented Michelson Interferometer, Bordeaux Geek Festival (BGF), May 2016 (Benoit Coulais, David Furio)
 Augmented Michelson Interferometer, Hall of ALPC region, June 2016 (David Furio)
 Demonstration of Teegi, Colloque Robotique et Education, Bordeaux, Juin 2016 (Jérémy Frey, Thibault Lainé).
 Demonstration of Teegi,, Bordeaux Geek Festival (BGF), May 2016 (Thibault Lainé)

10.3.5. Women In Science

Femmes et Sciences Deputy Board Member (« suppléante au conseil d'administration »), since 2016 (Anke Brock)
 Intervention in a high school in Valence d' Agen to present our research projects and career paths , March 2016 (Anke Brock with fellow members of Femmes et Sciences Aquitaine).
 "Digit'elles -témoignages de femmes scientifiques" , Fête de la Science, Bordeaux, October 2016 (Anke Brock with fellow members of Femmes et Sciences Aquitaine)
 Django girls, Django workshops for young participants, April and June 2016 (Julia Chatain)
 Filles et Maths, Speed meeting with female highschool students ti speak about careers in mathematics, May 2016 (Julia Chatain)
 Member of Inria Comité Parité et Egalité (Pascal Guitton)

10.3.6. Other

Conference on Brain-Computer Interfaces and how to become a research scientist, in a High School in Tulle, December 2016 (Fabien Lotte)
 Radio interview on BCI for "L'oeuf ou la poule", on CHOQ, a Montréal Radio from UQAM (Université du Québec à Montréal), Montreal, Canada, June 2016 (Fabien Lotte, Camille Jeunet)
 Radio interview on BCI and VR on Radio Canada, in Vancouver, Canada, June 2016 (Fabien Lotte)
 Radio interview about BCI and the Brain and Computers Digital Media Conference on the Vancouver-based Round House Radio, June 2016 (Fabien Lotte)
 Nuit des Chercheurs, Cap Sciences, Bordeaux, Septembre 2016 (Camille Jeunet)

11. Bibliography

Major publications by the team in recent years

- [1] A. BROCK, P. TRUILLET, B. ORIOLA, D. PICARD, C. JOUFFRAIS. *Interactivity Improves Usability of Geographic Maps for Visually Impaired People*, in "Human-Computer Interaction", 2015, vol. 30, n^o 2, p. 156-194 [DOI : 10.1080/07370024.2014.924412], <https://hal.archives-ouvertes.fr/hal-01077434>.
- [2] J. FREY, M. DANIEL, J. CASTET, M. HACHET, F. LOTTE. *Framework for Electroencephalography-based Evaluation of User Experience*, in "CHI '16 - SIGCHI Conference on Human Factors in Computing System", San Jose, United States, ACM (editor), May 2016 [DOI : 10.1145/2858036.2858525], <https://hal.inria.fr/hal-01251014>.
- [3] J. FREY, R. GERVAIS, S. FLECK, F. LOTTE, M. HACHET. *Teegi: Tangible EEG Interface*, in "UIST-ACM User Interface Software and Technology Symposium", Honolulu, United States, ACM, October 2014, <https://hal.inria.fr/hal-01025621>.

- [4] R. GERVAIS, J. FREY, A. GAY, F. LOTTE, M. HACHET. *TOBE: Tangible Out-of-Body Experience*, in "TEI'16 - Tangible, Embedded and Embodied Interaction", Eindhoven, Netherlands, ACM, February 2016 [DOI : 10.1145/2839462.2839486], <https://hal.archives-ouvertes.fr/hal-01215499>.
- [5] R. GERVAIS, J. SOL ROO, M. HACHET. *Tangible Viewports: Getting Out of Flatland in Desktop Environments*, in "Tangible, Embedded and Embodied Interaction (TEI)", Eindhoven, Netherlands, February 2016, <https://hal.archives-ouvertes.fr/hal-01215502>.
- [6] M. HACHET, J.-B. DE LA RIVIÈRE, J. LAVIOLE, A. COHÉ, S. CURSAN. *Touch-Based Interfaces for Interacting with 3D Content in Public Exhibitions*, in "IEEE Computer Graphics and Applications", March 2013, vol. 33, n° 2, p. 80-85 [DOI : 10.1109/MCG.2013.34], <http://hal.inria.fr/hal-00789500>.
- [7] J. JANKOWSKI, M. HACHET. *A Survey of Interaction Techniques for Interactive 3D Environments*, in "Eurographics 2013 - STAR", Girona, Spain, May 2013, <https://hal.inria.fr/hal-00789413>.
- [8] F. LOTTE, F. LARRUE, C. MÜHL. *Flaws in current human training protocols for spontaneous Brain-Computer Interfaces: lessons learned from instructional design*, in "Frontiers in Human Neurosciences", September 2013, vol. 7, n° 568 [DOI : 10.3389/FNHUM.2013.00568], <http://hal.inria.fr/hal-00862716>.

Publications of the year

Doctoral Dissertations and Habilitation Theses

- [9] F. LOTTE. *Towards Usable Electroencephalography-based Brain-Computer Interfaces*, Univ. Bordeaux, September 2016, Habilitation à diriger des recherches, <https://hal.inria.fr/tel-01416980>.

Articles in International Peer-Reviewed Journal

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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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1. Members

Research Scientists

Olivier Beaumont [Inria, Senior Researcher, HDR]

Lionel Eyraud-Dubois [Inria, Researcher]

Ruslan Sadykov [Inria, Researcher]

Faculty Members

Francois Vanderbeck [Team leader, Univ. Bordeaux, Professor, HDR]

François Clautiaux [Univ. Bordeaux, Professor, HDR]

Boris Detienne [Univ. Bordeaux I, Associate Professor]

Arnaud Pecher [Univ. Bordeaux I, Professor, HDR]

Pierre Pesneau [Univ. Bordeaux I, Associate Professor]

Technical Staff

Guillaume Marques [Inria, since Feb 2016]

Issam Tahiri [Inria, contract with ERTUS CONSULTING]

Kevin Barreau [Inria, until Oct 2016]

PhD Students

Thomas Bellitto [Univ. Bordeaux]

Imen Ben Mohamed [Kedge]

Rodolphe Griset [EDF, CIFRE]

Jérémy Guillot [Univ. Bordeaux]

Thomas Lambert [ENS Lyon]

Quentin Viaud [Saint-Gobain, CIFRE]

Post-Doctoral Fellows

Ayse Nur Arslan [Inria, from Nov 2016]

Agnès Le Roux [Univ. Bordeaux]

Halil Sen [Inria]

Visiting Scientists

Michael Romer [Martin Luther University, Halle-Wittenberg, Visiting Scientist, from Feb 2016 until Apr 2016]

Gautier Stauffer [INP Grenoble, Prof, Collaborator]

Administrative Assistants

Sabine Delarboulas Cusin [INRA]

Nicolas Jahier [Inria]

Nathalie Robin [Inria]

2. Overall Objectives

2.1. Overall Objectives

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, Lagrangian and Bender's decomposition methods to produce powerful relaxations, multi-level programming to model a hierarchy of decision levels or recourse decision in the case of data adjustment, 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. 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 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 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. More broadly, to contribute to theoretical and methodological developments of exact approaches in combinatorial optimization, while extending the scope of applications.
- (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 methods and heuristics.
- (iii) Software platform: To provide prototypes of specific model solvers and generic software tools that build on our research developments, writing proof-of-concept code, while transferring our research findings to internal and external users.

3. Research Program

3.1. Introduction

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 fractional 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, Dantzig-Wolfe decomposition, mixed integer programming, 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.

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* [64]. 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 $\text{conv}(X)$ is a polyhedron that can be described in terms of linear constraints, i.e. it writes as $\text{conv}(X) = \{x \in \mathbb{R}^{n+p} : Cx \leq d\}$ 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 $\text{conv}(X)$: if $\tilde{x} \notin \text{conv}(X)$, find a linear inequality $\pi x \geq \pi_0$ satisfied by all points in $\text{conv}(X)$ but violated by \tilde{x} . Hence, for NP-hard problems, one can not hope to get a compact description of $\text{conv}(X)$ nor a polynomial time exact separation routine. Polyhedral studies focus on identifying

some of the inequalities that are involved in the polyhedral description of $\text{conv}(X)$ and derive efficient *separation procedures* (cutting plane generation). Only a subset of the inequalities $Cx \leq d$ 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 [1], [4], [5], [3]. 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 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, ...).

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. 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. Introduction

Our group has tackled applications in logistics, transportation and routing [63], [62], [58], [60], in production planning [79] and inventory control [58], [60], in network design and traffic routing [40], [49], [56], [82], [37], [50], [68], [75], in cutting and placement problems [65], [66], [76], [77], [78], [80], and in scheduling [2], [69], [35].

4.2. 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 [49]. 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-electronic system installation cost. We developed and compared several decomposition approaches [84], [83], [82] 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 [81]. 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 [56], [57].

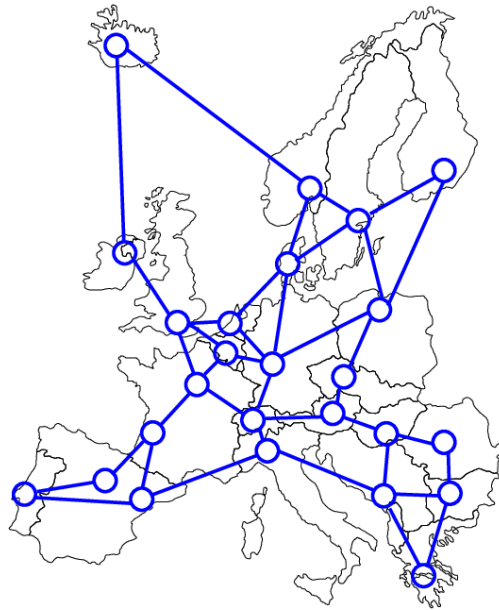


Figure 1. Design of a SDH/SONET european network where demands are multiplexed.

We studied several time dependent formulations for the unit demand vehicle routing problem [42], [41]. 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 [74] 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.

4.3. Packing and Covering Problems

Realoft 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 [73]. 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 [60]: we faced a multiple-class integer knapsack problem with setups [59] (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 [52], [51], [54], [53]. 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. 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: see <http://challenge-esicup-2015.org/>. This challenge is about loading trucks under practical constraints.

4.4. 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 [61]. 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 [63]).

Together with our partner company GAPSO from the associate team SAMBA, we worked on the equipment routing task scheduling problem [67] 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 [48] 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 [69]. A dominant class of schedules for malleable parallel jobs was discovered in the NP-hard problem to minimize the total weighted completion time [71]. We proved that a special case of the scheduling problem at cross docking terminals to minimize the storage cost is polynomially solvable [72], [70].

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 [36] 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 [44], [43], 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 [38]. We considered train timetabling problems and their re-optimization after a perturbation in the network [46], [45]. 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. 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 [47]. 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 [39].

5. Highlights of the Year

5.1. Highlights of the Year

The Inria Innovation Lab with Ertus-consulting has reached the state of outputting a strategic planner for phytosanitary treatments in viticulture, showing significant potential saving margins. The prototype was presented to the press and the wine-making industry in September 2016. This event has been followed by some articles in the specialized press (such as “Réussir Vigne”) and more generalist output (such as “Les Echos”). Industrial partnerships are being pursued with EDF (on nuclear maintenance planning) and Saint Gobain (on glass cutting optimization) and a new project has been launched with SNCF.

François Clautiaux published a book [24] about dual-feasible functions, their use to improve the resolution of several combinatorial optimization problems involving knapsack inequalities like cutting and packing, scheduling, and vehicle routing problems, and their strong links with column generation models and the underlying Dantzig-Wolfe decomposition. This book explores the general properties that identify the best dual-feasible functions, describes the general approaches that can be followed to derive new non-dominated functions, which leads on several problems to the best results reported in the literature.

Our research on decomposition based math-heuristics has led to new benchmarks, highlighting the performance of our generic procedures: for instance, we have managed to improve the best known solutions for several open Generalized Assignment Problem (GAP) instances of the literature. Similarly, our algorithms based on aggregation and disaggregation techniques [6] allowed us to outperform previous approaches for the cutting-stock problem, which is a classical benchmark problem. On the most difficult instances to date, we were able to solve optimally 240 instances out of 250, whereas previous algorithms were only able to solve 29 instances. In a more practical setting, we have developed algorithms to compute team schedules for a roster of employees [9], and these algorithms are now embedded in a professional employee **scheduling software** of the Asys company. We have also obtained strong results for scheduling problems in a high performance computing context [27], [19], which allowed to significantly improve the performance of linear algebra routines on high-end heterogeneous systems.

6. New Software and Platforms

6.1. BaPCod : A generic Branch-And-Price 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) algorithm, Benders approaches, or network flow algorithms.

- Participants: Francois Vanderbeck, Ruslan Sadykov, Issam Tahiri, Romain Leguay, Artur Alves Pessoa, Boris Detienne, Franck Labat, François Clautiaux, Pierre Pesneau, Eduardo Uchoa Barboza, Michael Poss and Halil Sen
- Partners: CNRS - IPB - Universidade Federal Fluminense - Université de Bordeaux
- Contact: François Vanderbeck
- URL: <https://wiki.bordeaux.inria.fr/realopt/pmwiki.php/Project/BaPCod>

7. New Results

7.1. Improving Branch-and-Price Methods

We have made progress on stabilization techniques and math-heuristics that are essential components for generic Branch-and-Price methods.

The convergence of a column generation algorithm can be improved in practice by using stabilization techniques. Smoothing and proximal methods based on penalizing the deviation from the incumbent dual solution have become standards of the domain. Interpreting column generation as cutting plane strategies in the dual problem, we have analyzed [29] the mechanisms on which stabilization relies. In particular, the link is established between smoothing and in-out separation strategies to derive generic convergence properties. For penalty function methods as well as for smoothing, we describe proposals for parameter self-adjusting schemes. Such schemes make initial parameter tuning less of an issue as corrections are made dynamically. Such adjustments also allow to adapt the parameters to the phase of the algorithm. Extensive test reports validate our self-adjusting parameter scheme and highlight their performances. Our results also show that using smoothing in combination with penalty function yields a cumulative effect on convergence speed-ups.

Math heuristics have become an essential component in mixed integer programming (MIP) solvers. Extending MIP based heuristics, we have studied [18], [30] generic procedures to build primal solutions in the context of a branch-and-price approach. As the Dantzig-Wolfe reformulation of a problem is typically tighter than that of the original compact formulation, heuristics based on rounding its linear programming (LP) solution can be more competitive. We focus on the so-called diving methods that used re-optimization after each LP rounding. We explore combination with diversification- intensification paradigms such as Limited Discrepancy Search, sub-MIPing, relaxation induced neighborhood search, 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.

7.2. Aggregation Techniques

We have developed [6] a general solution framework based on aggregation techniques to solve NP-Hard problems that can be formulated as a circulation model with specific side constraints. The size of the extended Mixed Integer Linear Programming formulation is generally pseudo-polynomial. To efficiently solve exactly these large scale models, we propose a new iterative aggregation and disaggregation algorithm. At each iteration, it projects the original model onto an aggregated one, producing an approximate model. The process iterates to refine the current aggregated model until the optimality is proved.

The computational experiments on two hard optimization problems (a variant of the vehicle routing problem and the cutting-stock problem) show that a generic implementation of the proposed framework allows us to outperform previous known methods.

We have applied this aggregation method to reduce the size of column generation (CG) models for covering problems in which the feasible subsets depend on a resource constraint [10]. The aggregation relies on a correlation between the resource consumption of the elements and the corresponding optimal dual values. The resulting aggregated dual model is a restriction of the original one, and it can be rapidly optimized to obtain a feasible dual solution. A primal bound can also be obtained by restricting the set of columns to those saturated by the dual feasible solution obtained by aggregation. The convergence is realized by iterative disaggregation until the gap is closed by the bounds. Computational results show the usefulness of our method for different cutting-stock problems. An important advantage is the fact that it can produce high-quality dual bounds much faster than the traditional lagrangian bound used in stabilized column generation.

7.3. Review of Algorithmic Enhancements for Benders Decomposition

In Benders decomposition approach to mixed integer programs, the optimization is carried in two stages: key first-stage decision variables are optimized using a polyhedral approximation of the full-blown problem projection, then a separation problem expressed in the second-stage variables is solved to check if the current first-stage solution is truly feasible, and otherwise, it produces a violated inequality. Such cutting-plane algorithms suffer from several drawbacks and may have very bad convergence rates. We have reviewed [23] the battery of approaches that have been proposed in the literature to address these drawbacks and to speed-up the algorithm. Our contribution consists in explaining these techniques in simple terms and unified notations, showing that in several cases, different proposals of the literature boil down to the same key ideas. We classify methods into specific initialization mode, stabilization techniques, strategies to select the separation point, and cut generation strategies. Where available, we highlight numerical benchmarks that have resulted from such enhancements.

7.4. Vehicle Routing Problems

Given a directed graph $G = (V, A)$, a cost function c associated with the arcs of A , and a set of precedence constraints $B \subset V \times V$, the Precedence Constrained Asymmetric Traveling Salesman Problem (PCATSP)

seeks for a minimum cost Hamiltonian circuit, starting at node 1, and such that for each $(i, j) \in B$, the node i is visited before node j . There are many ways of modelling the ATSP and several for the PCATSP. In [20] we present new formulations for the two problems that can be viewed as resulting from combining precedence variable based formulations with network flow based formulations. Indeed, the former class of formulations permits to integrate linear ordering constraints. The motivating formulation for this work is a complicated and “ugly” formulation that results from the separation of generalized subtour elimination constraints presented. This so called “ugly” formulation exhibits, however, one interesting feature, namely the “disjoint subpaths” property that is further explored to create more complicated formulations that combine two (or three) “disjoint path” network flow based formulations and have a stronger linear programming bound. Some of these stronger formulations are related to the ones presented for the PCATSP and can be viewed as generalizations in the space of the precedence based variables. Several sets of projected inequalities in the space of the arc and precedence variables are obtained by projection from these network flow based formulations. Computational results for the ATSP and PCATSP evaluate the quality of the new models and inequalities.

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 [17], 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 [22], [21], 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.

7.5. Production Scheduling Problems

We have considered [7] the flowshop problem on two machines with sequence-independent setup times to minimize total completion time. Large scale network flow formulations of the problem are suggested together with strong Lagrangian bounds based on these formulations. To cope with their size, filtering procedures are developed. To solve the problem to optimality, we embed the Lagrangian bounds into two branch-and-bound algorithms. The best algorithm is able to solve all 100-job instances of our testbed with setup times and all 140-job instances without setup times, thus significantly outperforming the best algorithms in the literature.

In [9], we address a multi-activity tour scheduling problem with time varying demand. The objective is to compute a team schedule for a fixed roster of employees in order to minimize the over-coverage and the under-coverage of different parallel activity demands along a planning horizon of one week. Numerous complicating constraints are present in our problem: all employees are different and can perform several different activities during the same day-shift, lunch breaks and pauses are flexible, demand is given for 15 minutes periods. Employees have feasibility and legality rules to be satisfied, but the objective function does not account for any quality measure associated with each individual’s schedule. More precisely, the problem mixes simultaneously days-off scheduling, shift scheduling, shift assignment, activity assignment, pause and lunch break assignment.

To solve this problem, we developed four methods: a compact Mixed Integer Linear Programming model, a branch-and-price like approach with a nested dynamic program to solve heuristically the subproblems, a diving heuristic and a greedy heuristic based on our subproblem solver. The computational results, based on both real cases and instances derived from real cases, demonstrate that our methods are able to provide good quality solutions in a short computing time. Our algorithms are now embedded in a commercial software, which is already in use in a mini-mart company.

7.6. Scheduling and Placement for HPC

With the complexification of the architecture of HPC nodes (multicores, non uniform memory access, GPU and accelerators), a recent trend in application development is to explicitly express the computations as a task graph, and rely on a specialized middleware stack to make scheduling decisions and implement them. Traditional algorithms used in this community are dynamic heuristics, to cope with the unpredictability of execution times. In [12], we analyze the performance of static and hybrid strategies, obtained by adding more static (resp. dynamic) features into dynamic (resp. static) strategies. Our conclusions are somehow unexpected in the sense that we prove that static-based strategies are very efficient, even in a context where performance estimations are not very good. We also present and generalize HeteroPrio, a semi-static resource-centric strategy based on the acceleration factors of tasks. In [19], we generalize this strategy to platforms with more than two types of resources. This allows to use intra-task parallelism by grouping several CPU cores together. In [27], we prove tight approximation ratios for HeteroPrio in the context of independent tasks, providing a theoretical insight to its good practical performance.

Another study [26] focuses on the memory-constrained case, where tasks may produce large data. A task can only be executed if all input and output data fit into memory, and a data can only be removed from memory after the completion of the task that uses it as an input data. There is a known, polynomial time algorithm [55] to minimize the peak memory used on one machine for the cases where the input graph is a rooted tree. We generalize in [26] to the variant where the input graph is a directed series-parallel graph, and propose a polynomial time algorithm. This allows to solve this practical problem in two important classes of applications.

