RESEARCH CENTER
Bordeaux - Sud-Ouest

FIELD

Activity Report 2015

Section Application Domains

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LFANT Project-Team (section vide)

POSET Team

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 SCRIME [0]. 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).

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.

[0] Studio de Création et de Recherche en Informatique et Musiques Expérimentales

CAGIRE Team

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 was developed by P. Bruel in that framework 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. 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.

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, 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.

CARDAMOM Team

4. Application Domains

4.1. De-anti icing systems

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

In [75] it has bee 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 [65], [122]. In these methods we compensate for the error at solid walls introduced by the penalization by using anisotropic mesh adaptation [94], [113], [114]. 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 [77]. 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 [79], [74] 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 [125], 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 [144], 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 accomodation 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 accomodation 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 [78], [117]. 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 [124] 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 sing 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

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

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

The simulation of these gases requires accurate thermodynamic models, such as Span-Wagner or Peng-Robinson (see [87]). 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 [143], 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 [98], we will develop, analyse, compare, and use for multi-fidelity optimization,non-linear models of different scales (fidelity) ranging from simple linear hydrodynamics over asymptotic discrete nonlinear wave models, to non-hydrostatic anisoptropic Euler free surface solvers. We will not work on the development of small scale models (VOF-RANS or LES) but may use such models, developed by our collaborators, for validation purposes. These developments will benefit from all our methodological work on asymptotic modelling and high order discretizations. As shown in [98], asymptotic models foe WECs involve an equation for the pressure on the body inducing a PDE structure similar to that of incompressible flow equations. The study of appropriate stable and efficient high order approximations (coupling velocity-pressure, efficient time stepping) will be an important part of this activity. Moreover, the flow-floating body interaction formulation introduces time stepping issues similar to those encountered in fluid structure interaction problems, and require a clever handling of complex floater geometries based on adaptive and ALE techniques. For this application, the derivation of fully discrete asymptotics may actually simplify our task.

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

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

4.4. 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 [128].

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

In collaboration wit the LCTS laboratory (a joint CNRS-CEA-SAFRAN-Bordeaux University lab devoted to the study of thermo-structural materials in Bordeaux), we are developing a multi-scale model in which a structural mechanics solver is coupled with a closure model for the crack physico chemistry. This model is obtained as a multi-dimensional asymptotic crack averaged approximation fo the transport equations (Fick's laws) with chemical reactions sources, plus a potential model for the flow of oxide [90], [95], [126]. We have demonstrated the potential of this model in showing the importance of taking into account the multi-dimensional topology of a fibre bundle (distribution of fibres) in the rupture mechanism. This means that the 0-dimensional model used in most of the studies (se e.g. [86]) 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 [110], [132], [123], [92], to hybrid methods coupling dispersive PDEs with hyperbolic ones, and trying to mimic wave breaking with travelling bores [136], [137], [135], [107], [100]. In both cases, numerical dissipation plays an important role and the activation or not of the breaking closure, as the quantitative contribution of numerical dissipation to the flow has not been properly investigated. These elements must be clarified to allow full control of adaptive techniques for the models used in this type of applications.

Another point we want to clarify is how to optimize the discretization of asymptotic PDE models. In particular, when adding mesh size(s) and time step, we are in presence of at least 3 (or even more) small parameters. The relations between physical ones have been more or less investigates, as have been the ones between purely numerical ones. We plan to study the impact of numerics on asymptotic PDE modelling by reverting the usual process and studying asymptotic limits of finite element discretizations of the Euler equations. Preliminary results show that this does allow to provide some understanding of this interaction and to possibly propose considerably improved numerical methods [76].

CQFD Project-Team

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.

GEOSTAT Project-Team

4. Application Domains

4.1. Application Domains

Application aspects in GEOSTAT encompass biomedical data (heartbeat signal analysis with IHU LIRYC, biomedical applications in speech signal analysis) and the study of universe science datasets. GEOSTAT's objectives in analysis of biomedical data hinge on the following observations:

- The analysis and detection of cardiac arrhythmia and pathological voice disorders is a paradigm in nonlinear methodologies applied to these types of signals.
- The classical hypothesis under linear approaches are confronted with strong nonlinearities, aperiodicity and chaotic phenomena present in theses signals.
- Existing nonlinear approaches are lacking physiological interpretation. Our objective in this part is to propose new measures based on low-level transition characteristics, these transition phenomena being related to general concepts associated to predictability in complex systems.