In [13], we consider the static problem of data placement for matrix multiplication in heterogeneous machines, so as to optimize both load balancing and communication volume. This is modeled as a partitioning of a square into a set of zones of prescribed areas, while minimizing the overall size of their projections onto horizontal and vertical axes. We combine two ideas from the literature (recursive partitioning, and optimal solution structure for low number of processors) to obtain a non-rectangular recursive partitioning (NRRP), whose approximation ratio is $\frac{2}{\sqrt{3}} \simeq 1.15$, improving over the previous 1.25 ratio. Moreover, we observe on a large set of realistic platforms built from CPUs and GPUs that this proposed NRRP algorithm allows to achieve very efficient partitionings on all considered cases. In [14], we consider the generalization of this problem to the three dimensional case. We prove the NP-completeness of the problem, and propose a generalisation of NRRP with a $(\frac{5}{6})^{\frac{2}{3}}$ approximation ratio.

7.7. Network Design Problems

The delivery of freight from manufacturing platforms to demand zones is often managed through one or more intermediate locations where storing, merging, transshipment and consolidation activities are performed. In [15], we design a Two-Echelon Distribution Network that helps synchronize different flows of product. Under demand uncertainty, our model integrates decisions on the locations and the size of second echelon facilities and decisions on the flows assignment between the echelons, and on delivery routes to serve the demand zones.

In [8], we study the k -edge-connected L -hop-constrained network design problem. Given a weighted graph $G = (V, E)$, a set D of pairs of nodes, two integers $L \geq 2$ and $k \geq 2$, the problem consists in finding a minimum weight subgraph of G containing at least k edge-disjoint paths of length at most L between every pair $\{s, t\} \in D$. We consider the problem in the case where $L = 2, 3$ and $|D| \geq 2$. We first discuss integer programming formulations introduced in the literature. Then, we introduce new integer programming formulations for the problem that are based on the transformation of the initial undirected graph into directed layered graphs. We present a theoretical comparison of these formulations in terms of LP-bound. Finally, these formulations are tested using CPLEX and compared in a computational study for $k = 3, 4, 5$.

7.8. Strategic Planning of Phytosanitary treatments in Wineries

In [16], we consider planning phytosanitary treatments in a vineyard. We are given a set of diseases (or requests) that must be treated for each site. Product mixtures are defined by their composition of active components, and their duration of protective power for each request. Machines are available to spread the

mixtures on the sites. The time horizon is divided in time periods. Sites are partitioned in sectors. The objective of the problem is to minimize the machine leasing costs, their travel cost to sectors and the costs related to the product use. To solve this problem, we use a column generation approach where the machine policy and the product order policy are pure master decisions, while treatment planning decisions are made in individual pricing subproblems associated with each site. We developed a dedicated dynamic program to solve the pricing subproblems.

7.9. Two-dimensional Guillotine-cut Bounded Knapsack Problem

The two-dimensional knapsack problem consists in packing a set of small rectangular items into a given large rectangle while maximizing the total reward associated with selected items. In [28], we restrict our attention to packings that emanate from a k -stage guillotine-cut process. We introduce a generic model where a knapsack solution is represented by a flow in a directed acyclic hypergraph. This hypergraph model derives from a forward labeling dynamic programming recursion that enumerates all non-dominated feasible cutting patterns. To reduce the hypergraph size, we make use of further dominance rules and a filtering procedure based on Lagrangian reduced costs fixing of hyperarcs. Our hypergraph model is (incrementally) extended to account for explicit bounds on the number of copies of each item. Our exact forward labeling algorithm is numerically compared to solving the max-cost flow model in the base hyper-graph with side constraints to model production bounds. Benchmarks are reported on instances from the literature and on datasets derived from a real-world application.

7.10. Matching-Based Allocation Strategies in Cloud Platforms

MapReduce is a well-know framework for distributing data-processing computations on parallel clusters. In MapReduce, a large computation is broken into small tasks that run in parallel on multiple machines, and scales easily to very large clusters of inexpensive commodity computers. Before the Map phase, the original dataset is first split into chunks, that are replicated (a constant number of times, usually 3) and distributed onto the computing nodes. During the Map phase, nodes request tasks and are allocated first tasks associated to local chunks (if any). Communications take place when requesting nodes do not hold any local chunk anymore. In [25], we provide the first complete theoretical data locality analysis of the Map phase of MapReduce, and more generally, for bag-of-tasks applications that behaves like MapReduce. We show that if tasks are homogeneous (in term of processing time), once the chunks have been replicated randomly on resources with a replication factor larger than 2, it is possible to find a priority mechanism for tasks that achieves a quasi-perfect number of communications using a sophisticated matching algorithm. In the more realistic case of heterogeneous processing times, we prove using an actual trace of a MapReduce server that this priority mechanism enables to complete the Map phase with significantly fewer communications, even on realistic distributions of task durations.

7.11. On Sets Avoiding Distance 1

In a joint work with C. Bachoc, T. Bellitto and P. Moustrou [11], we consider the maximum density of sets avoiding distance 1 in \mathbb{R}^n . Let $\|\cdot\|$ be a norm of \mathbb{R}^n and $G_{\|\cdot\|}$ be the so-called unit distance graph with the points of \mathbb{R}^n as vertex set and for edge set, the set of pairs $\{x, y\}$ such that $\|x - y\| = 1$. An independent set of $G_{\|\cdot\|}$ is said to avoid distance 1.

Let $\|\cdot\|_E$ denote the Euclidean norm. For $n = 2$, the chromatic number of $G_{\|\cdot\|_E}$ is still wide open: it is only known that $4 \leq \chi(G_{\|\cdot\|_E}) \leq 7$ (Nelson, Isbell 1950). The *measurable* chromatic number χ_m of the graph $G_{\|\cdot\|}$ is the minimal number of *measurable* stable sets of $G_{\|\cdot\|}$ needed to cover all its vertices. Obviously, we have $\chi(G_{\|\cdot\|_E}) \leq \chi_m(G_{\|\cdot\|_E})$. For $n = 2$, $5 \leq \chi_m(G_{\|\cdot\|_E})$ (Falconer 1981).

Let $m_1(G_{\|\cdot\|})$ denote the maximum density of a measurable set avoiding distance 1. We have $\frac{1}{m_1(G_{\|\cdot\|})} \leq \chi_m(G_{\|\cdot\|})$. We study the maximum density m_1 for norms defined by polytopes: if P is a centrally symmetric polytope and x is a point of \mathbb{R}^n , $\|x\|_P$ is the smallest positive real t such that $x \in tP$. Polytope norms include some usual norms such as the L^1 and L^∞ norms.

If P tiles the space by translation, then it is easy to see that $m_1(G_{\|\cdot\|_P}) \geq \frac{1}{2^n}$. C. Bachoc and S. Robins conjectured that equality always holds. We show that this conjecture is true for $n = 2$ and for some polytopes in higher dimensions.

8. Bilateral Contracts and Grants with Industry

8.1. Contract with EDF on robust maintenance planning

Our project with EDF concerns the optimization of the long term energy production planning, allowing for nuclear power plants maintenance. The challenges are to handle the large-scale instance of a five year planning and to handle the stochastic aspects of the problem: the stochastic variation of the electricity demand, the production capacity and the duration of maintenance period. The key decisions to be optimized are the dates of outages (for maintenance) and the level refuelling that determines the production of the year to come. We previously developed a column generation approach based on extended formulation which enables to solve within a few minutes a deterministic instance of the problem, which is within the time frame of the operational tools currently used by EDF. We now investigate stochastic and robust versions of the problem, where the duration of maintenance operations and the power demand are uncertain. Our approaches shall be evaluated on real life instances within a rolling horizon framework.

8.2. Collaboration with ERTUS on phytosanitary treatment planning

In planning winery operations (most importantly phytosanitary treatments on the wine tree) under weather forecast uncertainty, one searches for solutions that remain feasible and “cheap” in case of perturbation in the data. We consider the planning and scheduling of the operations that arise over a one-year horizon. More precisely, the operations to be scheduled include tasks related to soil care, or grape tree care: cutting, line building, thinning out leaves, ..., and chemical treatments. The latter are a main focus of our study since one of the principal goals of better planning is to reduce the amount of chemical treatments by selecting the appropriate products and schemes, but also by spacing out treatments while guarantying a disease free vineyard with some confidence. Each of the scheduled tasks requires its own resource, so the planning also triggers equipment and raw products selection decisions. The objective is to minimize both equipment and product costs augmented by an evaluation of the hazard of chemical product use. The planning should be “robust” to seasonal variations on the proper time frame for scheduling tasks.

8.3. Collaboration with St-Gobain Recherche on glass cutting

Through the PhD of Quentin Viaud, we study a hard glass-cutting problem. The objective is to minimize the quantity of trim loss when rectangular pieces are cut from large rectangles. This first study has shown that our methodologies are able to cope with this problem for medium-size instances. Solving the problem with large instances is a scientific challenge that we will address in the a follow-up contract.

8.4. Collaboration with Greycon Ltd. on industrial cutting

Through a research internship, we have studied a hard one-dimensional industrial cutting problem with many practical constraints. We have designed a non-standard diving heuristic, where some complicating constraints are handled through branching. Our heuristic was able to improve the solutions found by the industrial partner for several hard instances.

8.5. Collaboration with SNCF on timetable and rolling stock rotation planning

Our projet with SNCF concerns the optimisation of timetable and rolling stock rotation planning. The railway production planning process combines heterogeneous resources and is usually decomposed into different sequential sub-problems, beginning by line planning, timetabling, rolling stock rotations and crew scheduling. Our goal is to solve the timetable and rolling stock problems in an integrated manner. Given a line planning and service requirement constraints, the problem is to produce a timetable for a set of trains and the objective is to minimize the cost of the railcars used. An originality of our approach is to deal with railcars composed of multiple units, which can be coupled or decoupled at some stations. The PhD thesis of Mohamed Benkirane is funded by this project.

9. Partnerships and Cooperations

9.1. Regional Initiatives

We have received support from the regional authorities (Region Aquitaine) for a research project on the planning under uncertainty. A postdoc, Agnès Leroux, has been recruited on this project. She currently develops dynamic programming approaches for scheduling problems and their application to building planning for phytosanitary treatments.

9.2. National Initiatives

9.2.1. ANR

9.2.1.1. ANR Solhar (ANR-13-MONU-0007)

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 computing platforms equipped with accelerators. This project proposes an innovative approach which relies on the efficiency and portability of runtime systems, such as the StarPU tool. The focus of RealOpt in this project is on the scheduling aspect. Indeed, executing a heterogeneous workload with complex dependencies on a heterogeneous architecture is a very challenging problem that demands the development of effective scheduling algorithms. These will be confronted with possibly limited views of dependencies among tasks and multiple, and potentially conflicting objectives, such as minimizing the makespan, maximizing the locality of data or, where it applies, minimizing the memory consumption.

See also: <http://solhar.gforge.inria.fr/>

9.2.1.2. ANR SONGS (ANR 11 INFRA 13)

The goal of the SONGS project is to extend the applicability of the SimGrid simulation framework from Grids and Peer-to-Peer systems to Clouds and High Performance Computation systems. Any sound study of such systems through simulations relies on the following pillars of simulation methodology: Efficient simulation kernel; Sound and validated models; Simulation analysis tools; Campaign simulation management. The contribution of RealOpt in this project revolves around enabling peer-to-peer simulation, and providing use cases for Cloud Computing simulations.

See also: <http://infra-songs.gforge.inria.fr/>

9.3. International Initiatives

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

9.3.1.1. SAMBA

Title: Synergies for Ameliorations and Mastering of Branch-and-Price Algorithms

International Partner (Institution - Laboratory - Researcher):

Universidade Federal Fluminense (Brazil) - LIGOS - Eduardo Uchoa

Start year: 2011

See also: https://realopt.bordeaux.inria.fr/?page_id=573

SAMBA is a research project between the Inria project team ReAIOpt (Bordeaux, France), the ADT-Lab Pontifícia Universidade Católica do Rio de Janeiro, and the LOGIS at the Universidade Federal Fluminense. The project is supported by Inria under the “associate team” framework for an initial period of three years (2011-2013) and was renewed for another three years period (2014-2016) with additional partners at the Operations Research and Complex Systems Group School of Business, Universidad Adolfo Ibáñez, Chile, and the LIRMM at the University of Montpellier.

Quantitative models are important tools for strategic, tactical, and operational decision-making. Many underlying optimization problems are discrete in nature. They are modeled as linear programs with integer variables, so called Mixed Integer Programs (MIP). Their solution is essentially based on enumeration techniques, which is notoriously difficult given the huge size of the solution set. Powerful generic commercial solvers for MIP are available, but despite continuous progress, the existing tools can be overwhelmed when problem complexity or size increases.

Decomposition approaches are primary tools to expand the capabilities of MIP solution techniques. When the application presents a decomposable constraint system, the so-called “Dantzig-Wolfe decomposition” consists in reformulating the problem as a selection of a specific solution for each individual subsystems that together satisfy the linking constraints. In practice, the individual subsystem solutions are brought in the formulation in the course of the optimization if they can lead to improvement in the objective value. On the other hand, “Benders’ decomposition applies when the the application presents a decomposable system of variables, as traditional in stochastic two-stage optimization models where main decisions are taken prior to knowing the realization of random data, while second stage decision are adjustments that can be done once the true value of data is revealed. In this context, one solves the first stage model and check a posteriori the feasibility of the second stage. In case the second stage is infeasible, a constraint on the first stage variables is induced that aim to account for the cause of second stage infeasibility, and the processus reiterates.

Both of these decomposition approaches are perceived as requiring an application specific implementation for tractability in scaling-up to real-life applications. Our research aim at developing generic methods for these and algorithmic enhancements to can yield significant speed-ups in practice and have sound theoretical basis. Such research includes methodological developments (such as stabilization techniques for improved convergence, preprocessing rules, dynamic aggregation-and-disaggregation), algorithms strategies (such as multi-column/cut generation strategies, pre-evaluation of enumerated subproblem strategies – so-called strong branching), and efficient implementations (code re-engineering of our software platform BaPCod).

Beyond the methodological developments, our motivations are to set new benchmarks on standard combinatorial problems and industrial applications. In particular, we proceed to extend our techniques to the context of dynamic optimization. In a stochastic environment, the aim is to build a planning that are robust to perturbations in the sense that it can be adapted dynamically in reaction to the observed changes in the predicted data.

The project builds on the accumulated experience of both the Brazilian, the Chilean and the French teams that have done pioneering work in tackling complex applications and deriving generic solution strategies using this decomposition approach.

9.4. International Research Visitors

9.4.1. Visits of International Scientists

- LEITE BULHOES Teobaldo, from Universidade Federal Fluminense (Niteroi, Brazil), visited the team from November 2nd to December 9th.

9.4.2. Visits to International Teams

9.4.2.1. Sabbatical programme

Sadykov Ruslan

Date: Aug 2015 - Jul 2016

Institution: [Universidade Federal Fluminense](#) (Brazil)

9.4.2.2. Research Stays Abroad

- Thomas Lambert
Date: Feb 8 - Mar 4
Institution: [University College of Dublin](#) (Ireland)

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

10.1.1.1. Member of the Organizing Committees

- Pierre Pesneau has organized the workshop “Polyhedral Approaches for Combinatorial Optimization”, December 8-9 2016, Paris
- Arnaud Pêcher has organized the workshop “Bordeaux Graph Workshop”, Novembre 7-10 2016, Bordeaux.

10.1.2. Scientific Events Selection

10.1.2.1. Chair of Conference Program Committees

- Lionel Eyraud-Dubois is Chair of the “Cloud Computing and Data Center Management” track of I-SPAN 2017: the 14th International Symposium on Pervasive Systems, Algorithms, and Networks
- Olivier Beaumont is Co-Chair of the Algorithms track of ICPP 2016: 2016 International Conference on Parallel Processing

10.1.2.2. Member of the Conference Program Committees

The team members are members of the following program committees:

- François Clautiaux: ROADEF 2016: French Operational Research Society Conference.
- Lionel Eyraud-Dubois: ICPP 2016: 2016 International Conference on Parallel Processing
- Lionel Eyraud-Dubois and Olivier Beaumont: HiPC 2016: 23rd IEEE International Conference on High Performance Computing, Data, and Analytics
- Olivier Beaumont: IPDPS 2016, 30th IEEE International Parallel & Distributed Processing Symposium
- Olivier Beaumont: Euro-EDUPAR 2016, Parallel and Distributed Computing Education for Undergraduate Students, a EuroPar workshop
- Olivier Beaumont: HeteroPar 2016: Algorithms, Models, and Tools for Parallel Computing on Heterogeneous Platforms, a EuroPar Workshop

10.1.3. Journal

10.1.3.1. Member of the Editorial Boards

- Olivier Beaumont is editor for IEEE Transactions on Parallel and Distributed Systems (TPDS)
- François Vanderbeck is Associate Editor for the EURO Journal on Computational Optimization
- François Clautiaux is Associate Editor for Mathematical Programming and Exact Methods in the journal ISTE “Recherche Opérationnelle”

10.1.3.2. Reviewer - Reviewing Activities

The team members are regular referees for the best journals of the field.

10.1.4. Invited Talks

Arnaud Pêcher: *On sets avoiding distance 1*, 2016 International Conference on Graph Theory, Jinhua, Chine, 2016

10.1.5. Scientific Expertise

- Olivier Beaumont is a member of the **INCITE (math-comp track) panel**
- Olivier Beaumont is an expert for the H2020-FET-OPEN-2016 projects

10.1.6. Research Administration

- Olivier Beaumont is the scientific deputy of Inria Bordeaux Sud-Ouest and a member of the Evaluation Committee of Inria.
- François Vanderbeck is taking care of the team OptimAI (“Optimisation Mathématique Modèle Aléatoire et Statistique”) at the Mathematics Institute of Bordeaux.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

Licence : A. Pêcher, Programmation Impérative, 10h, DUT, Université de Bordeaux, France
 Licence : A. Pêcher, Conception Objet, 42h, DUT, Université de Bordeaux, France
 Licence : A. Pêcher, Programmation objet en Java, 44h, DUT, Université de Bordeaux, France
 Licence : A. Pêcher, Algorithmique Avancée, 32h, DUT, Université de Bordeaux, France
 Licence : A. Pêcher, Assembleur, 24h, DUT, Université de Bordeaux, France
 Licence : A. Pêcher, Programmation Mobile, 24h, DUT, Université de Bordeaux, France
 Master : F. Clautiaux, Gestion des Opérations et Planification de la Production, 20h, M2, Université de Bordeaux, France
 Master : F. Clautiaux, Flot et Combinatoire, 10h, M2, Institut Polytechniques de Bordeaux, France
 Master : F. Clautiaux, Introduction à la Programmation en Variables Entières, 20h, M1, Université de Bordeaux, France
 Master : F. Clautiaux, Projet d’optimisation pour l’insertion professionnelle, M2, Université de Bordeaux, France
 Master : L. Eyraud-Dubois, Optimisation en Cloud Computing et Big Data, 15h, M2, Université de Bordeaux, France
 Master : L. Eyraud-Dubois, Algorithmique et Programmation, 30h, M1, Université de Bordeaux, France
 Master : L. Eyraud-Dubois, Introduction à la Programmation en Variables Entières, 15h, M1, Université de Bordeaux, France
 Licence : P. Pesneau, Modèles et Méthodes d’Optimisation, 30h, L2, Université de Bordeaux, France

Licence : P. Pesneau, Système et programmation en Fortran 90, 24h, L2, Université de Bordeaux, France

Licence : P. Pesneau, Recherche Opérationnelle, 24h, DUT, Université de Bordeaux, France

Master : P. Pesneau, Algorithmique et Programmation 1, 60h, M1, Université de Bordeaux, France

Master : P. Pesneau, Algorithmique et Programmation 2, 30h, M1, Université de Bordeaux, France

Master : P. Pesneau, Programmation linéaire, 15h, M1, Université de Bordeaux, France

Master : P. Pesneau, Optimisation dans les graphes (partie flots), 15h, M1, Université de Bordeaux, France

Master : O. Beaumont, Approximation et Big Data, 15h, M2, Université de Bordeaux, France

Master : O. Beaumont, Distributed Computing and Data Mining, 4h, M2, Institut National Polytechnique de Bordeaux, France

Master : B. Detienne, Optimisation continue, 29h, M1, Université de Bordeaux, France

Master : B. Detienne, Recherche Opérationnelle, 16h, M1, Institut National Polytechnique de Bordeaux, France

Master : B. Detienne, Introduction à la Programmation en Variables Entières, 14h, M1, Université de Bordeaux, France

Master : B. Detienne, Gestion des Opérations et Planification de la Production, 28h, M2, Université de Bordeaux, France

Master : B. Detienne, Optimisation dans l'incertain, 58h, M2, Université de Bordeaux, France

Master : B. Detienne, Problèmes combinatoires et routage, 14h, M1, Université de Bordeaux, France

Master : I. Tahiri, Outils et Logiciels pour l'Optimisation, 30h, M1, Université de Bordeaux, France

Master : F. Vanderbeck, Recherche Opérationnelle, 15h, M1, Institut National Polytechnique de Bordeaux, France

Master : F. Vanderbeck, Programmation Entière, 58h, M2, Université de Bordeaux, France

10.2.2. Supervision

PhD in progress : Jérémy Guillot, Optimisation de problèmes de partitionnement, September 2014, François Clautiaux (dir) and Pierre Pesneau (dir).