MEMPHIS Team

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 realisation 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. The background method for fluid structure interface is the volume penalization method where the level set functions is used to improve the degree of accuracy of the method and also to follow the object. The simulations are unsteady, three dimensional, with $O(10^8)$ grid points on 512 CPUs.

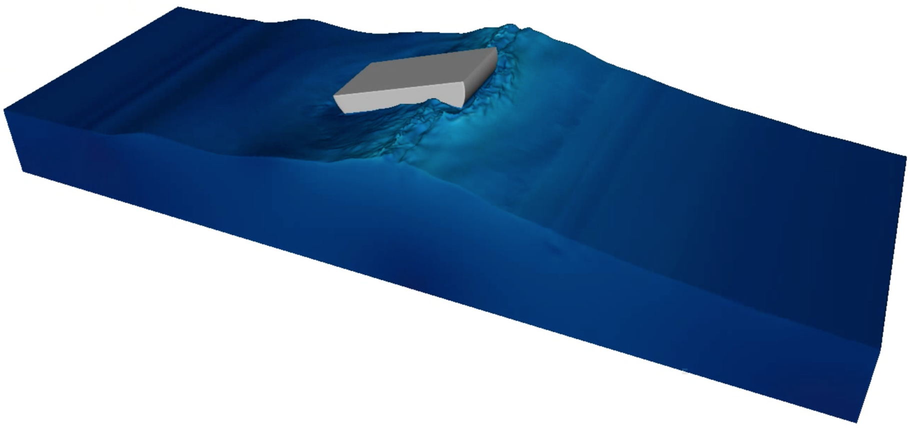

Figure 1. Numerical modeling of a sea-wave converter by a monolithic model and Cartesian meshes.

4.2. Impacts

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.

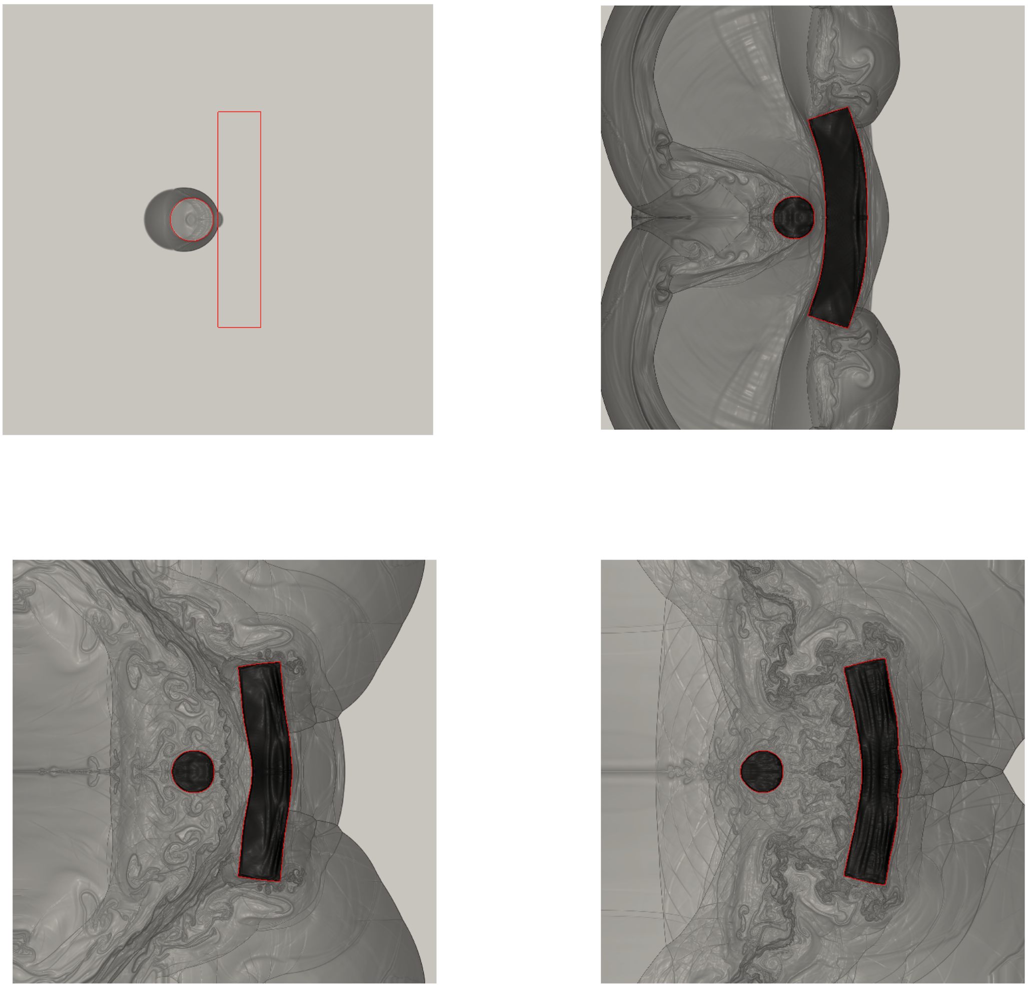

Figure 2. Impact and rebound of a copper projectile on a copper plate. Interface and schlieren at $50\mu s$, $199\mu s$, $398\mu s$ and $710\mu s$. From left to right, top to bottom.

4.3. New materials

Thanks to the multiscale schemes that we develop, we can charcterize 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 device 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).

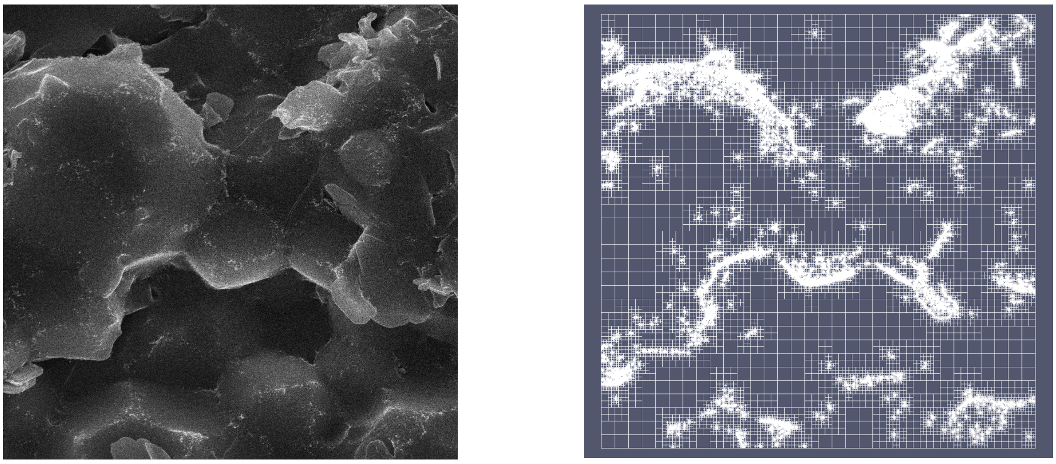

Figure 3. A micrography of an electrostrictive material is shown on the left: the bright regions visualize the carbon nanotubes. The hierarchical grid adapted to the nanotubes is shown on the right. The ratio between the largest and the smallest cell side is 2^7. Project developed in collaboration with the CRPP physics and chemistry lab of the CNRS in Bordeaux (Annie Colin, Philippe Poulin).

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.

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.