PhD in progress : Quentin Viaud, Méthodes de programmation mathématiques pour des problèmes complexes de découpe, January 2015, François Clautiaux (dir), Ruslan Sadykov (dir), and François Vanderbeck (co-dir)).

PhD in progress : Martin Bué, Gestion du revenu dans le cadre du voyage professionnel, September 2012, François Clautiaux (dir), Luce Brotcorne (dir).

PhD in progress : Rodolphe Griset, Robust planning in Electricity production, November 2015, Boris Detienne (dir) and François Vanderbeck (dir).

PhD in progress : Imen Ben Mohamed, Location routing problems, October 2015, Walid Klibi (dir) and François Vanderbeck (dir).

PhD in progress : Thomas Bellitto, Infinite graphs, September 2015, Arnaud Pêcher (dir) and Christine Bachoc (dir).

PhD in progress : Philippe Moustrou, Codes, September 2014, Arnaud Pêcher (dir) and Christine Bachoc (dir).

PhD in progress : Thomas Lambert, September 2014, Placement de tâches et réplication de fichiers sur plates-formes parallèles, Olivier Beaumont (dir) and Lionel Eyraud-Dubois (co-dir)

PhD in progress : Suraj Kumar, December 2013, Scheduling of Dense Linear Algebra Kernels on Heterogeneous Resources, Olivier Beaumont (dir) and Lionel Eyraud-Dubois (co-dir)

10.2.3. Juries

- François Clautiaux: Evaluation (rapporteur) of the PhD thesis of Charly Lersteau (University Bretagne Sud)
- Ruslan Sadykov: Evaluation (examinateur) of the PhD thesis of Rian Gabriel Santos Pinheiro (University Federal Fluminense, Niteroi, Brazil), March 1st, 2016.

10.3. Popularization

François Clautiaux is a member of the board of AMIES, the French Agency for Interaction in Mathematics with Business and Society. AMIES is a national organization that aims to develop relations between academic research teams in mathematics and business, especially SMEs.

11. Bibliography

Major publications by the team in recent years

- [1] R. SADYKOV, F. VANDERBECK. *Column Generation for Extended Formulations*, in "EURO Journal on Computational Optimization", May 2013, vol. 1, n^o 1-2, p. 81-115 [DOI : 10.1007/s13675-013-0009-9], <https://hal.inria.fr/hal-00661758>.
- [2] R. SADYKOV, L. A. WOLSEY. *Integer Programming and Constraint Programming in Solving a Multimachine Assignment Scheduling Problem with Deadlines and Release Dates*, in "INFORMS Journal on Computing", 1 2006, vol. 18, n^o 2, p. 209–217.
- [3] F. VANDERBECK. *Branching in Branch-and-Price: a Generic Scheme*, in "Mathematical Programming, Series A", 2011, vol. 130, p. 249-294 [DOI : 10.1007/s10107-009-0334-1], <http://hal.inria.fr/inria-00311274>.
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- [5] F. VANDERBECK, L. WOLSEY. *Reformulation and Decomposition of Integer Programs*, in "50 Years of Integer Programming 1958-2008", Springer, 2010, CORE DP 2009/16 [DOI : 10.1007/978-3-540-68279-0_13], <http://hal.inria.fr/inria-00392254>.

Publications of the year

Articles in International Peer-Reviewed Journal

- [6] F. CLAUTIAUX, S. HANAFI, R. MACEDO, M.-É. VOGÉ, C. ALVES. *Iterative aggregation and disaggregation algorithm for pseudo-polynomial network flow models with side constraints*, in "European Journal of Operational Research", October 2016 [DOI : 10.1016/J.EJOR.2016.09.051], <https://hal.inria.fr/hal-01410170>.
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- [8] I. DIARRASSOUBA, V. GABREL, A. R. MAHJOUR, L. GOUVEIA, P. PESNEAU. *Integer programming formulations for the k-edge-connected 3-hop-constrained network design problem*, in "Networks", March 2016, vol. 67, n^o 2 [DOI : 10.1002/NET.21667], <https://hal.inria.fr/hal-01281958>.

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[10] D. PORUMBEL, F. CLAUTIAUX. *Constraint Aggregation in Column Generation Models for Resource-Constrained Covering Problems*, in "INFORMS Journal on Computing", 2016, <https://hal.inria.fr/hal-01410195>.

Invited Conferences

[11] C. BACHOC, T. BELLITTO, P. MOUSTROU, A. PÊCHER. *On sets avoiding distance 1*, in "2016 International Conference on Graph Theory, Combinatorics and Applications", Jinhua, China, October 2016, <https://hal.archives-ouvertes.fr/hal-01408959>.

International Conferences with Proceedings

[12] E. AGULLO, O. BEAUMONT, L. EYRAUD-DUBOIS, S. KUMAR. *Are Static Schedules so Bad ? A Case Study on Cholesky Factorization*, in "IEEE International Parallel & Distributed Processing Symposium (IPDPS 2016)", Chicago, IL, United States, IEEE, May 2016, <https://hal.inria.fr/hal-01223573>.

[13] O. BEAUMONT, L. EYRAUD-DUBOIS, T. LAMBERT. *A New Approximation Algorithm for Matrix Partitioning in Presence of Strongly Heterogeneous Processors*, in "30th IEEE International Parallel & Distributed Processing Symposium", Chicago, France, IEEE (editor), Proceedings of the 30th IEEE International Parallel & Distributed Processing Symposium, IPDPS'16, IEEE, May 2016, <https://hal.inria.fr/hal-01216245>.

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[15] I. BEN MOHAMED, W. KLIBI, F. VANDERBECK. *Designing Two-Echelon Distribution Network under Demand Uncertainty*, in "VEROLOG", Nantes, France, June 2016, <https://hal.inria.fr/hal-01425739>.

[16] A. LE ROUX, B. DETIENNE, R. SADYKOV, I. TAHIRI, A. TOULLAT, F. VANDERBECK. *Strategic Planning of Phytosanitary treatments in Wineries*, in "ROADEF", Compiègne, France, February 2016, <https://hal.inria.fr/hal-01425704>.

[17] N. RAHMANI, B. DETIENNE, R. SADYKOV, F. VANDERBECK. *A Column Generation Based Heuristic for the Dial-A-Ride Problem*, in "International Conference on Information Systems, Logistics and Supply Chain (ILS)", Bordeaux, France, June 2016, <https://hal.inria.fr/hal-01425755>.

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Conferences without Proceedings

[19] O. BEAUMONT, T. COJEAN, L. EYRAUD-DUBOIS, A. GUERMOUCHE, S. KUMAR. *Scheduling of Linear Algebra Kernels on Multiple Heterogeneous Resources*, in "International Conference on High Performance Computing, Data, and Analytics (HiPC 2016)", Hyderabad, India, December 2016, <https://hal.inria.fr/hal-01361992>.

- [20] L. GOUVEIA, P. PESNEAU, M. RUTHMAIR, D. SANTOS. *Network flow precedence based formulations for the asymmetric traveling salesman problem with precedence constraints*, in "4th International Symposium on Combinatorial Optimization (ISCO 2016)", Vietri sul Mare, Italy, May 2016, <https://hal.inria.fr/hal-01418319>.
- [21] P. PESNEAU, F. CLAUTIAUX, J. GUILLOT. *Aggregation technique applied to a clustering problem for waste collection*, in "ROADEF 2016", Compiègne, France, February 2016, <https://hal.inria.fr/hal-01418346>.
- [22] P. PESNEAU, F. CLAUTIAUX, J. GUILLOT. *Aggregation technique applied to a clustering problem*, in "4th International Symposium on Combinatorial Optimization (ISCO 2016)", Vietri sul Mare, Italy, May 2016, <https://hal.inria.fr/hal-01418337>.
- [23] H. ŞEN, B. DETIENNE, R. SADYKOV, F. VANDERBECK. *A review of algorithmic enhancements for Benders decomposition*, in "4th International Symposium on Combinatorial Optimization (ISCO 2016)", Vietri-sul-mare, Italy, May 2016, <https://hal.inria.fr/hal-01427944>.

Scientific Books (or Scientific Book chapters)

- [24] C. ALVES, F. CLAUTIAUX, J. M. VALÉRIO DE CARVALHO, J. RIETZ. *Dual-Feasible Functions for Integer Programming and Combinatorial Optimization*, Springer, January 2016, <https://hal.inria.fr/hal-01410180>.

Research Reports

- [25] O. BEAUMONT, T. LAMBERT, L. MARCHAL, B. THOMAS. *Matching-Based Allocation Strategies for Improving Data Locality of Map Tasks in MapReduce*, Inria - Research Centre Grenoble – Rhône-Alpes ; Inria Bordeaux Sud-Ouest, November 2016, n^o RR-8968, <https://hal.inria.fr/hal-01386539>.
- [26] E. KAYAASLAN, T. LAMBERT, L. MARCHAL, B. UÇAR. *Scheduling Series-Parallel Task Graphs to Minimize Peak Memory*, Inria Grenoble Rhône-Alpes, Université de Grenoble, November 2016, n^o RR-8975, <https://hal.inria.fr/hal-01397299>.

Other Publications

- [27] O. BEAUMONT, L. EYRAUD-DUBOIS, S. KUMAR. *Approximation Proofs of a Fast and Efficient List Scheduling Algorithm for Task-Based Runtime Systems on Multicores and GPUs*, October 2016, working paper or preprint, <https://hal.inria.fr/hal-01386174>.
- [28] F. CLAUTIAUX, R. SADYKOV, F. VANDERBECK, Q. VIAUD. *Combining dynamic programming with filtering to solve a four-stage two-dimensional guillotine-cut bounded knapsack problem*, December 2016, working paper or preprint, <https://hal.inria.fr/hal-01426690>.
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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
Computational Neuroscience and Medecine

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Project-Team SISTM

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Keywords:

Computer Science and Digital Science:

- 3.3.2. - Data mining
- 3.3.3. - Big data analysis
- 3.4.1. - Supervised learning
- 3.4.2. - Unsupervised learning
- 3.4.4. - Optimization and learning
- 3.4.5. - Bayesian methods
- 6.1.1. - Continuous Modeling (PDE, ODE)
- 6.2.4. - Statistical methods
- 6.3.1. - Inverse problems
- 6.3.4. - Model reduction
- 6.4.2. - Stochastic control

Other Research Topics and Application Domains:

- 1.1. - Biology
- 1.1.6. - Genomics
- 1.1.7. - Immunology
- 1.1.9. - Bioinformatics
- 1.1.11. - Systems biology
- 1.4. - Pathologies
- 2.2.4. - Infectious diseases, Virology
- 2.2.5. - Immune system diseases
- 2.3. - Epidemiology
- 2.4.1. - Pharmacokinetics and dynamics
- 2.4.2. - Drug resistance
- 2.8. - Sports, performance, motor skills

1. Members

Research Scientists

Daniel Commenges [INSERM, Senior Researcher, HDR]
Melanie Prague [Inria, Researcher]

Faculty Members

Rodolphe Thiébaud [Team leader, PUPH, Univ. Bordeaux, Professor, HDR]
Marta Avalos Fernandez [Univ. Bordeaux, Associate Professor]
Robin Genuer [Univ. Bordeaux, Associate Professor]
Laura Richert [MCUPH, Univ. Bordeaux, Associate Professor]
Boris Hejblum [Univ. Bordeaux, Associate Professor]

Technical Staff

Henri Bonnabau [Univ. Bordeaux]

Chariff Alkassim [INSERM, from Mar 2015]
Aaron Ayllon Benitez [INSERM, from until Oct 2016]

PhD Students

Perrine Soret [INSERM]
Laura Villain [Univ. Bordeaux]
Chloe Pasin [Univ. Bordeaux]
Edouard Lhomme [Univ. Bordeaux]
Hadrien Lorenzo [Univ. Bordeaux]

Post-Doctoral Fellow

Marius Kwemou [INSERM, from May 2016]

Administrative Assistants

Sandrine Darmigny [INSERM]
Catherine Cattaert Megrat [Inria]
Sylvie Embolla [Inria]
Anton Ottavi [INSERM, European Projects coordinator]
Destandau Eugénie [INSERM, Communication]

Others

David Myers [Master Internship, from Apr 2016 until Sep 2016]
Chloé Belguermi [Master Internship, from Apr 2016 until Sep 2016]
Thomas Esnaud [Master Internship, from Mar 2016 until Aug 2016]
Jean-Louis Palgen [Master Internship, from Feb 2016 until Jun 2016]
Hao Ren [Master Internship, from Mar 2016 until Aug 2016]
Madelyn Yiseth Rojas Castro [Master Internship, from Jul 2016 until Sep 2016]
Hugo Thiessard [Assistant ingenior Internship, Jul 2016]

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 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 technology, 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.

2.2. Overall Applied Objectives

Data are generated in clinical trials or biological experimentations. Our main application of interest is the immune response to vaccine or other immune interventions (such as exogenous cytokines), mainly in the context of HIV infection. The methods developed in this context can be applied in other circumstances but the focus of the team on immunology 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/fr/>). Examples of objectives related to this application field are:

- To understand how immune response is generated with immune interventions (vaccines or interleukines)
- To predict what would be the immune response to a given immune intervention for designing next studies and adapting interventions to individual patients

3. Research Program

3.1. Mechanistic modelling

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 summarising the dynamics over time in term of slopes of the trajectories [51]. These slopes can be compared between treatment groups or according to patients' characteristics. Another way for analysing 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 [41]. 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 [40].

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 [30]. 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 [28].

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 [44], [54], [33], [42], [36], [53], the difficulty associated with the complexity of ODE models and the sparsity of the data leading to identifiability issues need further research.

3.2. High dimensional data

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 become 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 become 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 network⁰. As an example, in a recent 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 [50]. 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 datasets.

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 datasets typically contain many variables, much more than observations. Hence, multiple testing is an obvious issue that needs to be taken into account [45]. 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 [52]. The integrative analysis of large datasets 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 [37]. The comprehensive analysis of these large datasets 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" [47], "Systems vaccinology" [43], "Systems medicine" [32]. From the statistician point of view, two main challenges appear: i) to deal with the massive amount of data ii) to find relevant models capturing observed behaviors.

4.2. The case of HIV immunology

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 [39]. 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) [31]. However, the implementation of such strategy is difficult especially in developing countries. Some HIV infected individuals do not tolerate antiretroviral regimen or did not

⁰see online at <http://www.eurocoord.net>

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. The case of Ebola vaccine development

In response to the recent outbreak of Ebola virus disease in West Africa, the clinical development of some candidate to Ebola vaccine has been accelerated. Several vectors, mostly encoding glycoprotein of the virus, were tested in Phase I-II studies in order to assess their safety and immunogenicity. One of the main question of interest there is the antibody response induced by vaccination, as some non-human primates studies have shown protection against the virus when antibody levels were high enough. Although bridging studies still have to be developed, antibodies are thus considered as a criterium of interest. The challenge is then to evaluate the durability of the antibody response, whether it be at an individual or population level, in order to evaluate the impact of a vaccine strategy in case of an epidemic. Moreover, we are interested in the factors associated to this antibody response, and even more the other immune markers (from both innate and adaptative immune response) able to predict antibody levels. As those relationship are non-linear, sophisticated statistical and mathematical methods are developed in order to address these questions. A systems medicine approach using multidimensional immunogenicity data from clinical trials and statistical models can help to understand vaccine mechanisms and improve the selection of optimised vaccine strategies for clinical trials.

5. Highlights of the Year

5.1. Highlights of the Year

Modeling clinical trials of IL7

We have published the results of two clinical trials [17] that are showing the feasibility of repeating IL-7 cycles and confirmed the predictions performed with our dynamical model published in [49]. This mecanistic modeling allow to propose protocol which decrease the number of injection within each IL-7 cycle while keeping the same efficacy [35].

Awards Mélanie Prague published an invited paper on her PhD works (which was supervized by Daniel Commenges and co-supervized by Rodolphe Thiébaud) as a perks for the attribution of the "Marie-Jeanne Laurent-Duhamel PhD award (2015) by the SFdS (Société Francaise de statistiques). [15]

6. New Software and Platforms

6.1. New software

6.1.1. *clogitLasso*

Lasso Estimation of Conditional Logistic Regression Models for Case-Crossover and Matched Case-Control Studies

- KEYWORDS: Classification , Statistics , Cluster , Machine learning , Regression
- FUNCTIONAL DESCRIPTION Fit a sequence of conditional logistic regression models with lasso, for small to large sized samples.
- Contact: Marius Kwémou
- URL: <https://github.com/robingenuer/>

6.1.2. *COVVSURF*

Combination of Clustering Of Variables and Variable Selection Using Random Forests

- KEYWORDS: Classification , Statistics , Cluster , Machine learning , Regression
- FUNCTIONAL DESCRIPTION This package implements a two stage strategy, where first we use ClustOfVar package to perform a clustering of variables and second we use VSURF package to select features (i.e. synthetic variables built in the first step).
- Contact: Robin Genuer
- URL: <https://github.com/robingenuer/CoVVSURF>

6.1.3. *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/web/packages/NPflow/>

6.1.4. *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/web/packages/tcgsaseq/>

6.1.5. *CD4 Shiny*

Reference curves for CD4 response to antiretroviral therapy in HIV infected patients

- KEYWORDS: HIV infection, antiretroviral therapy, cd4 response, reference curves, quantile regression
- FUNCTIONAL DESCRIPTION References curves for CD4 response to antiretroviral therapy in HIV infected patients derived from large cohorts and estimated according to known factors associated with the response to antiretroviral therapy.
- Contact: Rodolphe Thiébaud
- URL: <http://shiny.isped.u-bordeaux.fr/CD4refcurves/>

6.2. Older software still maintained by SISTM

6.2.1. *NIMROD*

Normal approximation Inference in Models with Random effects based on Ordinary Differential equations

- KEYWORDS: Biostatistics - Optimization
- FUNCTIONAL DESCRIPTION We have written a specific program called NIMROD for estimating parameter of ODE based population models.
- Contact: Rodolphe Thiebaut
- URL: <http://etudes.isped.u-bordeaux2.fr/BIOSTATISTIQUE/NIMROD/documentation/html/index.html>

6.2.2. *R2GUESS*

Graphical processing Unit Evolutionary Stochastic Search

- KEYWORDS: Bioinformatics - Biostatistics
- 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
- URL: <https://cran.r-project.org/web/packages/R2GUESS/index.html>

6.2.3. *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. Under development, and soon to be available on the CRAN website, 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/web/packages/TcGSA/index.html>

6.2.4. *VSURF*

Variable Selection Using Random Forests

- KEYWORD: Bioinformatics
- 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.
- Contact: Robin Genuer
- URL: <https://cran.r-project.org/web/packages/VSURF/index.html>

6.2.5. *marqLevAlg*

Function optimization (minimization or maximization)

- 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.
- Contact: Melanie Prague
- URL: <https://cran.r-project.org/web/packages/marqLevAlg/index.html>

7. New Results

7.1. High dimensional data

Approaches Applied in Genomics Context [13]

Motivation: The association between two blocks of 'omics' data brings challenging issues in computational biology due to their size and complexity. Here, we focus on a class of multivariate statistical methods called partial least square (PLS). Sparse version of PLS (sPLS) operates integration of two datasets while simultaneously selecting the contributing variables. However, these methods do not take into account the important structural or group effects due to the relationship between markers among biological pathways. Hence, considering the predefined groups of markers (e.g. genesets), this could improve the relevance and the efficacy of the PLS approach. Results: We propose two PLS extensions called group PLS (gPLS) and sparse gPLS (sgPLS). Our algorithm enables to study the relationship between two different types of omics data (e.g. SNP and gene expression) or between an omics dataset and multivariate phenotypes (e.g. cytokine secretion). We demonstrate the good performance of gPLS and sgPLS compared with the sPLS in the context of grouped data. Then, these methods are compared through an HIV therapeutic vaccine trial. Our approaches provide parsimonious models to reveal the relationship between gene abundance and the immunological response to the vaccine.

Combining clustering of variables and feature selection using random forests: the CoV/VSURF procedure [26]

High-dimensional data classification is a challenging problem. A standard approach to tackle this problem is to perform variables selection, e.g. using step-wise or LASSO procedures. Another standard way is to perform dimension reduction, e.g. by Principal Component Analysis or Partial Least Square procedures. The approach proposed in this paper combines both dimension reduction and variables selection. First, a procedure of clustering of variables is used to built groups of correlated variables in order to reduce the redundancy of information. This dimension reduction step relies on the R package ClustOfVar which can deal with both numerical and categorical variables. Secondly, the most relevant synthetic variables (which are numerical variables summarizing the groups obtained in the first step) are selected with a procedure of variable selection using random forests, implemented in the R package VSURF. Numerical performances of the proposed methodology called CoV/VSURF are compared with direct applications of VSURF or random forests on the original p variables. Improvements obtained with the CoV/VSURF procedure are illustrated on two simulated mixed datasets (cases $n > p$ and $n < p$)

Arbres CART et Forêts aléatoires, Importance et sélection de variables [27]

Two algorithms proposed by Leo Breiman : CART trees (Classification And Regression Trees for) introduced in the first half of the 80s and random forests emerged, meanwhile, in the early 2000s, are the subject of this article. The goal is to provide each of the topics, a presentation, a theoretical guarantee, an example and some variants and extensions. After a preamble, introduction recalls objectives of classification and regression problems before retracing some predecessors of the Random Forests. Then, a section is devoted to CART trees then random forests are presented. Then, a variable selection procedure based on permutation variable importance is proposed. Finally the adaptation of random forests to the Big Data context is sketched.

Comments on: " A Random Forest Guided Tour " [8]

This paper is a comment on the survey paper by Biau and Scornet (2016) about random forests. We focus on the problem of quantifying the impact of each ingredient of random forests on their performance. We show that such a quantification is possible for a simple pure forest , leading to conclusions that could apply more generally. Then, we consider " hold-out " random forests, which are a good middle point between " toy " pure forests and Breiman's original random forests.

Targeting HIV-1 Env gp140 to LOX-1 Elicits Immune Responses in Rhesus Macaques. [18]

Improved antigenicity against HIV-1 envelope (Env) protein is needed to elicit vaccine-induced protective immunity in humans. Here we describe the first tests in non-human primates (NHPs) of Env gp140 protein fused to a humanized anti-LOX-1 recombinant antibody for delivering Env directly to LOX-1-bearing antigen presenting cells, especially dendritic cells (DC). These data, as well as the safety of this protein vaccine, justify further exploration of this DC-targeting vaccine approach for protective immunity against HIV-1.

Significant changes in HIV-1 Capsid stability induced by common CTL-driven viral sequence mutations. [46]

HIV-1-infected individuals with protective HLA class I alleles exhibit better control of viremia and slower disease progression. Virus control in these individuals has been associated with strong and potent HIV-1-specific cytotoxic-T-lymphocyte (CTL) responses restricted by protective HLA alleles, but control of viremia also occurs in the presence of selected CTL escape mutations. Taken together, these data demonstrate that CTL-driven escape mutations within p24 Gag restricted by protective HLA class I alleles have a significant impact on capsid stability that might contribute to the persistent control of viral replication observed despite viral escape from CTL responses.

Optimization and evaluation of luminex performance with supernatants of Peripheral Blood Mononuclear Cell culture. [48]

The Luminex bead-based multiplex assay is useful for quantifying immune mediators such as cytokines and chemokines. Cross-comparisons of reagents for this technique from different suppliers have already been performed using serum or plasma but rarely with supernatants collected from antigen-stimulated peripheral blood mononuclear cells (PBMC). Here, we first describe an optimization protocol for cell culture including quantity of cells and culture duration to obtain reproducible cytokine and chemokine quantifications. Then, we compared three different Luminex kit suppliers.

7.2. Modeling biomarkers and Mechanistic modeling

- **Dynamic models for estimating the effect of HAART on CD4 in observational studies: Application to the Aquitaine Cohort and the Swiss HIV Cohort Study. [15]**

Highly active antiretroviral therapy (HAART) has proved efficient in increasing CD4 counts in many randomized clinical trials. Because randomized trials have some limitations (e.g., short duration, highly selected subjects), it is interesting to assess the effect of treatments using observational studies. This is challenging because treatment is started preferentially in subjects with severe conditions. This general problem had been treated using Marginal Structural Models (MSM) relying on the counterfactual formulation. Another approach to causality is based on dynamical models. We present three discrete-time dynamic models based on linear increments models (LIM): the first one based on one difference equation for CD4 counts, the second with an equilibrium point, and the third based on a system of two difference equations, which allows jointly modeling CD4 counts and viral load. We also consider continuous-time models based on ordinary differential equations with non-linear mixed effects (ODE-NLME). These mechanistic models allow incorporating biological knowledge when available, which leads to increased statistical evidence for detecting treatment effect. Because inference in ODE-NLME is numerically challenging and requires specific methods and softwares, LIM are a valuable intermediary option in terms of consistency, precision, and complexity. We compare the different approaches in simulation and in illustration on the ANRS CO3 Aquitaine Cohort and the Swiss HIV Cohort Study.

- **Use of dynamical models for treatment optimization in HIV infected patients : a sequential Bayesian analysis approach. [15]**

The use of dynamic mechanistic models based on ordinary differential equations (ODE) has greatly improved the knowledge of the dynamics of HIV and of the immune system. Their flexibility for fitting data and prediction abilities make them a good tool for optimization of the design delivery and efficacy of new intervention in the HIV field. We present the problem of inference in ODE

models with mixed effects on parameters. We introduce a Bayesian estimation procedure based on the maximization of the penalized likelihood and a normal approximation of posteriors, which is implemented in the NIMROD software. We investigate the impact of pooling different data by using a sequential Bayesian analysis (SBA), which uses posteriors of a previous study as new priors. We show that the normal approximation of the posteriors, which constrains the shape of new priors, leads to gains in accuracy of estimation while reducing computation times. The illustration is from two clinical trials of combination of antiretroviral therapies (cART): ALBI ANRS 070 and PUZZLE ANRS 104. This paper reproduces some unpublished work from my PhD thesis. It is an extension of my oral presentation on the same topic at the 47th Journées de Statistique organized by the French Statistical Society (SFdS) in Lille, France, May 2015, when being awarded the Marie-Jeanne Laurent-Duhamel prize.

- **Surveillance of $\gamma\delta$ T Cells Predicts Cytomegalovirus Infection Resolution in Kidney Transplants. [11]**

Cytomegalovirus (CMV) infection in solid-organ transplantation is associated with increased morbidity and mortality, particularly if a CMV mutant strain with antiviral resistance emerges. Monitoring CMV specific T cell response could provide relevant information for patient care. We assessed if V delta 2 neg gamma delta T cell kinetics in peripheral blood predict CMV infection resolution and emergence of a mutant strain in high risk recipients of kidney transplants, including 168 seronegative recipients receiving organs from seropositive donors and 104 seropositive recipients receiving antithymocyte globulins (R+/ATG). In conclusion, longitudinal surveillance of V delta 2 neg gamma delta T cells in recipients of kidney transplants may predict CMV infection resolution and antiviral drug resistance.

- **Early CD4+ T Cell Responses Are Associated with Subsequent CD8+ T Cell Responses to an rAd5-Based Prophylactic Prime-Boost HIV Vaccine Strategy. [12]**

Initial evaluation of a candidate vaccine against HIV includes an assessment of the vaccine's ability to generate immune responses. However, the dynamics of vaccine-induced immune responses are unclear. We hypothesized that the IFN-gamma producing cytotoxic CD8+ T cell responses could be predicted by early IL-2 producing CD4+ helper T cell responses, and we evaluated this hypothesis using data from a phase I/II prophylactic HIV vaccine trial. The objective was to assess the dynamics after vaccination with a recombinant adenoviral serotype 5 (rAd5) HIV vaccine. Regression models confirmed this relationship with a significant association between the two markers. These results suggest an early and leading role of CD4+ T cells in the cellular response to the rAd5-rAd5 vaccine and in particular the stimulation of cytotoxic CD8+ T cell responses. These results could inform better timing of CD4+ T cell measurements in future clinical trials.

- **Reference curves for CD4 T-cell count response to combination antiretroviral therapy in HIV-1-infected treatment-naïve patients. [29]**

The aim of this work was to provide a reference for the CD4 T-cell count response in the early months after the initiation of combination antiretroviral therapy (cART) in HIV-1-infected patients. All patients in the Collaboration of Observational HIV Epidemiological Research Europe (COHERE) cohort who were aged > 18 years and started cART for the first time between 1 January 2005 and 1 January 2010 and who had at least one available measurement of CD4 count and a viral load < 50 HIV-1 RNA copies/mL at 6 months (± 3 months) after cART initiation were included in the study. Unadjusted and adjusted reference curves and predictions were obtained using quantile regressions. Reference curves aid the evaluation of the immune response early after antiretroviral therapy initiation that leads to viral control.

- **Repeated Cycles of Recombinant Human Interleukin 7 in HIV-Infected Patients With Low CD4 T-Cell Reconstitution on Antiretroviral Therapy: Results of 2 Phase II Multicenter Studies. [17].**

Phase I/II studies in human immunodeficiency virus (HIV) infected patients receiving antiretroviral therapy have shown that a single cycle of 3 weekly subcutaneous injections of recombinant human interleukin 7 (r-hIL-7) is safe and improves immune CD4 T-cell restoration. Herein, we report data

from 2 phase II trials evaluating the effect of repeated cycles of r-hIL-7 (20 microg/kg) with the objective of restoring a sustained CD4 T-cell count >500 cells/microL. INSPIRE 2 was a single-arm trial conducted in the United States and Canada. INSPIRE 3 was a 2 arm trial with 3:1 randomization to r-hIL-7 versus control conducted in Europe and South Africa. Participants with plasma HIV RNA levels <50 copies/mL during antiretroviral therapy and with CD4 T-cell counts between 101 and 400 cells/microL were eligible. A repeat cycle was administered when CD4 T-cell counts fell to <550 cells/microL. A total of 107 patients were treated and received 1 (n = 107), 2 (n = 74), 3 (n = 14), or 4 (n = 1) r-hIL-7 cycles during a median follow-up of 23 months. r-hIL-7 was well tolerated. Four grade 4 events were observed, including 1 case of asymptomatic alanine aminotransferase elevation. After the second cycle, anti-r-hIL-7 binding antibodies developed in 82% and 77% of patients in INSPIRE 2 and 3, respectively (neutralizing antibodies in 38% and 37%), without impact on the CD4 T-cell response. Half of the patients spent >63% of their follow-up time with a CD4 T-cell count >500 cells/microL. CONCLUSIONS: Repeated cycles of r-hIL-7 were well tolerated and achieved sustained CD4 T-cell restoration to >500 cells/microL in the majority of study participants.

7.3. Implication in analysis of results from Clinical trials and cohorts

- **Superior efficacy of an HIV vaccine combined with ARV prevention in SHIV challenged non-human primates. [38]**

Although vaccines and antiretroviral (ARV) prevention have demonstrated partial success against human immunodeficiency virus (HIV) infection in clinical trials, their combined introduction could provide more potent protection. Furthermore, combination approaches could ameliorate the potential increased risk of infection following vaccination in the absence of protective immunity. We used a nonhuman primate model to determine potential interactions of combining a partially effective ARV microbicide with an envelope-based vaccine. These important findings suggest that combined implementation of new biomedical prevention strategies may provide significant gains in HIV prevention.

- **A Method to Estimate the Size and Characteristics of HIV-positive Populations Using an Individual-based Stochastic Simulation Model. [14]**

It is important not only to collect epidemiologic data on HIV but to also fully utilize such information to understand the epidemic over time and to help inform and monitor the impact of policies and interventions. We describe and apply a novel method to estimate the size and characteristics of HIV-positive populations. In the pseudo-epidemic example, HIV estimates have narrower plausibility ranges and are closer to the true number, the greater the data availability to calibrate the model. We demonstrate that our method can be applied to settings with less data, however plausibility ranges for estimates will be wider to reflect greater uncertainty of the data used to fit the model.

- **Immunologic response in treatment-naïve HIV-2-infected patients: the IeDEA West Africa cohort. [9]**

Response to antiretroviral therapy (ART) among individuals infected with HIV-2 is poorly described. We compared the immunological response among patients treated with three nucleoside reverse-transcriptase inhibitors (NRTIs) to boosted protease inhibitor (PI) and unboosted PI-based regimens in West Africa. In this observational study using African data, boosted PI-containing regimens had better immunological response compared to triple NRTI combinations and unboosted PI-based regimens at 12 months. A randomized clinical trial is still required to determine the best initial regimen for treating HIV-2 infected patients.

- **Intrinsic defect in keratinocyte function leads to inflammation in Hidradenitis suppurativa. [10]**

Hidradenitis suppurativa (HS) is a chronic, inflammatory, debilitating, follicular disease of the skin. Despite a high prevalence in the general population, the physiopathology of HS remains poorly understood. The use of antibiotics and immunosuppressive agents for therapy suggests a deregulated immune response to microflora. These findings point out a functional defect of keratinocytes in

HS leading to a balance prone to inflammatory responses. This is likely to favor a permissive environment for bacterial infections and chronic inflammation characterizing clinical outcomes in patients with HS.

- **Uptake of Home-Based HIV Testing, Linkage to Care, and Community Attitudes about ART in Rural KwaZulu-Natal, South Africa: Descriptive Results from the First Phase of the ANRS 12249 TasP Cluster-Randomised Trial. [34]**

The 2015 WHO recommendation of antiretroviral therapy (ART) for all immediately following HIV diagnosis is partially based on the anticipated impact on HIV incidence in the surrounding population. We investigated this approach in a cluster-randomised trial in a high HIV prevalence setting in rural KwaZulu-Natal. We present findings from the first phase of the trial and report on uptake of home-based HIV testing, linkage to care, uptake of ART, and community attitudes about ART. Home-based HIV testing was well received in this rural population, although men were less easily contactable at home; immediate ART was acceptable, with good viral suppression and retention. However, only about half of HIV-positive people accessed care within 6 mo of being identified, with nearly two-thirds accessing care by 12 mo. The observed delay in linkage to care would limit the individual and public health ART benefits of universal testing and treatment in this population.

7.4. Conferences

Members of the team were involved in more than 20 talks during conferences and colloquium. In particular, [20], [21], [23], [19], [22], [24] and [25] have proceedings.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

Implication in research for the development of vaccine has lead to a direct contracts with industry such as with Iliad Biotechnologies. This contract had been signed for the BPZE-1 pertussis vaccine trial. This study evaluates the safety and immunogenicity of a higher dose formulation of a new live attenuated vaccine, BPZE1, intended to prevent *Bordetella pertussis* nasopharyngeal colonization and pertussis disease, and investigates whether higher doses of BPZE1 induce the live vaccine to colonize subjects' nasopharynx. The study is a Phase Ib (high dose), single centre, dose-escalating, placebo-controlled study of the live attenuated *B. pertussis* strain BPZE1 given as a single intranasal dose to healthy adult volunteer. This contract is part of the EUCLID platform (via the CIC 1401) in which Laura Richert and Rodolphe Thiébaud are involved.

8.2. Bilateral Grants with Industry

Implication in research for the development of Ebola vaccine has lead to several indirect contracts with industry:

- The EBOVAC2 project, which is presented in Section 'FP7 & H2020 Projects', leads to collaboration with Janssen from Johnson et Johnson.
- The BPZE-1 pertussis vaccine trial, which is presented in Section 'Bilateral Contracts with Industry', leads to collaboration with Iliad Biotechnologies. (Via the EUCLID platform and CIC 1401)
- The Prevac trial vaccine trial leads to collaboration with Merck. 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. (Via the EUCLID platform and CIC 1401)

9. Partnerships and Cooperations

9.1. Regional Initiatives

The team have strong links with :

Université de Bordeaux

ISPED (Institut de Santé Publique et du Développement)

Bordeaux CHU ("Centre Hospitalier Universitaire").

Limoges CHU ("Centre Hospitalier Universitaire").

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) and "Maladies infectieuses dans les pays à ressources limitées" (IDLIC).

Institut Bergonié, Univ Bordeaux through the EUCLID platform

Inria Project-team MONC and CQFD

9.2. National Initiatives

9.2.1. Labex Vaccine Research Institute (VRI)

There are strong collaborations with immunologists involved in the Labex Vaccine Research Institute (VRI) as Rodolphe Thiébaud is leading the Biostatistics/Bioinformatics division.

9.2.2. Expert Appraisals

Rodolphe Thiébaud 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).

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).

Rodolphe Thiébaud is a member of the Membre du CNU 46.04 (Biostatistiques, informatique médicale et technologies de communication).

Laura Richert is an expert for the PHRC (Programme hospitalier de recherche Clinique).

Laura Richert is a member of F-CRIN Steering Committee.

Marta Avalos is an expert for L'ASN (Agence nationale de sécurité du médicament et des produits de santé)

9.2.3. Various Partnership

The project team members are involved in:

Convention between the "Fédération française de natation" and Inria (18950 euros) for the R&D project "Quels schémas de périodisation pour la préparation des Jeux Olympiques à Rio ?" (Marta Avalos).

DRUGS-SAFE platform funded by ANSM (Marta Avalos).

F-CRIN (French clinical research infrastructure network) was initiated in 2012 by ANR under a PIA founding (Programme des Investissements d'avenir) named "INBS/Infrastructures nationales en biologie et en santé". (Laura Richert)

The project team members also collaborate with:

I-REIVAC is the French vaccine research network. This network is part of the Consortium de Recherche en Vaccinologie (CoReVac) created by the Institut de Microbiologie et des Maladies Infectieuses (IMMI). (Laura Richert)

9.3. European Initiatives

9.3.1. FP7 & H2020 Projects

The member of SISTM Team are involved in EHVA (European HIV Vaccine Alliance):

Program: Most information about this program can be found at <http://www.ehv-a.eu/>.

Coordinator: Rodolphe Thiébaud is Work Package leader of the WP10 "Data Integration".

Other partners: The EHVA encompasses 39 partners, each with the expertise to promote a comprehensive approach to the development of an effective HIV vaccine. The 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.

Abstract: With 37 million people living with HIV worldwide, and over 2 million 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 understanding, treatment and prevention of HIV made over the past 30 years, the development of broadly-effective HIV vaccine has remained unachievable. EHVA plans to develop and implement:

- Discovery Platform with the goal of generating novel vaccine candidates inducing potent neutralizing and non-neutralizing antibody responses and T-cell responses
- Immune Profiling Platform with the goal of ranking novel and existing (benchmark) vaccine candidates on the basis of the immune profile
- Data Management/Integration/Down-Selection Platform, with the goal of providing statistical tools for the analysis and interpretation of complex data and algorithms for the efficient selection of vaccines
- Clinical Trials Platform with the goal of accelerating the clinical development of novel vaccines and the early prediction of vaccine failure.

The member of SISTM Team and particularly Laura Richert are also involved in other H2020 projects such as SenseCog, Medit'aging and Orthunion.

9.3.2. Collaborations in European Programs, Except FP7 & H2020

Program: The EBOVAC2 project is one of 8 projects funded under IMI Ebola+ programme that was launched in response to the Ebola virus disease outbreak. The project aims to assess the safety and efficacy of a novel prime boost preventive vaccine regimen against Ebola Virus Disease (EVD).

Project acronym: EBOVAC2

Project title: EBOVAC2

Coordinator: Rodolphe Thiébaud

Other 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)

Abstract: Given the urgent need for an preventive Ebola vaccine strategy in the context of the current epidemic, the clinical development plan follows an expedited scheme, aiming at starting a Phase 2B large scale safety and immunogenicity study as soon as possible while assuring the safety of the trial participants.

- Phase 1 trials to assess the safety and immunogenicity data of the candidate prime-boost regimen in healthy volunteers are ongoing in the UK, the US and Kenya and Uganda. A further study site has been approved to start in Tanzania. Both prime-boost combinations (Ad26.ZEBOV prime + MVA-BN-Filo boost; and MVA-BN-Filo prime + Ad26.ZEBOV boost) administered at different intervals are being tested in these trials.

- Phase 2 trials (this project) are planned to start as soon as the post-prime safety and immunogenicity data from the UK Phase I are available. Phase 2 trials will be conducted in healthy volunteers in Europe (France and UK) and non-epidemic African countries (to be determined). HIV positive adults will also be vaccinated in African countries. 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.

9.3.3. Collaborations with Major European Organizations

University of Oxford;
London School of Hygiene and Tropical Medicine;
University Hospital Hamburg;
Heinrich Pette Institute for Experimental Virology, Hambourg;
MRC, University College London

9.4. International Initiatives

Scharp, Seattle;
Fred Hutchinson Cancer center, Seattle;
Baylor Institute;
NIH for the Prevac trial;
NGO Alima for the Prevac trial;
Several African clinical sites for Ebovac2 and Prevac trials.

9.5. International Research Visitors

9.5.1. Visits of International Scientists

Cristian Meza, Associate Professor of the Universidad de Valparaiso (Chili), member of the research center CIMFAV : <http://cmeza.cimfav.cl/> collaborates on the project entitled "Longitudinal high-dimensional data" (septembre)

David Conesa, Associate Professor of the Universidad de Valencia (Espagne), member of the research group GEEITEMA : <http://www.geeitema.org/conesa/> collaborates on the project entitled "Bayesian predictive methods with application to the home and leisure injuries in France study MAVIE" (septembre)

Sam Doerken, PhD student of the University of Freiburg (Allemagne), member of the Institute for Medical Biometry and Statistics : <http://portal.uni-freiburg.de/imbi/employees/persons/doerken> collaborates on the project entitled "Penalization regression methods for sparse exposures with application to pharmacoepidemiology" (septembre - octobre)

Jessica Grnsbell, PhD student of the Harvard T.H. Chan School of Public Health, came as a visiting scholar on a subject of "analysis of high dimensional genetic data" (May).

9.5.2. Visits to International Teams

Marta Avalos will be a research visitor at CSIRO's Data61 in Canberra, Australia from Dec. 2016 until June 2017. Collaboration with Cheng Soon Ong <http://www.ong-home.my/>

Marta Avalos (in April and October) visited David Conesa through the Erasmus+ program Universidad de Valencia (Espagne).