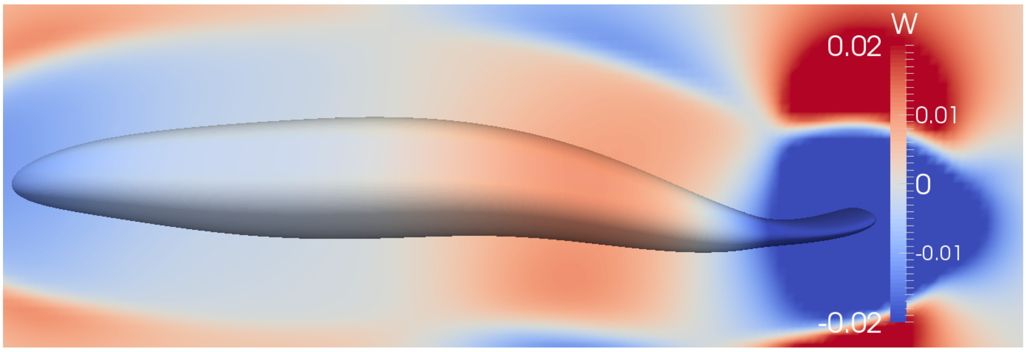

Figure 4. Comparison of the exact deformation velocity (presented inside the swimmer) and the approximated velocity identified using optimal transport (represented outside the fish). The error of the identification scheme is negligible for this component of the velocity, as it can be inferred by comparing the two velocities on the boundary of the swimmer.

For this reason, we will consider incompressible or rigid transports.

REALOPT Project-Team

4. Application Domains

4.1. Introduction

Our group has tackled applications in logistics, transportation and routing [60], [59], [55], [57], in production planning [77] and inventory control [55], [57], in network design and traffic routing [38], [47], [53], [80], [35], [48], [66], [73], in cutting and placement problems [63], [64], [74], [75], [76], [78], and in scheduling [6], [67], [33].

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 [47]. 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 [82], [81], [80] 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 [79]. 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 [53], [54].

We studied several time dependent formulations for the unit demand vehicle routing problem [40], [39]. 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 [72] 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 testes on a set of real-life instances coming from a Russian freight real transportation company. Our algorithmes have been faster on these instances than the current solution approach being used by the company.

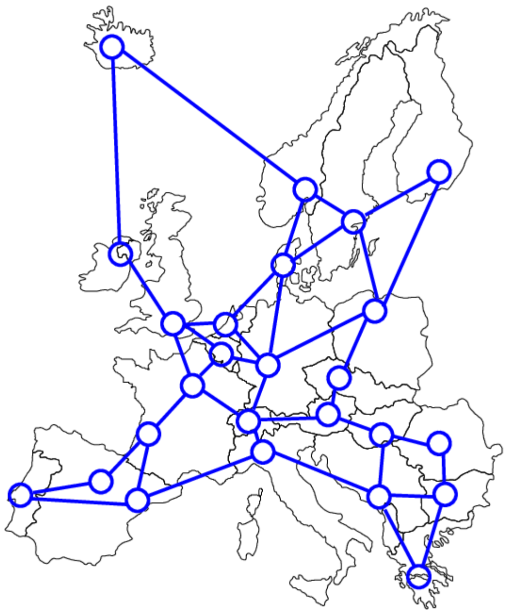

Figure 1. Design of a SDH/SONET european network where demands are multiplexed.

4.3. Packing and Covering Problems

Realopt team has a strong experience on exact methods for cutting and packing problems. These problems occur in logistics (loading trucks), industry (wood or steel cutting), computer science (parallel processor scheduling).

We developed a branch-and-price algorithm for the Bin Packing Problem with Conflicts which improves on other approaches available in the literature [71]. 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 developped a branch-and-price algorithm for a variant of the bin-packing problem where the items are fragile. In [31] 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 [57]: we faced a multiple-class integer knapsack problem with setups [56] (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 [50], [49], [52], [51]. 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 developping exacti 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. They are extra sequencing constraints regarding the production that make the problem even more complex.
Finally, let us add that we are now organizing a european challenge on packing with society Renault: see http://challenge-esicup-2015.org/. This challenge is about loading trucks under practical constraints. The final results will be announced in March 2015.

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. [58]. 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 [60].

Together with our partner company GAPSO from the associate team SAMBA, we worked on the equipment routing task scheduling problem [65] arising during port operations. In this problem, a set of tasks needs to be performed using equipments of different types with the objective to maximum the weighted sum of performed tasks.