Perrine Soret (from 26/12/15 to 28/01/16) visited Cristian Meza and Karine Bertin (Inria Chili) at CIMFAV (Centre for Research and Modeling of Random Phenomena, Valparaíso), Univ Valparaiso, Chili, concerning the project "New challenges in mixed-effects models".

Laura Richtert spent 6 months as visiting researcher at Heinrich Pette Institut for experimental virology, department virus immunology (Pr M. Altfeld), Hamburg Germany in 2016

Boris Hejblum is a Visiting Scientist appointment at Harvard University (not paid), Department of Biostatistics

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

Daniel Commenges organised a SFB (Société Française de Biometrie) in Montpellier (3 Juin 2016), Daniel Commenges Co-organised the "Journées GDR-SFB" in Lyon (27-28 Juin)

Robin Genuer Co-organised a reading group called Smiling in Bordeaux (<http://www.math.u-bordeaux.fr/~machaven/smiling>)

Rodolphe Thiébaud organized the scientific program of the Bordeaux Modelling Workshop (1 et 2 Juin 2016)

Rodolphe Thiébaud organised a 10 hours seminar on "Bayesian filters and particule methods" at Inria Bordeaux (Nov. and Dec. 2016)

10.1.2. General Chair, Scientific Chair

Rodolphe Thiébaud is a member of the scientific committee of the Muraz Center (Bobo-Dioulasso, Burkina Faso), since 2016

Rodolphe Thiébaud is a member of the Scientific Advisory Board de l'Institut Pierre Louis d'Epidémiologie et de Santé Publique (UPMC, Dir : Dominique Costagliola), since 2015

Daniel Commenges is a member of the scientific committee of de "Journée de la SFdS (Société Francaise de Statistiques)" (Montpellier, 30 Mai-3 Juin)

10.1.3. Member of the Organizing Committees

All the team members helped in the ground organisation of the Bordeaux Modelling Workshop

10.1.4. Member of the Journal Editorial Boards

Lifetime Data Analysis (Daniel Commenges)

Statistics Surveys (Daniel Commenges)

Journal de la Société Francaise de Statistique (Daniel Commenges)

Daniel Commenges DC Principales revues de Statistique (Biometrics, JASA, JRSS, Stat Med, LIDA,...)

10.1.5. Reviewer - Reviewing Activities

AIDS (Rodolphe Thiébaud)
 Annals of Applied Statistics (Boris Hejblum)
 BioData Mining (Boris Hejblum)
 Biometrics (Daniel Commenges, Mélanie Prague)
 International Journal of Biostatistics (Robin Genuer)
 International Journal of Epidemiology (Daniel Commenges)
 Journal of Applied Statistics (Marta Avalos)
 Journal of the Royal Statistical Society: Interaction (Mélanie Prague)
 Machine Learning (Robin Genuer)
 Neural Information Processing Systems (Robin Genuer)
 Pattern Recognition Letters (Robin Genuer)
 Statistics and Computing (Robin Genuer)
 Statistical Methods and Applications (Marta Avalos)
 Statistics in Medicine (Daniel Commenges, Rodolphe Thiébaud, Mélanie Prague)
 Statistics Surveys (Daniel Commenges)

10.1.6. Invited Talks

Daniel Commenges gave 3 invited talks in Vienne (19 Mai), Vigo (26 Octobre) and Berlin (25 Novembre).

Laura Richert gave 2 invited talks in Webinar about "big data in epidemiology" (20 juin) and in Paris for the Colloquium "One Health" about "Signature transcriptomique post-vaccinale chez l'Homme" (3 Novembre).

Rodolphe Thiébaud gave 3 invited talks

Mélanie Prague gave 2 invited talks one in Nancy (20 fev.) and one un Summer Sim (26 july).

10.1.7. Leadership within the Scientific Community

Daniel Commenges is the president of the SFB (Société Française de Biométrie) which is the French satellite for the IBS (International Biometrics society).

10.1.8. Research Administration

Daniel Commenges is the director of the Biostat-Info axis in the Inserm BPH (Bordeaux Public Health) institute.

Rodolphe Thiébaud is a member of the department of life science in University of Bordeaux

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

In class teaching

Master : Marta Avalos teaches in the two years of the Master of Public Health at ISPED, Univ. Bordeaux, France.

Master : Robin Genuer, teaches in the two years of the Master of Public Health (M1 Santé publique, M2 Biostatistique, M2 Informatique médicale, M2 Santé internationale, M2 épidémiologie).

Master : Boris Hejblum, teaches in the two years of the Master of Public Health (M1 Santé publique, M2 Biostatistique, M2 Informatique médicale, M2 Santé internationale, M2 épidémiologie).

Master : Robin Genuer, MSS du collège ST, intervention dans le cours de Statistique en grande dimension.

Master : Rodolphe Thiébaud, teaches in the two years of the Master of Public Health, and he is head of the Epidemiology specialty of the second year of the Master of Public Health.

Master : Laura Richert teaches in the two years of the Master of Public Health at ISPED, Univ. Bordeaux, France (M2 Biostatistiques).

Master : Laura Richert teaches in the Master of Vaccinology at UPEC (University Paris-Est-Créteil), France.

Master : Chloe Pasin is a teaching assistant for the two years of the Master of Public Health at ISPED, Univ. Bordeaux, France.

Master : Laura Villain is a teaching assistant for the two years of the Master of Public Health at ISPED, Univ. Bordeaux, France

Bachelor : Laura Richert teaches in PACES and DFASM1-3 for Medical degree at Univ. Bordeaux, France

Summer School: All the SISTM team member teach in the ISPED Summer school.

E-learning

Marta Avalos is head of the first year of the e-learning program of the Master of Public Health, and teaches in it.

Mélanie Prague teaches in the Diplôme universitaire "Méthodes statistiques de régression en épidémiologie".

Laura Richert teaches in the Diplôme universitaire "Recherche Clinique".

Rodolphe Thiébaud is head of the Epidemiology specialty of the second year of the e-learning program of the Master of Public Health, and teaches in it.

Robin Genuer and Perrine Soret participate to the IdEx Bordeaux University "Défi numérique" project "BeginR" (<http://beginr.moutault.net/>).

10.2.2. Supervision

PhD in progress : Wenjia Wang "Modèle de Rasch" (CIFRE, co-direction avec Mickael Guedj Pharnext), from Oct 2015, directed by Daniel Commenges.

PhD in progress : Laura Villain "Modélisation de l'effet du traitement par injection IL7" (CIFRE, co-direction avec Rodolphe Thiébaud), from Oct 2015, directed by Daniel Commenges.

PhD in progress : Perrine Soret, *Modélisation de données longitudinales en grande dimension*, from Oct 2014, directed by Marta Avalos.

PhD in progress : Mélanie Née *Recherche et caractérisation de profils attentionnels : mieux comprendre la place de l'attention dans la survenue des accidents de la vie courante*, from Oct 2015, co-directed by Emmanuel Lagarde (60%), Cédric Galera (20%), Marta Avalos (20%)

PhD in progress : Chloé Pasin, *Modelling the immune response to HIV vaccine*, from Sep 2015, co-directed by Rodolphe Thiébaud and Francois Dufour

PhD in progress : Edouard Lhomme, *Analyse des déterminants de la réponse immunitaire post-vaccination dans des stratégies vaccinales expérimentales*, from Oct 2016, directed by Laura Richert.

PhD in progress : Hadrien Lorenzo, *Analyses de données longitudinales de grandes dimensions appliquées aux essais vaccinaux contre le VIH et Ebola*, from Oct 2016, co-directed by Rodolphe Thiébaud and Jérôme Saracco.

Master internship : Hao Ren "Contribution au développement d'un outil statistique d'aide à la décision en sport de haut niveau", directed by Marta Avalos and Perrine Soret (01/03/2016-12/08/2016)

Master internship : Madelyn Rojas "Practices for the provision of prior information in Bayesian Logistic Regression: Application in MAVIE project", directed by Marta Avalos and David Conesa (11/07/2016-09/09/2016)

Master internship : Thomas Blondel "Application of Bayesian linear models to sports science data", directed by David Conesa and Marta Avalos (05/04/2016 - 04/06/2016)

Master internship : Julie Havas "Application of Bayesian Logistic Regression to the mavié study of home and leisure injury", directed by David Conesa and Marta Avalos (05/04/2016 - 04/06/2016)

Master internship : Thomas Esnaud "Etude de la méthode de clustering par forêts aléatoires, applications à la reconnaissance automatique de populations cellulaires.", directed by Robin Genuer (14/03/2016 - 31/08/2016)

Master internship : Lise Mandigny "Revue systématique et Méta-analyse des essais cliniques publiés de développement de vaccins contre le virus Ebola", directed by Rodolphe Thiébaud (1/04/2016 - 31/09/2016)

Master internship : Stella Huang "Modélisation de l'infection à pseudomonas aeruginosa dans les services de réanimation ? étude DYNAPYO", directed by Rodolphe Thiébaud (11/02/2016 - 15/08/2016)

Master project : B Dufoyer, A Chevalier, H Aassif, A Labchri, projet de programmation du Master 1 Informatique, Univ Bordeaux. Titre : " Développement d'un outil de prévention des accidents de la vie courante à partir de méthodes de machine learning : site web et bases de données ", directed by Marta Avalos and L Orriols, M Travanca, L Divert, INSERM U1219. (11/01/2016-12/04/2016)

Master project : N Craeye, C Elassaoui, F Elouazi, B Faltrept, projet de programmation du Master 1 Informatique, Univ Bordeaux. Titre : " Développement d'un outil de mesure de l'attention via internet ", directed by Marta Avalos and M Née, L Divert, E Lagarde, INSERM U1219. (11/01/2016-12/04/2016)

10.2.3. Juries

Daniel Commenges was involved in two PhD defences as president of the jury: Leila Azarang (Vigo), Anais Rouanet (Bordeaux).

Robin Genuer was in charge of the reports of the PhD of Havelund Welling, entitled "Characterization of absorption enhancers for orally administered therapeutic peptides in tablet formulations", defended on 30/09/2016 in Department of Applied Mathematics and Computer Science, Technical University of Denmark, Kongens Lyngby

Mélanie Prague is a member of the follow-up dissertation comity of Sébastien Benzckry's PhD student (Inria Bordeaux Sud-ouest, MONC team). Nicolo Chiara is working on "Mathematical modeling of systemic aspects of cancer and cancer therapy".

Rodolphe Thiébaud took part in the HDR committee of Vivian Viallon (2016) and Francesco Salvo (2016)

Robin Genuer took part in the recruitment commission MCF CNU 26 (Toulouse 2016)

Rodolphe Thiébaud took part in the recruitment commissions PU CNU 26 (Paris Descartes 2016), MCF CNU 26 (Bordeaux 2016), MCF CNU 85 (Bordeaux 2016).

10.3. Popularization

Marta Avalos, Marius Kwémou and Perrine Soret animated "Mais qui est le coupable ? (Ou comment les maths contribuent à conduire une enquête épidémiologique)" for high school students through the "Fête de la Science" organized at Inria, Oct 2016.

Laura Richert participated to "Nuit Européenne des Chercheurs" with speed dating and a radio interview, Cap Sciences, Bordeaux, September 2016.

11. Bibliography

Major publications by the team in recent years

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- [21] G. LEFORT, M. F. AVALOS, P. SORET, P. DAVID, J. F. TOUSSAINT, P. HELLARD. *A comparison of unsupervised curve classification methods for sport training data*, in "3rd conference of the International Society for Non-Parametric Statistics (ISNPS)", Avignon, France, The International Society for NonParametric Statistics (ISNPS), June 2016, <https://hal.inria.fr/hal-01396366>.
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Team **STORM**

STatic Optimizations, Runtime Methods

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
Distributed and High Performance Computing

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Team STORM

Creation of the Team: 2015 January 01

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- 2.1.6. - Concurrent programming
- 2.1.10. - Domain-specific languages
- 2.2.1. - Static analysis
- 2.2.3. - Run-time systems
- 2.2.4. - Parallel architectures
- 2.2.5. - GPGPU, FPGA, etc.
- 6.2.6. - Optimization
- 6.2.7. - High performance computing

Other Research Topics and Application Domains:

- 3.3.1. - Earth and subsoil
- 5.2.3. - Aviation

1. Members

Research Scientist

Olivier Aumage [Inria, Researcher]

Faculty Members

Denis Barthou [Team leader, Bordeaux INP, Professor, HDR]
Marie Christine Counilh [Univ. Bordeaux, Associate Professor]
Raymond Namyst [Univ. Bordeaux, Professor, HDR]
Samuel Thibault [Univ. Bordeaux, Associate Professor]
Pierre Andre Wacrenier [Univ. Bordeaux, Associate Professor]

Technical Staff

Adrien Cassagne [Inria]
Jerome Clet-Ortega [Inria]
Nathalie Furmento [CNRS]
Samuel Pitoiset [Inria]
Chiheb Sakka [Inria from Jul 2016]
Corentin Salingue [Inria]

PhD Students

Hugo Brunie [CEA]
Terry Cojean [Inria]
Christopher Haine [Inria]
Pierre Huchant [Univ. Bordeaux]
Suraj Kumar [Inria]
Raphaël Prat [CEA, from Oct 2016]
Arthur Loussert [CEA, from Oct 2016]
Marc Sergent [Univ. Bordeaux, until Dec 2016]
Gregory Vaumourin [CEA, until Oct 2016]

Post-Doctoral Fellow

Luka Stanisic [Inria]

Administrative Assistant

Sylvie Embolla [Inria]

Others

Thomas Caroff [Inria, Intern, from Jun 2016 until Jul 2016]

Arthur Chevalier [Inria, Intern, from May 2016 until Jul 2016]

Berenice Faltrept [Inria, Intern, from May 2016 until Jul 2016]

Loris Lucido [Inria, Intern, from Jun 2016 until Aug 2016]

Berangere Subervie [Inria, Intern, from Jun 2016 until Jul 2016]

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, fit 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.
- **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.

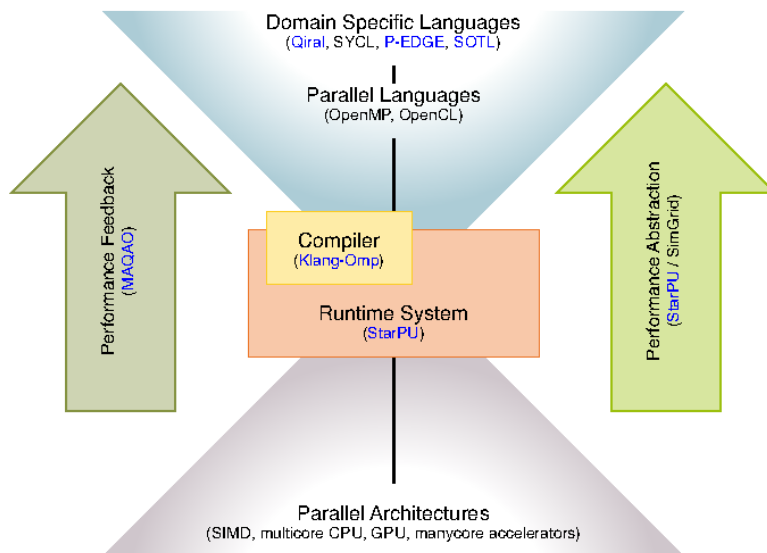


Figure 1. STORM Big Picture

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 at horizon 2020 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 adaptive 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. 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. 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.

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. We recall in the following section the expertise of the team.

4. Application Domains

4.1. Application Fields

The application of our work concerns linear algebra, solvers and fast-multipole methods, in collaboration with other Inria teams and with industry. This allows a wide range of scientific and industrial applications possibly interested in the techniques we propose, in the domain of high performance computing but also in order to compute intensive embedded applications. In terms of direct application, the software developed in the team are used in applications in various fields, ranging from seismic, mechanic of fluids, molecular dynamics, high energy physics or material simulations. Similarly, the domains of image processing and signal processing can take advantage of the expertise and software of the team.

5. New Software and Platforms

5.1. Chameleon

KEYWORDS: HPC - Dense linear algebra - Task-based algorithm - Runtime system - 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.

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 (e.i. 4 min).

- Participants: Emmanuel Agullo, Mathieu Faverge, Cédric Castagnede and Florent Pruvost
- Partners: Innovative Computing Laboratory (ICL) - King Abdullha University of Science and Technology - University of Colorado Denver
- Contact: Emmanuel Agullo
- URL: <https://project.inria.fr/chameleon/>

5.2. KLANG-OMP

The KStar OpenMP Compiler

KEYWORDS: Compilers - Task scheduling - OpenMP - Source-to-source compiler - Data parallelism

FUNCTIONAL DESCRIPTION

The Klang-Omp compiler, now renamed KStar following the recommendation of the local experimentation and development service, 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: Olivier Aumage, Nathalie Furmento, Samuel Pitoiset and Samuel Thibault
- Contact: Olivier Aumage
- URL: <http://kstar.gforge.inria.fr/#!index.md>

5.3. 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: Olivier Aumage, François Broquedis, Pierrick Brunet, Nathalie Furmento, Thierry Gautier, Samuel Thibault and Philippe Virouleau
- Contact: Thierry Gautier
- URL: <http://kastors.gforge.inria.fr/#!/index.md>

5.4. MORSE

- Contact: Emmanuel Agullo
- URL: <http://icl.cs.utk.edu/morse/>

5.5. AFF3CT

A Fast Forward Error Correction Tool (previously named P-Edge).

KEYWORDS: Code generation - Error Correction Code

FUNCTIONAL DESCRIPTION

The AFF3CT library joins genericity techniques together with code generation capabilities to enable implementing efficient and portable error correction codes. The genericity offered allows to easily experiment with a large panel of algorithmic variants.

- Previous name: P-Edge
- Authors: Adrien Cassagne, Olivier Aumage, Bertrand Le Gal, Camille Leroux and Denis Barthou
- Partner: IMS
- Contact: Adrien Cassagne
- URL: <https://aff3ct.github.io/>

5.6. StarPU

The StarPU Runtime System

KEYWORDS: HPC - Scheduling - GPU - Multicore - 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: Cédric Augonnet, Samuel Thibault, Nathalie Furmento, Simon Archipoff, Jérôme Clet-Ortega, Nicolas Collin, Ludovic Courtes, Mehdi Juhour, Xavier Lacoste, Benoît Lize, Ludovic Stordeur, Cyril Roelandt, Corentin Salingue, Chiheb Sakka, Samuel Pitoiset, François Tessier, Pierre-André Wacrenier, Andra Hugo, Terry Cojean, Raymond Namyst, Olivier Aumage and Marc Sergent
- Contact: Olivier Aumage
- URL: <http://starpu.gforge.inria.fr/>

5.7. hwloc

Hardware Locality

KEYWORDS: HPC - Topology - Open MPI - Affinities - GPU - Multicore - NUMA - 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.

- Participants: Brice Goglin and Samuel Thibault
- Partners: AMD - Intel - Open MPI consortium
- Contact: Brice Goglin
- URL: <http://www.open-mpi.org/projects/hwloc/>

6. New Results

6.1. Automatic OpenCL Task Adaptation for Heterogeneous Architectures

OpenCL defines a common parallel programming language for all devices, although writing tasks adapted to the devices, managing communication and load-balancing issues are left to the programmer. In this work [11], we propose a novel automatic compiler and runtime technique to execute single OpenCL kernels on heterogeneous multi-device architectures. Our technique splits computation and data automatically across the computing devices. The technique proposed is completely transparent to the user, does not require off-line training or a performance model. It handles communications and load-balancing issues, resulting from hardware heterogeneity, load imbalance within the kernel itself and load variations between repeated executions of the kernel, in an iterative computation. We present our results on benchmarks and on an N-body application over two platforms, a 12-core CPU with two different GPUs and a 16-core CPU with three homogeneous GPUs.

6.2. Fast Forward Error Correction Codes

Error Correction Codes are essential for preserving data integrity in communications. These algorithms find errors due to noise in transmissions and correct these errors with a high probability. Several algorithms are used, with different capacities in term of correction and most of them are implemented in cell phones or satellites as ASICS. The need to handle many different usages, different contexts of use pushes towards software solutions. A larger spectrum of algorithms can be explored, in order to meet the expectations in terms of performance, power consumption and error correcting power. These new algorithms, for the 5G for instance, can then be either implemented in software (for large antenna for instance) or in hardware. In both case, software simulation is necessary in order to evaluate the properties of the new algorithms. We developed in collaboration with IMS new versions of algorithms and a new software, AFF3CT <http://aff3ct.github.io/index.html>, that allows the exploration of many different algorithmic variants and their evaluation. Two conference papers have been published on these new results [7][6].

6.3. Resource aggregation for task-based Cholesky Factorization

Hybrid computing platforms are now commonplace, featuring a large number of CPU cores and accelerators. This trend makes balancing computations between these heterogeneous resources performance critical. In a recent paper [8] we propose aggregating several CPU cores in order to execute larger parallel tasks and thus improve the load balance between CPUs and accelerators. Additionally, we present our approach to exploit internal parallelism within tasks. This is done by combining two runtime systems: one runtime system to handle the task graph and another one to manage the internal parallelism. We demonstrate the relevance of our approach in the context of the dense Cholesky factorization kernel implemented on top of the StarPU task-based runtime system. We present experimental results showing that our solution outperforms state of the art implementations. In addition, we realized an extended version of this paper submitted for review to the Parallel Computing journal special issue for HCW and HeteroPar 2016 workshops. In this new paper [19] we provide additional details on our contribution and propose a brand new study on the recent Intel Xeon Phi Knights Landing (KNL) where we show that we are able to outperform existing state of the art implementations on this platform thanks to our proposed technique.

6.4. Scheduling of Linear Algebra Kernels on Multiple Heterogeneous Resources

In this paper [5], we consider task-based dense linear algebra applications on a single heterogeneous node which contains regular CPU cores and a set of GPU devices. Efficient scheduling strategies are crucial in this context in order to achieve good and portable performance. HeteroPrio, a resource-centric dynamic scheduling strategy has been introduced in a previous work and evaluated for the special case of nodes with exactly two

types of resources. However, this restriction can be limiting, for example on nodes with several types of accelerators, but not only this. Indeed, an interesting approach to increase resource usage is to group several CPU cores together, which allows to use intra-task parallelism. We propose a generalization of HeteroPrio to the case with several classes of heterogeneous workers. We provide extensive evaluation of this algorithm with Cholesky factorization, both through simulation and actual execution, compared with HEFT-based scheduling strategy, the state of the art dynamic scheduling strategy for heterogeneous systems. Experimental evaluation shows that our approach is efficient even for highly heterogeneous configurations and significantly outperforms HEFT-based strategy.

6.5. Analyzing Dynamic Task-Based Applications on Hybrid Platforms: An Agile Scripting Approach

In this paper [10], we present visual analysis techniques to evaluate the performance of HPC task-based applications on hybrid architectures. Our approach is based on composing modern data analysis tools (pjdump, R, ggplot2, plotly), enabling an agile and flexible scripting framework with minor development cost. We validate our proposal by analyzing traces from the full-fledged implementation of the Cholesky decomposition available in the MORSE library running on a hybrid (CPU/GPU) platform. The analysis compares two different workloads and three different task schedulers from the StarPU runtime system. Our analysis based on composite views allows to identify allocation mistakes, priority problems in scheduling decisions, GPU tasks anomalies causing bad performance, and critical path issues.

6.6. Distributed StarPU Scalability on Heterogeneous Platforms

The emergence of accelerators as standard computing resources on supercomputers and the subsequent architectural complexity increase revived the need for high-level parallel programming paradigms. Sequential task-based programming model has been shown to efficiently meet this challenge on a single multicore node possibly enhanced with accelerators, which motivated its support in the OpenMP 4.0 standard. In this paper, we show that this paradigm can also be employed to achieve high performance on modern supercomputers composed of multiple such nodes, with extremely limited changes in the user code. To prove this claim, we have extended the StarPU runtime system with an advanced inter-node data management layer that supports this model by posting communications automatically [16]. We illustrate our discussion with the task-based tile Cholesky algorithm that we implemented on top of this new runtime system layer. We show that it allows for very high productivity while achieving a performance competitive with both the pure Message Passing Interface (MPI)-based ScaLAPACK Cholesky reference implementation and the DPLASMA Cholesky code, which implements another (non sequential) task-based programming paradigm.

6.7. Controlling the Memory Subscription of Distributed Applications with a Task-Based Runtime System

The ever-increasing supercomputer architectural complexity emphasizes the need for high-level parallel programming paradigms. Among such paradigms, task-based programming manages to abstract away much of the architecture complexity while efficiently meeting the performance challenge, even at large scale. Dynamic run-time systems are typically used to execute task-based applications, to schedule computation resource usage and memory allocations. While computation scheduling has been well studied, the dynamic management of memory resource subscription inside such run-times has however been little explored. This paper [12] studies the cooperation between a task-based distributed application code and a run-time system engine to control the memory subscription levels throughout the execution. We show that the task paradigm allows to control the memory footprint of the application by throttling the task submission flow rate, striking a compromise between the performance benefits of anticipative task submission and the resulting memory consumption. We illustrate the benefits of our contribution on a compressed dense linear algebra distributed application.

6.8. StarPU Interfacing with GASPI/GPI2

A version of the distributed dependence support of StarPU has been ported by Corentin Salingue, under the supervision of Olivier Aumage on the high performance GASPI/GPI2 networking layer developed by the Fraunhofer institute in Germany. The GPI2 framework offers a lightweight communication interface specifically designed for thread enabled HPC applications. This work has been conducted as part of the H2020 INTERTWinE european project.

6.9. A Stencil DSEL for Single Code Accelerated Computing with SYCL

Stencil kernels arise in many scientific codes as the result from discretizing natural, continuous phenomena. Many research works have designed stencil frameworks to help programmer optimize stencil kernels for performance, and to target CPUs or accelerators. However, existing stencil kernels, either library-based or language-based necessitate to write distinct source codes for accelerated kernels and for the core application, or to resort to specific keywords, pragmas or language extensions. SYCL is a C++ based approach designed by the Khronos Group to program the core application as well as the application kernels with a single unified, C++ compliant source code. A SYCL application can then be linked with a CPU-only runtime library or processed by a SYCL-enabled compiler to automatically build an OpenCL accelerated application. Our contribution [13] is a stencil domain specific embedded language (DSEL) which leverage SYCL together with expression template techniques to implement statically optimized stencil applications able to run on platforms equipped with OpenCL devices, while preserving the single source benefits from SYCL.

6.10. Bridging the gap between OpenMP 4.0 and native runtime systems for the fast multipole method

With the advent of complex modern architectures, the low-level paradigms long considered sufficient to build High Performance Computing (HPC) numerical codes have met their limits. Achieving efficiency, ensuring portability, while preserving programming tractability on such hardware prompted the HPC community to design new, higher level paradigms. The successful ports of fully-featured numerical libraries on several recent runtime system proposals have shown, indeed, the benefit of task-based parallelism models in terms of performance portability on complex platforms. However, the common weakness of these projects is to deeply tie applications to specific expert-only runtime system APIs. The OpenMP specification, which aims at providing a common parallel programming means for shared-memory platforms, appears as a good candidate to address this issue thanks to the latest task-based constructs introduced as part of its revision 4.0. The goal of this paper [15] is to assess the effectiveness and limits of this support for designing a high-performance numerical library. We illustrate our discussion with the ScalFMM library, which implements state-of-the-art fast multipole method (FMM) algorithms, that we have deeply re-designed with respect to the most advanced features provided by OpenMP 4. We show that OpenMP 4 allows for significant performance improvements over previous OpenMP revisions on recent multicore processors. We furthermore propose extensions to the OpenMP 4 standard and show how they can enhance FMM performance. To assess our statement, we have implemented this support within the Klang-OMP source-to-source compiler that translates OpenMP directives into calls to the StarPU task-based runtime system. This study shows that we can take advantage of the advanced capabilities of a fully-featured runtime system without resorting to a specific, native runtime port, hence bridging the gap between the OpenMP standard and the very high performance that was so far reserved to expert-only runtime system APIs.

6.11. Hierarchical Tasks

Modern computing platforms are heterogeneous and the load balancing is more complex to reach high performance. We decided to deal with the granularity problem in the context of task parallelism and in a dynamic way through the implementation of hierarchical tasks in StarPU runtime. The idea is to give the runtime the ability to control tasks submission in order to choose the good granularity at the right moment.

The application describes a control graph and the runtime generates the computation tasks graph on-the-fly according to the state of the machine (available computing resources, memory consumption, ...). As a consequence the runtime is able to limit the size of the computation tasks graph without losing parallelism. Some experiments have been done on a Cholesky application and in the qr-mumps software and show that the work of an application programmer can be alleviated and the granularity choice could be easily delegated to the task based runtime.

6.12. Software-Hardware Exploration for Read-Only Data

We have proposed a new way of managing the cache by exploiting the difference of behavior in the memory system between read-only data and read-write data. A division of the existing cache-based memory hierarchy is proposed in order to create a dedicated data path for read-only data. This proposition is similar to the existing separation at the L1-level between instruction and data caches. In order to justify this approach, an analysis performed on a set of benchmarks shows that read-only data count for significant part of the working set and are less reused than read-write data. A transparent solution is proposed based on specific compilation support to separate automatically the memory accesses of read-only data at L1-level. This organization exploits the properties of the different sub- workloads in order to increase the overall data locality and data reuse. Simulated in a multicore environment, the evaluation of the new memory organization shows reduction of L1 misses up to 28.5%. Moreover, the messages issued on the interconnection network can be reduced up to 14.7% without any penalty on the performance.

Besides the reduced miss-rate allows maintaining performance with smaller cache size on the read-write path while the properties of the read- only part can benefit of a simplified cache implementation despite a shared multicore access [1].

7. Bilateral Contracts and Grants with Industry

7.1. Bilateral Contracts with Industry

- HiBOX project, with Airbus and IMACS (2013-2017).
- CEA contracts:
 - Several PhD contracts: for Hugo Brunie, Raphaël Prat, Marc Sergent and Arthur Loussert.
 - Industrial contract with CEA-DAM on particle simulation.

8. Partnerships and Cooperations

8.1. National Initiatives

8.1.1. PIA

ELCI The ELCI 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.

8.1.2. ANR

ANR SOLHAR (<http://solhar.gforge.inria.fr/doku.php?id=start>).
ANR MONU 2013 Program, 2013 - 2016 (36 months)
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 Songs Simulation of next generation systems (<http://infra-songs.gforge.inria.fr/>).

ANR INFRA 2011, 01/2012 - 12/2015 (48 months)

Identification: ANR-11INFR01306

Coordinator: Martin Quinson (Inria Nancy)

Other partners: Inria Nancy, Inria Rhône-Alpes, IN2P3, LSIT, Inria Rennes, I3S.

Abstract: The goal of the SONGS project is to extend the applicability of the SimGrid simulation framework from Grids and Peer-to-Peer systems to Clouds and High Performance Computation systems. Each type of large-scale computing system will be addressed through a set of use cases and lead by researchers recognized as experts in this area.

8.1.3. ADT - Inria Technological Development Actions

ADT K'Star (<http://kstar.gforge.inria.fr/#!/index.md>)

Participants: Olivier Aumage, Nathalie Furmento, Samuel Pitoiset, Samuel Thibault.

Inria ADT Campaign 2013, 10/2013 - 9/2015 (24 months)

Coordinator: Thierry Gautier (team AVALON, Inria Grenoble - Rhône-Alpes) and Olivier Aumage (team RUNTIME, Inria Bordeaux - Sud-Ouest)

Abstract: The Inria action ADT K'Star is a joint effort from Inria teams AVALON and RUNTIME to design the Klang-Omp source-to-source OpenMP compiler to translate OpenMP directives into calls to the API of AVALON and RUNTIME respective runtime systems (XKaaapi for AVALON, StarPU for RUNTIME).

8.1.4. IPL - Inria Project Lab

C2S@Exa - Computer and Computational Sciences at Exascale **Participant:** Olivier Aumage.

Inria IPL 2013 - 2017 (48 months)

Coordinator: Stéphane Lantéri (team Nachos, Inria Sophia)

Since January 2013, the team is participating to the C2S@Exa http://www-sop.inria.fr/c2s_at_exa Inria Project Lab (IPL). This national initiative aims at the development of numerical modeling methodologies that fully exploit the processing capabilities of modern massively parallel architectures in the context of a number of selected applications related to important scientific and technological challenges for the quality and the security of life in our society. This collaborative effort involves computer scientists that are experts of programming models, environments and tools for harnessing massively parallel systems, algorithmists that propose algorithms and contribute to generic libraries

and core solvers in order to take benefit from all the parallelism levels with the main goal of optimal scaling on very large numbers of computing entities and, numerical mathematicians that are studying numerical schemes and scalable solvers for systems of partial differential equations in view of the simulation of very large-scale problems.

HAC-SPECIS - High-performance Application and Computers, Studying PErformance and Correctness In Simulation

Participants: Samuel Thibault, Luka Stanisic.

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.

8.2. European Initiatives

8.2.1. FP7 & H2020 Projects

8.2.1.1. INTERTWinE

Title: Programming Model INTERoperability ToWards Exascale

Programm: H2020

Duration: October 2015 - October 2018

Coordinator: EPCC

Partners:

Barcelona Supercomputing Center - Centro Nacional de Supercomputacion (Spain)

Deutsches Zentrum für Luft - und Raumfahrt Ev (Germany)

Fraunhofer Gesellschaft Zur Forderung Der Angewandten Forschung Ev (Germany)

Institut National de Recherche en Informatique et en Automatique (France)

Kungliga Tekniska Hoegskolan (Sweden)

T-Systems Solutions for Research (Germany)

The University of Edinburgh (United Kingdom)

Universitat Jaume I de Castellon (Spain)

The University of Manchester (United Kingdom)

Inria contact: Olivier Aumage

This project addresses the problem of programming model design and implementation for the Exascale. The first Exascale computers will be very highly parallel systems, consisting of a hierarchy of architectural levels. To program such systems effectively and portably, programming APIs with efficient and robust implementations must be ready in the appropriate timescale. A single, “silver bullet” API which addresses all the architectural levels does not exist and seems very unlikely to emerge soon enough. We must therefore expect that using combinations of different APIs at different system levels will be the only practical solution in the short to medium term. Although there remains room for improvement in individual programming models and their implementations, the main challenges lie in interoperability between APIs. It is this interoperability, both at the specification level and at the implementation level, which this project seeks to address and to further the state of the art. INTERTWinE brings together the principal European organisations driving the evolution of programming models and their implementations. The project will focus on seven key programming APIs: MPI, GASPI, OpenMP, OmpSs, StarPU, QUARK and PaRSEC, each of which has a project partner with extensive experience in API design and implementation. Interoperability requirements, and evaluation of implementations will be driven by a set of kernels and applications, each of which has a project partner with a major role in their development. The project will implement a co- design cycle, by feeding back advances in API design and implementation into the applications and kernels, thereby driving new requirements and hence further advances.

8.2.1.2. *Mont-Blanc 2*

Title: Programming Model INTERoperability ToWards Exascale

Programm: FP7

Duration: September 2013 - January 2017

Coordinator: BSC

Partners: Atos/Bull, ARM, Jülich, LRZ, Univ. Stuttgart, CINECA, CNRS, CEA, Univ. Bristol, Allinea Software, Univ. Cantabria

Inria contact: Olivier Aumage

The Mont-Blanc project aims to develop a European Exascale approach leveraging on commodity power-efficient embedded technologies. The project has developed a HPC system software stack on ARM, and will deploy the first integrated ARM-based HPC prototype by 2014, and is also working on a set of 11 scientific applications to be ported and tuned to the prototype system. Team STORM has been involved in porting the MAQAO binary code analyzer and instrumenter on ARM platforms and interfacing it with the kernel autotuning framework BOAST.

8.3. International Initiatives

8.3.1. *Inria International Partners*

8.3.1.1. *Declared Inria International Partners*

- Team STORM is supervising the membership of Inria as part of the OpenMP Architecture Review Board (ARB), the international body in charge of the standardisation of the OpenMP parallel programming language. The membership has been supported by an InriaHUB/Standardisation grant.
- Team STORM is member of the Khronos Group Advisory Panel about the standardization of the OpenCL and SYCL programming languages.

9. Dissemination

9.1. Promoting Scientific Activities

9.1.1. *Scientific Events Selection*

9.1.1.1. *Chair of Conference Program Committees*

- Samuel Thibault was a Program Committee chair for EuroPar'16.

9.1.1.2. *Member of the Conference Program Committees*

- Samuel Thibault was a member of the Program Committee for Compas'16, HCW'16, MuCoCos'16, P³MA'16
- Olivier Aumage was a member of the Program Committee for HUCAA 16'
- Raymond Namyst was a member of the Program Committees for Cluster'16, EuroPar'16 and SAC/MUSEPAT'16
- Denis Barthou was a Program Committee chair for UCHPC'16

9.1.1.3. *Reviewer*

The members of the team reviewed numerous papers for various international conferences such as IPDPS, Super-Computing, Euro-Par, ICPP.

9.1.2. *Journal*

The members of the team review papers from many high-level journals such as TPDS, CCPE, TACO, JPDC.

9.1.3. Invited Talks

- Samuel Thibault was invited to present StarPU advances at the "Scalable Task-based Programming Models" workshop of SIAM-PP 2016
- Samuel Thibault was invited to participate to the "What Do You Need to Know About Task-Based Programming for Future Systems?" panel of SIAM-PP 2016
- Samuel Thibault was invited to make a talk on StarPU at an meeting for the H2020 NLAFFET project
- Samuel Thibault was then invited to make a talk at the CCDSC-2016 workshop
- Samuel Thibault was invited to make a talk at Jussieu for a APR seminar
- Terry Cojean was invited to present his work at the "Task-based Scientific, High Performance Computing on Top of Runtime Systems" workshop of SIAM-PP 2016
- Terry Cojean was invited to present his work by the research group of Prof. Benkner at the University of Vienna.
- Terry Cojean was invited to give a talk on StarPU at the RESPA workshop of Super-Computing 2016, details available in [2]
- Luka Stanisic was invited to present an effective methodology for reproducible research on dynamic task-based runtime systems at the "Task-based Scientific, High Performance Computing on Top of Runtime Systems" workshop of SIAM-PP 2016
- Luka Stanisic was invited to present advanced usage of Git at the "Reproducible Research" webinars
- Olivier Aumage was invited to present StarPU at the Parallel Programming Frameworks: Technologies, Performance and Applications track of SIAM-PP 2016 in Paris.
- Olivier Aumage was invited to present StarPU at CERFACS in Toulouse.
- Olivier Aumage was invited to present StarPU at the workshop Building a European/American Community for the Development of Dynamic Runtimes in Extreme-Scale Systems, as part of ISC'2016 in Frankfurt.
- Olivier Aumage and Samuel Thibault presented a tutorial session on runtime systems and StarPU as part of the Prace Advanced Training Center (PATC) program in Paris, in partnership with La Maison de la simulation.
- Olivier Aumage was invited to present StarPU by the research group of Prof. Benkner at the university of Vienna.
- Olivier Aumage was invited to give a training session on advanced parallel programming models for HPC platforms as part of the EoCoE European Center of Excellence face-to-face meeting in Rome
- Raymond Namyst was invited to give a talk about Heterogeneous Programming at the RoMoL Workshop, Barcelona, March 2016
- Raymond Namyst was invited to give a talk about StarPU at the CEA 2016 HPC Worshop, Cargèse

9.2. Teaching - Supervision - Juries

9.2.1. Teaching administration

Samuel Thibault is responsible for the computer science topic of the first university semester.

Samuel Thibault is responsible for the creation of the new Licence Pro ADSILLH (Administrateur et Développeur de Systèmes Informatiques sous Licences Libres et Hybrides)

Denis Barthou is responsible for the cyber-security, systems and networks 3rd year of the ENSEIRB-MATMECA engineering school.

Raymond Namyst is Vice-chair of the Computer Science Training Department of University of Bordeaux

9.2.2. Teaching

Licence : Marie-Christine Counilh, Introduction to Computer Science, 64HeTD, L1, University of Bordeaux

Licence : Marie-Christine Counilh, Introduction to C Programming, 52HeTD, L1, University of Bordeaux

Licence : Samuel Thibault, Introduction to Computer Science, 32HeTD, L1, University of Bordeaux

Licence : Samuel Thibault, Networking, 51HeTD, L3, University of Bordeaux

Licence : Samuel Thibault, Computer Architecture, 77HeTD, L2, University of Bordeaux

Licence : Samuel Thibault, Tutored project, 10HeTD, L3, University of Bordeaux

Licence : Pierre-André Wacrenier, Introduction to Computer Science, 64HeTD, L1, University of Bordeaux

Licence : Terry Cojean, Networking, 40HeTD, L1, IUT Bordeaux

Licence : Terry Cojean, Object Oriented Programming, 24HeTD, L3, IUT Bordeaux

Master : Luka Stanisic, Operating Systems, 22HeTD, M1, University of Bordeaux

Master : Samuel Thibault, Operating Systems, 22HeTD, M1, University of Bordeaux

Master : Marie-Christine Counilh, Object Oriented Programming, 30HeTD, M1, University of Bordeaux

Master : Raymond Namyst, Operating Systems, M1, University of Bordeaux

Master : Pierre-André Wacrenier and Raymond Namyst, Parallel Programming, M1, University of Bordeaux

Engineering School: Samuel Thibault, Information System Security, 13HeTD, M1, ENSEIRB-MATMECA/IPB

Engineering School: Olivier Aumage, Languages and Supports for Parallelism, 14HeTD, M2, ENSEIRB-MATMECA/IPB joint with University of Bordeaux

Engineering School: Olivier Aumage, High Performance Communication Libraries, 20HeTD, M2, ENSEIRB-MATMECA/IPB joint with University of Bordeaux

Engineering School: Denis Barthou, Compilation, Architecture, Architecture for HPC, real-time 3D at ENSEIRB-MATMECA (around 200HeTD), from L3 to M2.