We participated to the project on an airborne radar scheduling. For this problem, we developed fast heuristics [46] and exact algorithms [33]. A substantial research has been done on machine scheduling problems. A new compact MIP formulation was proposed for a large class of these problems [32]. An exact decomposition algorithm was developed for the NP-hard maximizing the weighted number of late jobs problem on a single machine [67]. A dominant class of schedules for malleable parallel jobs was discovered in the NP-hard problem to minimize the total weighted completion time [69]. We proved that a special case of the scheduling problem at cross docking terminals to minimize the storage cost is polynomially solvable [70], [68].

Another application area in which we have successfully developed MIP approaches is in the area of tactical production and supply chain planning. In [30], we proposed a simple heuristic for challenging multi-echelon problems that makes effective use of a standard MIP solver. [29] 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 [34] 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 [42], [41], 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 [36]. We considered train timetabling problems and their re-optimization after a perturbation in the network [44], [43]. 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 [45]. 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 adressed 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 [37].

CARMEN Team

4. Application Domains

4.1. Scientific context: the LIRYC

Our fields of application are naturally: electrophysiology and cardiac physiopathology at the tissue scale on one side; medical and clinical cardiology on the other side.

The team's research project is part of the IHU LIRYC project, initiated by Pr. M. Haissaguerre. It is concerned by the major issues of modern electrocardiology: atrial arrhythmias, sudden death due to ventricular fibrillation and heart failure related to ventricular dyssynchrony.

We aim at bringing applied mathematics and scientific computing closer to biomedical research applied to cardiac rhythmology and clinical cardiology. It aims at enhancing our fundamental knowledge of the normal and abnormal cardiac electrical activity, 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 the 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:

At the atrial level, we apply our models to understand the mechanisms of complex arrythmias and the relation with the heterogeneities at the insertion of the pulmonary vein.

At the ventricula level, we focus on (1) modeling the complex coupling between the Purkinje network and the ventricles and (2) modeling the structural heterogeneities at the cellular scale, taking into account the complex organisation and disorganisation 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.

MAGIQUE-3D Project-Team

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. Modeling of Multiperforated plates in turboreactors

In the turbo-engine, the temperature can reach 2000 K inside the combustion chamber. To protect its boundary, “fresh” air at 800 K is injected through thousands of perforations. The geometry of the network of perforations is chosen in order to optimize the cooling and the mechanical properties of the chamber. It has been experimentally observed that these perforations have a negative impact on the stability of the combustion. This is due to the interaction with an acoustic wave generated by the combustion. Due to the large number of holes (2000) and their small sizes (0.5 mm) with respect to the size of the combustion chamber (50 cm), it is not conceivable to rely on numerical computations (even with supercomputers) to predict the influence of these perforations.

In collaboration with ONERA, we develop new models which allow to take into account these multiperforated plates at the macroscopic scale.

4.3. Helioseismology

This collaboration with the Max Planck Institute for solar system, 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.

MNEMOSYNE Project-Team

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 mnesic and cognitive deficits, require a systemic view of the cerebral architecture and associated functions, very consistent with our approach.

Of course, numerical sciences are also impacted by our researches, at several levels. At a global level, we will propose new control architectures aimed at providing a higher degree of autonomy to robots, as well as machine learning algorithms working in more realistic environment. More specifically, our focus on some cognitive functions in closed loop with a real environment will address currently open problems. This is obviously the case for planning and decision making; this is particularly the case for the domain of affective computing, since motivational characteristics arising from the design of an artificial physiology allow to consider not only cold rational cognition but also hot emotional cognition. The association of both kinds of cognition is undoublty an innovative way to create more realistic intelligent systems but also to elaborate more natural interfaces between these systems and human users.

At last, we think that our activities in well-founded distributed computations and high performance computing are not just intended to help us design large scale systems. We also think that we are working here at the core of informatics and, accordingly, that we could transfer some fundamental results in this domain.

Monc Team

4. Application Domains

4.1. Introduction

We now present our contribution to these above challenges. We do an investigation of particular cancers:

- Gliomas (brain tumors),
- Meningioma,
- Colorectal cancers,
- Lung and liver metastasis,
- Breast cancer.