9.2.3. Supervision

- PhD: Gregory Vaumourin, Hybrid Memory Hierarchy and Dynamic Data Handling in Embedded Parallel Architectures, University of Bordeaux, defended in Nov 2016, advisors: Denis Barthou, Alexandre Guerre (CEA), Thomas Dombek (CEA)
- PhD: Marc Sergent, Passage à l'échelle d'un support d'exécution à base de tâches pour l'algèbre linéaire dense, University of Bordeaux, defended in Dec 2016, advisors: Raymond Namyst, Olivier Aumage, Samuel Thibault, David Goudin (CEA)
- PhD in progress: Suraj Kumar, Task-based programming paradigms and scheduling, 2013/12, Emmanuel Agullo, Olivier Beaumont, Samuel Thibault
- PhD in progress: Terry cojean, Programming heterogeneous machines using moldable tasks, 2014/09, Pierre-André Wacrenier, Abdou Guermouche, Raymond Namyst
- PhD in progress: Christopher Haine, Estimating efficiency and automatic restructuration of data layout, 2014/01, Olivier Aumage, Denis Barthou
- PhD in progress: Arthur Loussert, Ressource (co)Allocation in HPC systems, 2016/10, Raymond Namyst, Marc Perache (CEA), Benoît Welterlen (ATOS)
- PhD in progress: Raphaël Prat, Load Balancing in Molecular Dynamics, 2016/10, Raymond Namyst, Laurent Colombet (CEA)

9.2.4. Juries

Denis Barthou has participated to the following PhD juries

- Abdul Wahid MEMON, U. Versailles St Quentin, Jun 2016 (reviewer)
- Abderrahmane Nassim HALLI, U. of Grenoble, Sep 2016 (reviewer)
- Milan KABAC, U. Bordeaux, Oct 2016 (president)
- Nans ODRY, U. Aix Marseille, Oct 2016 (reviewer)

Raymond Namyst has participated to the following PhD juries

- David Beniamine, U. Grenoble, Dec 2016 (reviewer)
- Alban Rousset, U. Besançon, Oct 2016 (reviewer)
- Naweiluo Zhou, U. Grenoble, Oct 2016 (reviewer)
- Béranger Bramas, U. Bordeaux, Feb 2016 (president)
- Oleg Iegorov, U. Grenoble, Apr 2016 (president)

9.3. Popularization

- Samuel Thibault made a Inria talk about « Building Debian/Ubuntu packages to make it easy for users to install your software »

10. Bibliography

Publications of the year

Doctoral Dissertations and Habilitation Theses

- [1] G. VAUMOURIN. *Read Only Data Specific Management for an Energy Efficient Memory System*, Université de Bordeaux, October 2016, <https://tel.archives-ouvertes.fr/tel-01402354>.

Invited Conferences

- [2] T. COJEAN. *The StarPU Runtime System at Exascale ? : Scheduling and Programming over Upcoming Machines*, in "RESPA workshop at SC16", Salt Lake City, Utah, United States, November 2016, <https://hal.inria.fr/hal-01410103>.

International Conferences with Proceedings

- [3] E. AGULLO, O. BEAUMONT, L. EYRAUD-DUBOIS, S. KUMAR. *Are Static Schedules so Bad ? A Case Study on Cholesky Factorization*, in "IEEE International Parallel & Distributed Processing Symposium (IPDPS 2016)", Chicago, IL, United States, IEEE, May 2016, <https://hal.inria.fr/hal-01223573>.
- [4] P.-A. ARRAS, D. FUIN, E. JEANNOT, S. THIBAUT. *DKPN: A Composite Dataflow/Kahn Process Networks Execution Model*, in "24th Euromicro International Conference on Parallel, Distributed and Network-based processing", Heraklion Crete, Greece, February 2016, <https://hal.inria.fr/hal-01234333>.
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Team TADAAM

Topology-Aware System-Scale Data Management for High-Performance Computing

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
Distributed and High Performance Computing

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Team TADAAM

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- 1.1.1. - Multicore
- 1.1.2. - Hardware accelerators (GPGPU, FPGA, etc.)
- 1.1.3. - Memory models
- 1.1.4. - High performance computing
- 1.1.5. - Exascale
- 1.2. - Networks
- 2.1.7. - Distributed programming
- 2.2.2. - Memory models
- 2.2.3. - Run-time systems
- 2.6.1. - Operating systems
- 2.6.2. - Middleware
- 3.1.3. - Distributed data
- 6.2.7. - High performance computing
- 7.1. - Parallel and distributed algorithms
- 7.3. - Optimization
- 7.9. - Graph theory

Other Research Topics and Application Domains:

- 6.3.2. - Network protocols
- 6.5. - Information systems
- 9.4.1. - Computer science

1. Members

Research Scientists

- Emmanuel Jeannot [Team leader, Inria, Senior Researcher, HDR]
- Guillaume Aupy [Inria, Researcher, from Dec. 2016]
- Alexandre Denis [Inria, Researcher]
- Brice Goglin [Inria, Researcher, HDR]

Faculty Members

- Guillaume Mercier [INP Bordeaux, Associate Professor]
- François Pellegrini [Univ. Bordeaux, Professor, HDR]

Technical Staff

- Clément Foyer [Inria, from Feb. 2016]
- Cedric Lachat [Inria]
- François Tessier [Inria, until Jan. 2016]

PhD Students

- Remi Barat [CEA]
- Raphaël Blanchard [ONERA, until Oct. 2016]
- Nicolas Denoyelle [Bull, granted by CIFRE]

Benjamin Lorendeau [EDF, granted by CIFRE]
Romain Prou [Inria, until Oct. 2016]
Hugo Taboada [CEA]
Adèle Villiermet [Inria]

Post-Doctoral Fellows

Farouk Mansouri [Inria]
Cyril Bordage [Inria]

Visiting Scientist

Juan Luis García Zapata [University of Extremadura, from Sep. 2016 to Nov. 2016]

Administrative Assistants

Cecile Boutros [Inria]
Sylvie Embolla [Inria]

Others

Arnaud Bardoux [Intern from University of Strasbourg, from Apr. 2016 to Sep. 2016]
Ahmad Boissetri Binzagr [Intern from University of Bordeaux, from May 2016 to Jul. 2016]
Francois Candela [Inria, Intern from University of Bordeaux, from May 2016 to Jul. 2016]
Paul Jeanmaire [Intern from ENS Cachan, from Jun. 2016 to Jul. 2016]

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 through 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 nodes⁰. However, very few applications use the whole machine. In general, an application runs only on a subset of the nodes⁰. 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.

⁰More 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.

⁰In 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

The NETLOC (See Section 6.1) tools have been run on one of the largest European supercomputers (the TGCC/Genci CURIE machine) and successfully modeled its 5200 nodes and its interconnection network (more than 800 switches). This is a joint work with CEA and the COLOC European project.

6. New Software and Platforms

6.1. NetLoc

Network Locality

FUNCTIONAL DESCRIPTION

⁰<http://www.prace-ri.eu/prace-9th-regular-call/>

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 application 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. NETLOC is distributed within HWLOC releases starting with HWLOC 2.0.

- Participants: Cyril Bordage and Brice Goglin
- Contact: Brice Goglin
- URL: <http://www.open-mpi.org/projects/netloc/>

6.2. NewMadeleine

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 Mad-MPI fully supports the MPI_THREAD_MULTIPLE multi-threading level.

- Participants: Alexandre Denis, Nathalie Furmento, Raymond Namyst and Clement Foyer
- Contact: Alexandre Denis
- URL: <http://pm2.gforge.inria.fr/newmadeleine/>

6.3. 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 43 million elements to more than 1 billion elements 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.

- Participants: Cedric Lachat, François Pellegrini and Cécile Dobrzynski
- Partners: CNRS - IPB - Université de Bordeaux
- Contact: Cedric Lachat
- URL: <http://project.inria.fr/pampa/>

6.4. SCOTCH

KEYWORDS: High-performance computing - Graph algorithms - Domain decomposition - Static mapping - Mesh partitioning - Sparse matrix ordering

SCIENTIFIC DESCRIPTION

SCOTCH is a software package and libraries for sequential and parallel graph partitioning, static mapping and clustering; sequential mesh and hypergraph partitioning; and sequential and parallel sparse matrix block ordering.

Its main use is to subdivide a scientific problem, expressed as a graph, into a set of subproblems as independent as possible from each other (in terms of connecting edges).

FUNCTIONAL DESCRIPTION

SCOTCH takes the form of a set of libraries, plus additional standalone programs. The sequential and parallel libraries provide a set of interfaces to describe centralized and distributed graphs to partition, the target architectures to map onto, the resulting centralized and distributed mapping and ordering structures, etc. SCOTCH takes advantage of Posix threads, and its parallel version, PT-SCOTCH, uses the MPI interface.

- Participants: François Pellegrini, Cédric Lachat, Rémi Barat and Cédric Chevalier
- Partners: CNRS - IPB - Region Aquitaine
- Contact: François Pellegrini
- URL: <http://www.labri.fr/~pelegrin/scotch/>

6.5. TreeMatch

KEYWORDS: Intensive parallel computing - High-Performance Computing - Hierarchical architecture - Placement

SCIENTIFIC DESCRIPTION

TreeMatch provides a permutation of the processes to the 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.

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: Emmanuel Jeannot, François Tessier, Adele Villiermet, Guillaume Mercier and Pierre Celor
- Partners: CNRS - IPB - Université de Bordeaux
- Contact: Emmanuel Jeannot
- URL: <http://treematch.gforge.inria.fr/>

6.6. hwloc

Hardware Locality

KEYWORDS: HPC - Topology - Open MPI - Affinities - GPU - Multicore - NUMA - 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.

- Participants: Brice Goglin and Samuel Thibault
- Partners: AMD - Intel - Open MPI consortium
- Contact: Brice Goglin
- URL: <http://www.open-mpi.org/projects/hwloc/>

7. New Results

7.1. Network Modeling

NETLOC (see Section 6.1) is a tool in HWLOC to discover the network topology. Our first work with NETLOC was to redesign it to be more efficient and more adapted to the needs. The code was cleaned and some dependencies were removed. We have added a display tool, that is able to show a network topology in a web browser where a user can interact with. It ran on one of the largest European supercomputer (the TGCC/Genci CURIE machine) and successfully modeled its 5200 nodes and its interconnection network (more than 800 switches).

Moreover, it is now possible to interact with Scotch from netloc. The first feature is to export a network topology, or even the current available topology given by the resource manager, into a SCOTCH architecture. Conversely, we can use SCOTCH tools in NETLOC for building a process mapping based on resources found by NETLOC and a process graph describing communications between processes. Tests conducted on a stencil mini-app have shown that the benefits are real and still needs more work.

7.2. Communication and computation overlap

To amortize the cost of communication in HPC application, programmers want to overlap communications with computation. To do so, they assume non-blocking MPI communications will progress in background. NewMadeleine, our communication library, is actually able to make communication progress in background so as to actually have overlap happen. However, not all MPI implementations are able to overlap communication and computation.

We have proposed [8] a benchmark to measure what really happens when trying to overlap non-blocking point-to-point communications with computation. The benchmark measures how much overlap happen in various cases: sender-side, receiver-side, datatypes likely to be offloaded onto NIC or not, multi-threaded computation, multi-threaded communication or not. We have benchmarked a wide panel of MPI libraries and hardware platforms, and thanks to low-level traces, explained the results.

7.3. Topology Aware Performance Monitoring

A tool has been developed to abstract performance metrics and map them onto the HWLOC (see Section 6.6) topology model of the system. During the year 2016, the tool has been entirely rewritten to release a more meaningful and stable programming abstraction, with off the shelf performance abstraction plugins and raw performance acquisition plugin [16]. A special effort has been carried out on output presentation by extending lstopo tool from hwloc into a library embedded in the monitoring tool to display performance metrics on the system topology. Another backend using R has also been developed for the purpose of post-mortem analysis and model extraction from abstract metrics of the topology.

7.4. Locality Aware Roofline Model

The years 2016 marked the achievement of our extension of the famous Cache Aware Roofline Model(CARM) and the associate tool. The latter model targets deep platform and application analysis on multicore processors. Its model consist into a two-dimensions plane bound by several machine ceils and representative of scientific application workloads. Our extension validate the use of the CARM on emerging processors with heterogeneous memory subsystem, and extend the CARM methodology to encompass interconnection network, thus, enabling full modeling of shared memory systems [17]. This work is a collaboration with the INESC-ID research center under the NESUS project.

7.5. Performance Analysis of Electromagnetic Field Application on Large SMP Node

In the scope of the COLOC project we worked on understanding scalability issues of the efield application on a large shared memory system. Our analysis with above mentionned tools highlighted a potential bandwidth bottleneck. This problem can usually be tackled by the mean of threads and data mapping on respectively the machine cores and the memories. Unfortunately, those techniques can't be applied with this (closed source) application since the system does not allow to monitor memory accesses and traffic on the system.

7.6. Structural Modeling of Heterogeneous Memory Architectures

HWLOC (see Section 6.6) is the de facto standard tool for gathering information of parallel platform topologies. The advent of new memory architecture, with high-bandwidth and/or non-volatile memories cause the memory management subsytem complexity to increase. Indeed, besides taking care of allocating data buffers locally, developers also have to choose between different local memories with different performance and persistence characteristics. Moreover, the operating systems still cannot expose the full details about these technologies to applications. We modified the HWLOC tool to cope with these new needs in collaboration with Intel. This work led to the design a new structural model for platforms with heteregeneous memories [10].

7.7. Scalable Management of Platform Topologies

HWLOC (see Section 6.6) is used for gathering the topology of thousands of nodes in large clusters. Those nodes are now growing to hundreds of cores, making the overall amount of topology information non-negligible. We designed new ways to compress topologies, either lossless or lossy, for easier transfer between compute nodes and front nodes and more compact storage and manipulation [20]. We also studied the overhead of topology discovery on the overall execution time and showed that the Linux kernel is bottleneck on large nodes. It raised the need to use exported and/or abstracted topologies to factorize this overhead [11].

7.8. MPI One-side operations

MPI one-sided operations, aka Remote Memory Access (RMA), are direct read/write memory access to a remote node. Only one node (the origin) explicitly calls MPI operations, while communication progression is implicit for the other node (the target). These operations assume that the communication library is able to make communication progress in background.

Since MadMPI, the MPI implementation of NewMadeleine (see Section 6.2), extensively uses event-driven mechanism to reach asynchronous progression, we have [24] taken advantage of this property to implement MPI RMA operations in the library. This implementation keeps the overlap properties by asynchronously handle the messages exchanged by the applications. The addition also supports `MPI_THREAD_MULTIPLE`, for both shared and distributed memory contexts.

7.9. Topology and affinity aware hierarchical and distributed load-balancing

The evolution of massively parallel supercomputers make palpable two issues in particular: the load imbalance and the poor management of data locality in applications. Thus, with the increase of the number of cores and the drastic decrease of amount of memory per core, the large performance needs imply to particularly take care of the load-balancing and as much as possible of the locality of data. One mean to take into account this locality issue relies on the placement of the processing entities and load balancing techniques are relevant in order to improve application performance. With large-scale platforms in mind, we developed a hierarchical and distributed algorithm which aim is to perform a topology-aware load balancing tailored for Charm++ applications. This algorithm is based on both LibTopoMap for the network awareness aspects and on Treematch to determine a relevant placement of the processing entities. We show that the proposed algorithm improves the overall execution time in both the cases of real applications and a synthetic benchmark as well. For this last experiment, we show a scalability up to one millions processing entities [12].

7.10. Topology-Aware Data Aggregation for Intensive I/O on Large-Scale Supercomputers

Reading and writing data efficiently from storage systems is critical for high performance data-centric applications. These I/O systems are being increasingly characterized by complex topologies and deeper memory hierarchies. Effective parallel I/O solutions are needed to scale applications on current and future supercomputers. Data aggregation is an efficient approach consisting of electing some processes in charge of aggregating data from a set of neighbors and writing the aggregated data into storage. Thus, the bandwidth use can be optimized while the contention is reduced. In [13], we have taken into account the network topology for mapping aggregators and we propose an optimized buffering system in order to reduce the aggregation cost. We have validated our approach using micro-benchmarks and the I/O kernel of a large-scale cosmology simulation. We have showed improvements up to 15× faster for I/O operations compared to a standard implementation of MPI I/O.

7.11. Communication monitoring in OpenMPI

Monitoring data exchanges is critical when it comes to optimize process placement in a large scale environment. We participated in adding in Open-MPI, which is one of the major MPI implementation, a fine grain, point-to-point monitoring component that keeps track of message exchanges. Unlike implementations using PMPI operations, the layer in which this monitoring acts allow us to record at a lower level the effective data communications, for example, after the covering tree has been calculated. This component has been enriched with a complete coverage of collectives, point-to-point and one-sided communications. This component also reports informations about message sizes distribution. Monitored informations can be accessed by using `MPI_Tools` interface, or by dumping data in files.

7.12. Process Placement with TreeMatch

We released TreeMatch ver 0.4 in August. The new features are: a new API, the handling of oversubscribing (being able to map more processes than computing resources), fast exhaustive search (for small cases), K-partitioning in case of large arity of the tree, and a set of extensive tests.

7.13. Topology Aware Resource Management

SLURM is a Resource and Job Management System, a middleware in charge of delivering computing power to applications in HPC systems. Our goal is to take into account in SLURM placement process hardware topology but application communication pattern too. We have a new [9], [19] selection option for the `cons_res` plugin in SLURM. In this case the usually `best_fit` algorithm used to choose nodes is replaced by TreeMatch, an algorithm to find the best placement among the free nodes list in light of a given application communication matrix. We plan to release this work in the next release SLURM 17.02.

Fragmentation in cluster is one of the criteria important for administrator. Indeed, the way jobs are allocated impacts the global resource usage. Usually it is observed through utilization of a cluster for a fixed load rate, but no metrics dedicated to fragmentation exist in literature. Hence we construct several metrics to measure it. Our goal is to study the impact of our selection algorithm on fragmentation in comparison with other.

7.14. Impact of progress threads placement for MPI Non-Blocking Collectives

MPI Non-Blocking Collectives (NBC) allow communication overlap with computation. A good overlapping ratio is obtained when computation and communication are running in parallel. To achieve this, some implementations use progress threads to manage communication tasks. These threads should be bound on different cores to maximize the overlap. Thus, we elaborate several threads placement algorithms. These algorithms have been implemented within the MPC framework, using the HWLOC software to get a global view of the machine topology. We propose [18] a thread placement algorithm taking into account the NUMA topology of the machine in order to improve the overlapping ratio of non-blocking collective communications.

7.15. Hierarchical Communication Management in MPI

MPI, in its current state provides only a very limited set of functionalities so as to allow the programmer to effectively leverage the physical characteristics of the underlying hardware, such as the potentially complex memory hierarchy. The MPI philosophy being to be a hardware-agnostic interface, the challenge is therefore to propose an interface extension that offers the programmer significant control over the hardware without dwelling too much into hardware details. We seek the right level of abstraction for this interface and the goal is to push this proposal to the MPI Forum. This new interface is based on the concept of communicators, expands an already existing function available in the standard and also introduces a couple of helper functions. We have prototyped and drafted our proposal for the 2017 meetings of the forum.

7.16. Fully-abstracted approach for efficient thread binding in task-based model of programming

Task-based models and runtimes are quite popular in the HPC community. They help to implement applications with a high level of abstraction while still applying different types of optimizations. An important optimization target is hardware affinity, which concerns to match application behavior (thread, communication, data) to the architecture topology (cores, caches, memory). In fact, realizing a well adapted placement of threads is a key to achieve performance and scalability, especially on NUMA-SMP machines. However, this type of optimization is difficult: architectures become increasingly complex and application behavior changes with implementations and input parameters, *e.g.* problem size and number of thread. Thus, by themselves task based runtimes often deal badly with this optimization and leave a lot of fine-tuning to the user. In this work [21], [25], [14], we propose a fully automatic, abstracted and portable affinity module. It produces and implements an optimized affinity strategy that combines knowledge about application characteristics and the

architecture's topology. Implemented in the backend of our task-based runtime ORWL, our approach was used to enhance the performance and the scalability of several unmodified ORWL-coded applications: matrix multiplication, a 2D stencil (Livermore Kernel 23), and a video tracking real world application. On two SGI SMP machines with quite different hardware characteristics, our tests show spectacular performance improvements for this unmodified application code due to a dramatic decrease of cache misses. A comparison to reference implementations using OpenMP confirms this performance gain of almost one order of magnitude.

7.17. Multi-criteria graph partitioning for multi-physics simulations load balancing

A new set of algorithms has been designed to compute multi-criteria static mappings for the load balancing of multi-physics simulations. The multi-criteria graph partitioning is known to be NP-hard, and there exist very few multi-criteria graph partitioners. Moreover, they focus on the edge-cut minimization instead of enforcing load balance. In practice, this strategy often leads to very unbalanced partitions, which are not useful for multi-physics simulations.

We have designed algorithms that focus on balancing several criteria at the same time to ensure that our results always match all balance criteria. We have implemented a prototype in Python to test these different heuristics. One of them, called PIERE, obtained good results [15], in term of balance as well as communication costs. PIERE uses the classic multilevel framework, but implements a new initial partitioning algorithm, which allows to find a balanced partition of the graph. The partition is then refined by local optimization heuristics that ensure the balance is kept for all criteria. This allow us to return a partition respecting the balance constraints. In [15], we compare against well-known partitioners that are SCOTCH and METIS, and highlight that, for a small mesh, the results exhibit a high discrepancy: each tool lacks of robustness.

PIERE outperformed the existing software METIS in our test cases, but there is room for improvement. We also verified the superiority of the hypergraph model over the graph model used by most partitioners. Meanwhile, we studied the source code of well known partitioners, namely METIS and SCOTCH, and we have identified a lot of algorithmic choices and internal parameters that are not described in their documentations. Carefully analyzing them helps us to clearly understand the differences of the different algorithms.

7.18. Scotch

In order to prepare for the inclusion of multi-criteria graph partitioning algorithms in SCOTCH, in the context of the PhD thesis of Rémi Barat, a new branch has been created in the SCOTCH repository. This new branch, labeled as 6.1, is the basis for the next main release of SCOTCH. The sequential graph structure has been adapted to handle graphs with multiple loads per vertex, and all the related algorithms have been adapted to take into account multiple vertex loads. This resulted in minimal updates in the interface of Scotch, with full ascending compatibility. All of these modifications have been performed so as not to slow down significantly the algorithms in the most common case of graphs with single vertex loads.

7.19. PaMPA

Parallel remeshing has been improved. PaMPA coupled with Mmg (v5) remeshed a tetrahedral mesh from 43Melements to more than 1Belements on 280 Broadwell processors in 20 minutes. The resulted mesh, used by CERFACS, permitted one of the most finest simulation computed with LES (Large Eddy Simulation) on combustion.

The scalability of PT-SCOTCH scalability has been tested on the Curie cluster and compared to that of PARMETIS. These tests used DARI resources.

7.20. Originality of software works

Most judges have very little, if not none, knowledge on software development. This results in misconceptions and mistakes regarding the application of copyright/author right (*droit d'auteur*) in court cases related to software. More generally, the concept of originality is misunderstood. While this criterion is meant in theory to separate works of the mind that are personal to an author (e.g., literary works), from creations of form that cannot, by nature, reflect the personality of their creator (e.g. mathematical tables), it is often used to qualify the degree of similarity between two different works, in the context of plagiarism. Also, the distinction between the realm of programs, that is, works of the mind, and that of algorithms, is not mastered. Algorithms belong to the *fonds commun*, a French term that has no equivalent in English and might be translated as “common pool”. In order to help judges and lawmakers in understanding these notions, and articulate them, we have proposed a methodology for ruling software disputes. This methodology is solely based on the study of similarities in software code, since author right exclusively pertains to the level of the form [22].

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contract with CEA

CEA is granting the PhD thesis of Hugo Taboada on specialized thread management in the context of multi programming models, and the PhD thesis of Rémi Barat on multi-criteria graph partitioning.

8.2. Bilateral Grant with Bull/Atos

Bull/ATOS is granting the CIFRE PhD thesis on Nicolas Denoyelle on advanced memory hierarchies and new topologies.

8.3. Bilateral Grant with Onera

Onera is granting the PhD thesis of Raphaël Blanchard on the parallelization and data distribution of discontinuous Galerkin methods for complex flow simulations.

8.4. Bilateral Grant with EDF

EDF is granting the CIFRE PhD thesis of Benjamin Lorendeau on new programming models and optimization of Code Saturn.

8.5. Bilateral Grant with Intel

Intel is granting \$30k and providing 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.

9. Partnerships and Cooperations

9.1. National Initiatives

9.1.1. ANR

ANR *MOEBUS* Scheduling in HPC (<http://moebus.gforge.inria.fr/doku.php>).

ANR INFRA 2013, 10/2013 - 9/2017 (48 months)

Coordinator: Denis Trystram (Inria Rhône-Alpes)

Other partners: Inria Bordeaux Sud-Ouest, Bull/ATOS

Abstract: This project focuses on the efficient execution of parallel applications submitted by various users and sharing resources in large-scale high-performance computing environments

ANR SATAS SAT as a Service.

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.

9.1.2. IPL - Inria Project Lab

MULTICORE - Large scale multicore virtualization for performance scaling and portability

Participants: Emmanuel Jeannot and Farouk Mansouri.

Multicore processors are becoming the norm in most computing systems. However supporting them in an efficient way is still a scientific challenge. This large-scale initiative introduces a novel approach based on virtualization and dynamicity, in order to mask hardware heterogeneity, and to let performance scale with the number and nature of cores. It aims to build collaborative virtualization mechanisms that achieve essential tasks related to parallel execution and data management. We want to unify the analysis and transformation processes of programs and accompanying data into one unique virtual machine. We hope delivering a solution for compute-intensive applications running on general-purpose standard computers.

9.2. European Initiatives

9.2.1. Collaborations in European Programs, Except FP7 & H2020

COLOC: the Concurrency and Locality Challenge (<http://www.coloc-itea.org>).

Program: ITEA2

Project acronym: COLOC

Project title: The Concurrency and Locality Challenge

Duration: November 2014 - November 2017

Coordinator: BULL/ATOS

Other partners: BULL/ATOS (France); Dassault Aviation (France) ; Enfeild AB (Sweden); Scilab entreprise (France); Teratec (France); Inria (France); Swedish Defebnse Research Agency - FOI (France); UVSQ (France).

Abstract: The COLOC project aims at providing new models, mechanisms and tools for improving applications performance and supercomputer resources usage taking into account data locality and concurrency.

NESUS: Network for Ultrascale Computing (<http://www.nesus.eu>)

Program: COST

Project acronym: NESUS

Project title: Network for Ultrascale Computing

Duration: April 2014 - April 2018

Coordinator: University Carlos III de Madrid

Other partners: more than 35 countries

Abstract: Ultrascale systems are envisioned as large-scale complex systems joining parallel and distributed computing systems that will be two to three orders of magnitude larger than today's systems. The EU is already funding large scale computing systems research, but it is not coordinated across researchers, leading to duplications and inefficiencies. The goal of the NESUS Action is to establish an open European research network targeting sustainable solutions for ultrascale computing aiming at cross fertilization among HPC, large scale distributed systems, and big data management. The network will contribute to glue disparate researchers working across different areas and provide a meeting ground for researchers in these separate areas to exchange ideas, to identify synergies, and to pursue common activities in research topics such as sustainable software solutions (applications and system software stack), data management, energy efficiency, and resilience. Some of the most active research groups of the world in this area are members of this proposal. This Action will increase the value of these groups at the European-level by reducing duplication of efforts and providing a more holistic view to all researchers, it will promote the leadership of Europe, and it will increase their impact on science, economy, and society.

9.2.2. Collaborations with Major European Organizations

Partner 1: INESC-ID, Lisbon, (Portugal)

Subject 1: Application modeling for hierarchical memory system

Partner 2: Argonne National Lab

Subject 2: Topology-aware data aggregation for I/O intensive application

Partner 3: BSC, Barcelona (Spain)

Subject 3: High-performance communication on new architectures; load-balancing and meshing: improve the distribution of data across the processors for a flow and particle simulation in the human nasal cavity.

Partner 4: University of Liege (Belgium), Université Catholique de Louvain (Belgium), Weierstrass Institute for Applied Analysis and Stochastics (WIAS) (Germany)

Subject 4: Coupling sequential remeshers with PaMPA began in 2016. The work [23] is in progress and it concerns Tetgen developed by Hang Si, and Gmsh by Christophe Geuzaine and Jean-François Remacle.

9.3. International Initiatives

9.3.1. Inria International Labs

Joint-Lab on Extreme Scale Computing (JLESC):

Coordinators: Franck Cappello and Marc Snir.

Other partners: Argonne National Lab, University of Urbana Champaign, Tokyo Riken, Jülich Supercomputing Center, Barcelona Supercomputing Center.

Abstract: The Joint Laboratory is based at Illinois and includes researchers from Inria, and the National Center for Supercomputing Applications, ANL, Riken, Jülich, and BSC. It focuses on software challenges found in extreme scale high-performance computers.

9.3.2. Inria International Partners

9.3.2.1. Declared Inria International Partners

Partner 1: AMD Research

Subject 1: Managing locality in the Heterogeneous System Architecture.

AMD provided hardware and details about its future architectures and programming models (HSA) to improve locality support for its products in the HWLOC software.

9.3.2.2. Informal International Partners

Partner 1: ICL at University of Tennessee

Subject 1: 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 2: Cisco Systems

Subject 2: network topologies and platform models

Partner 3: University of Tokyo and RIKEN

Subject 3: Adaptation of MPI and runtime systems to lightweight kernels used on clusters of manycores. This action has been submitted as a JLESC project proposal, currently beeing evaluated.

Partner 4: Lawrence Livermore National Laboratory

Subject 4: Testing of the mapping features of SCOTCH on very large process graphs (more than two billion vertices) and very large target architectures (more than 200,000 parts).

Partner 5: Sandia National Lab

Subject 5: Topology-aware management and allocation of computing resources in runtime systems.

9.4. International Research Visitors

9.4.1. Visits of International Scientists

- Balazs Gerofi from RIKEN visited us to present his work on micro-kernels for HPC. His visit led to a project proposal for JLESC.
- Jose-Luiz Garcia Zapata, stayed for three months in the team to work on spectral partitioning and mapping. He implemented a spectral bipartitioning method in SCOTCH.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

10.1.1.1. General Chair, Scientific Chair

Guillaume AUPY was the Technical Program vice-chair of SC'17.

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

Guillaume AUPY was the co-chair of the Parallel and Distributed Algorithms track of ICA3PP'17.

Emmanuel JEANNOT was the Program chair of the Heterogeneity in Computing Workshop (HCW'17).

Emmanuel JEANNOT was the Program chair of the track parallelism of COMPAS 2016.

10.1.2.2. Member of the Conference Program Committees

Alexandre DENIS was a member of the program committee of Compas'16 and CCGrid 2017.

Brice GOGLIN was a member of the program committee of CCGrid 2016, Cluster 2016, EuroMPI 2017, HotInterconnect 24 and of the Exacomm workshop.

Emmanuel JEANNOT was a member of the program committee of IPDPS 2017, CCGRID 2017,

Guillaume MERCIER was a member of the program committee of EuroMPI 2016 and EuroMPI 2017.

10.1.2.3. Reviewer

Cyril BORDAGE was reviewer for Cluster 2016.

Alexandre DENIS was a reviewer for Cluster 2016.

Brice GOGLIN was a reviewer for IEEE Micro.

Farouk MANSOURI was a reviewer for Cluster 2016.

Guillaume MERCIER was a reviewer for IPDPS 2017.

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).

Guillaume MERCIER is editor of the EuroMPI 2016 Special issue of the Journal of High Performance Computing Applications (IJHPCA).

10.1.3.2. Reviewer - Reviewing Activities

Guillaume AUPY was a reviewer for EURASIP Journal of Embedded Systems, Cluster Computing and Transactions on Parallel and Distributed Systems (TPDS).

Alexandre DENIS was a reviewer for the Journal of Parallel and Distributed Computing (JPDC).

Emmanuel JEANNOT was reviewer of IEEE TPDS.

Guillaume MERCIER was a reviewer for the EuroMPI 2016 Special Issue of the Parallel Computing journal.

François PELLEGRINI was a reviewer for SIAM Journal on Scientific Computing (SISC).

10.1.4. Invited Talks

Brice GOGLIN gave a talk about managing hardware locality in HPC during an AMD Tech Talk at AMD Research (Austin, TX).

Emmanuel JEANNOT gave a talk about topology-aware data management at the Workshop on Clusters, Clouds, and Data for Scientific Computing (CCDSC 2016).

Emmanuel JEANNOT gave a talk about metrics and models for process placement at the Third Workshop on Programming Abstractions for Data Locality (PADAL'16).

François PELLEGRINI delivered a keynote speech on freedom in the digital age, during the annual congress of *Société informatique de France*, Strasbourg.

François PELLEGRINI gave a talk on software law at Université de Nice Sophia-Antipolis.

François PELLEGRINI participated in a round-table on *Big data, compliance and personal data* during the JInov meeting, Paris.

François PELLEGRINI gave a talk on *Free software, a tool for sustainable development in countries of the Souths* law at the *Colloque international sur le logiciel libre dans les pays du Sud*, organized by Université Moulay Ismaïl & École nationale supérieure d'arts et métiers de Meknès.

François PELLEGRINI delivered a talk on freedom in the digital age, during the Defense Security Cyber summer school organized by Université de Bordeaux.

François PELLEGRINI delivered a talk on freedom and the ethics of informatics during the summer school for young researchers on the ethics of informatics, organized by CERNA and Allistene in Arcachon.

François PELLEGRINI participated in a round-table on the legal criteria for software originality in the colloquium on protection and infringement of software : the notion of digital common pool, organized by AFDIT at Conseil national des barreaux, Paris.

François PELLEGRINI delivered a talk on the issues of rights on immaterial goods for digital development, during the international seminar of training for trainers on internet and information systems governance, organised by ITICC with the support of Organisation Internationale de la Francophonie and ARCEP-BF, in Ouagadougou.

François PELLEGRINI delivered the opening conference on the legal and economic bases of the digital economy, for a training seminar for Members of the Parliament of Benin on the issues of laws on digital matters, organized by Organisation Internationale de la Francophonie at Grand-Popo.

François PELLEGRINI gave a talk on the operational solutions to digital security issues, during the 4th NGO forum organized by the French embassy in Moscow.

François PELLEGRINI delivered a keynote speech on the governance of open and free innovation, at the invitation of the French ministry of Foreign affairs, during the workshop on open innovation which took place within the French-German inter-governmental conference on digital issues, in Berlin.

Adèle VILLIERMET has been invited to give a talk at the summer school of GDR RO.

10.1.5. Scientific Expertise

Emmanuel JEANNOT was member of the hiring committee for an assistant professor position in informatics at Université de Bordeaux.

Brice GOGLIN was also a member of the hiring committee for Inria Bordeaux - Sud-Ouest research scientists.

François PELLEGRINI was a member of the hiring committee for a full professor position in informatics at Université de Nice Sophia-Antipolis (PR27-327). He also reviewed a PR1 promotion file at Université de Bordeaux.

10.1.6. Standardization Activities

TADAAM attends the MPI Forum meetings on behalf of Inria (where the MPI standard for communication in parallel applications is developed and maintained).

A proposal is currently under early discussion for submission to the forum [7.15](#).

10.1.7. Tutorials

Brice GOGLIN gave a tutorial about managing hardware affinities on hierarchical platforms with HWLOC during a PRACE Advanced Training Center session.

François PELLEGRINI gave a “hands-on” tutorial on SCOTCH during a meeting of the European project COLOC.

10.1.8. Research Administration

Emmanuel JEANNOT is member of the scientific committee of the Labex IRMIA (Université de Strasbourg).

Emmanuel JEANNOT is the head of the young researcher commission of Inria Bordeaux Sud-Ouest in charge of supervising the hiring of the PhDs and post-doc of the center.

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 and C programming to advanced topics such as computer architecture, operating systems, parallel programming and high-performance runtime systems, as well as software law.

10.2.2. Supervision

PhD in progress: Remi Barat, multi-criteria graph partitioning, started in 2014. Advisor: François Pellegrini.

PhD in progress: Raphaël Blanchard, parallelization and data distribution of discontinuous Galerkin methods for complex flow simulations, started in 2013. Advisor: François Pellegrini.

PhD in progress: Nicolas Denoyelle, advanced memory hierarchies and new topologies, started in 2015. Advisor: Brice Goglin and Emmanuel Jeannot.

PhD in progress: Benjamin Lorendeau, new programming models and optimization of Code Saturn, started in 2015. Advisor: Yvan Fournier and Emmanuel Jeannot.

PhD in progress: Hugo Taboada, communication progression in runtime systems, started in 2015. Advisor: Alexandre Denis and Emmanuel Jeannot.

PhD in progress: Adèle Villiermet, topology-aware resource management, started in 2014. Advisor: Emmanuel Jeannot and Guillaume Mercier.

PhD stopped: Romain Prou, communication management based on remote memory access, student resigned in october 2016. Advisor: Alexandre Denis and Emmanuel Jeannot.

10.2.3. Juries

Brice GOGLIN was member of the PhD defense committee of:

- Mohamed Lamine Karaoui (Université Pierre et Marie Curie, Reviewer).

Emmanuel JEANNOT was member of the PhD defense committee of:

- Loïc Thiébault (Université de Versailles Saint-Quentin, Reviewer).

François PELLEGRINI was member of the PhD defense committee of:

- Karl-Eduard Berger (Université de Versailles Saint-Quentin);
- Alessandro Fanfarillo (Università degli Studi di Roma Tor Vergata, Reviewer);
- Thomas Hume, Université de Bordeaux;
- Sébastien Morais (Université Évry Val d'Essonne, Reviewer).

10.3. Popularization

Brice GOGLIN is in charge of the diffusion of the scientific culture for the Inria Research Center of Bordeaux. He organized several popularization activities in the center. He also gave several talks about computer architecture, high performance computing, and research careers to general public audience, school students, teachers, or even to non-expert Inria colleagues.

Brice GOGLIN was involved in the design of the section about fundamentals of computer science in the 2017 massive open online course that will help teachers of the new ICN section in schools (*Informatique et Création Numérique*). It was filmed for 10 video sequences (about an hour in total).

François PELLEGRINI was filmed during a 3-hour conference on author's rights, in the context of the MAPI'Days, to serve as an on-line training for personnel and students of Université de Bordeaux (<https://fad.u-bordeaux.fr/course/view.php?id=740>).

François PELLEGRINI is the author of an opinion piece on digital sovereignty in newspaper Le Monde (http://www.lemonde.fr/idees/article/2016/06/24/la-souverainete-numerique-passe-par-le-logiciel-libre_4957781_3232.html).

François PELLEGRINI is the co-author of a booklet on free/libre software licenses edited by Pôle Systematic Paris Région & Pôle Aquinetic, which is now in its second edition (http://systematic-paris-region.org/sites/default/files/content/page/attachments/LivretBleu_Juridique_GT-LogicielLibre_Systematic_Mai2016_web.pdf).

In the context of the decree authorizing the TES (*Titres Électroniques Sécurisés*) file, François PELLEGRINI published a set of three blog posts (starting with <http://www.pellegrini.cc/2016/11/la-biometrie-des-honnetes-gens/>), which have been cited and linked by several French newspapers (Libération, Mediapart, NextInpact). He also participated in a debate on the same subject, organised by the Ligue des droits de l'Homme de Gironde (<http://dh-gironde.org/jeudi-15-decembre-2016-a-18h30-rencontre-debat-autour-du-mega-fichier-tes/>).

François PELLEGRINI delivered a talk on *Freedom and the ethics of informatics* during a seminar on *Technologies, ethics and cognition* organized by the bouddhist group Dhagpo Bordeaux, in partnership with Cap Sciences and Université de Bordeaux (<http://www.dhagpo-bordeaux.org/seminaire-technologies-ethique-cognition/>).

François PELLEGRINI was filmed, during an interview on *Innovation and free/libre licenses*, for the ULab Innov+ MOOC.

11. Bibliography

Publications of the year

Articles in International Peer-Reviewed Journal

- [1] L.-C. CANON, E. JEANNOT. *Correlation-Aware Heuristics for Evaluating the Distribution of the Longest Path Length of a DAG with Random Weights*, in "IEEE Transactions on Parallel and Distributed Systems", 2016, <https://hal.inria.fr/hal-01412922>.

Articles in Non Peer-Reviewed Journal

- [2] J. CARRETERO, R. ČIEGIS, E. JEANNOT, L. LEFÈVRE, G. RÜNGER, D. TALIA, Ž. JULIUS. *HeteroPar 2014, APCIE 2014, and TASUS 2014 Special Issue*, in "Concurrency and Computation: Practice and Experience", 2016, 2, <https://hal.inria.fr/hal-01253278>.

Invited Conferences

- [3] F. PELLEGRINI. *L'enjeu du big data pour la gouvernance*, in "Journée d'Etude : Transition numérique et action publique : focus sur la loi pour une République numérique", Paris, France, Centre d'études et de Recherches de sciences administratives et politiques de l'Université Paris II and Chaire Mutations de l'Action Publique et du Droit Public, November 2016, <https://hal.inria.fr/hal-01418990>.
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International Conferences with Proceedings

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- [7] I. CORES, P. GONZÁLEZ, E. J. JEANNOT, M. J. MARTÍN, G. RODRÍGUEZ. *An application-level solution for the dynamic reconfiguration of MPI applications*, in "12th International Meeting on High Performance Computing for Computational Science", Porto, Portugal, June 2016, <https://hal.inria.fr/hal-01424263>.
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- [9] Y. GEORGIU, E. JEANNOT, G. MERCIER, A. VILLIERMET. *Topology-aware resource management for HPC applications*, in "ICDCN 2017", Hyderabad, India, January 2017 [DOI : 10.1145/3007748.3007768], <https://hal.inria.fr/hal-01414196>.
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National Conferences with Proceeding

- [14] F. MANSOURI, J. GUSTEDT. *Le modèle de programmation ORWL pour la parallélisation d'une application de suivi vidéo HD sur architecture multi-coeurs*, in "Conférence d'informatique en Parallélisme, Architecture et Système (COMPAS)", Lorient, France, July 2016, accepted for publication in Compas' 16, <https://hal.inria.fr/hal-01325850>.

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