4.2. Axis 1: Tumor modeling for patient-specific simulations

- Patient-specific simulations
- Parameter estimations (with the help of low order models)

4.3. Axis 2: Bio-physical modeling for personalized therapies

- Modelling of electrochemotherapy

4.4. Axis 3: Quantitative cancer modeling for biological and preclinical studies

- 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

PLEIADE Team

4. Application Domains

4.1. Genome and transcriptome annotation, to model function

Sequencing genomes and transcriptomes provides a picture of how a biological system can function, or does function under a given physiological condition. Simultaneous sequencing of a group of related organisms is now a routine procedure in biological laboratories for studying a behavior of interest, and provides a marvelous opportunity for building a comprehensive knowledge base of the relations between genomes. Key elements in mining these relations are: classifying the genes in related organisms and the reactions in their metabolic networks, recognizing the patterns that describe shared features, and highlighting specific differences.

PLEIADE will develops applications in comparative genomics of related organisms, using new mathematical tools for representing compactly, at different scales of difference, comparisons between related genomes. New methods based on computational geometry refine these comparisons. Compact representations can be stored, exchanged, and combined. They will form the basis of new simultaneous genome annotation methods, linked directly to abductive inference methods for building functional models of the organisms and their communities.

Our ambition in biotechnology is to permit the design of synthetic or genetically selected organisms at an abstract level, and guide the modification or assembly of a new genome. Our effort is focused on two main applications: genetic engineering and synthetic biology of oil-producing organisms (biofuels in CAER, palm oils), and improving and selecting starter microorganisms used in winemaking (collaboration with the ISVV and the BioLaffort company).

4.2. Molecular based systematics and taxonomy

Defining and recognizing myriads of species in biosphere has taken phenomenal energy over the past centuries and remains a major goal of Natural History. It is an iconic paradigm in pattern recognition (clustering has coevolved with numerical taxonomy many decades ago). Developments in evolution and molecular biology, as well as in data analysis, have over the past decades enabled a profound revolution, where species can be delimited and recognized by data analysis of sequences. We aim at proposing new tools, in the framework of E-science, which make possible (i) better exploration of the diversity in a given clade, and (ii) assignment of a place in these patterns for new, unknown organisms, using information provided by sets of sequences. This will require investment in data analysis, machine learning, and pattern recognition to deal with the volumes of data and their complexity.

One example of this project is about the diversity of trees in Amazonian forest, in collaboration with botanists in French Guiana. Protists (unicellular Eukaryots) are by far more diverse than plants, and far less known. Molecular exploration of Eukaryotes diversity is nowadays a standard in biodiversity studies. Data are available, through metagenomics, as an avalanche and make molecular diversity enter the domain of Big Data. Hence, an effort will be invested, in collaboration with other Inria teams (GenScale, HiePACS) for porting to HPC algorithms of pattern recognition and machine learning, or distance geometry, for these tools to be available as well in metagenomics. This will be developed first on diatoms (unicellular algae) in collaboration with INRA team at Thonon and University of Uppsala), on pathogens of tomato and grapewine, within an existing network, and on bacterial communities, in collaboration with University of Pau. For the latter, the studies will extend to correlations between molecular diversity and sets of traits and functions in the ecosystem.

4.3. Community ecology and population genetics

Community assembly models how species can assemble or diassemble to build stable or metastable communities. It has grown out of inventories of countable organisms. Using *metagenomics* one can produce molecular based inventories at rates never reached before. Most communities can be understood as pathways of carbon exchange, mostly in the form of sugar, between species. Even a plant cannot exist without carbon exchange with its rhizosphere. Two main routes for carbon exchange have been recognized: predation and parasitism. In predation, interactions–even if sometimes dramatic–may be loose and infrequent, whereas parasitism requires what Claude Combes has called intimate and sustainable interactions [17]. About one decade ago, some works [21] have proposed a comprehensive framework to link the studies of biodiversity with community assembly. This is still incipient research, connecting community ecology and biogeography.

We aim at developping graph-based models of co-occurence between species from NGS inventories in metagenomics, i.e. recognition of patterns in community assembly, and as a further layer to study links, if any, between diversity at different scales and community assemblies, starting from current, but oversimplified theories, where species assemble from a regional pool either randomly, as in neutral models, or by environmental filtering, as in niche modeling. We propose to study community assembly as a multiscale process between nested pools, both in tree communities in Amazonia, and diatom communities in freshwaters. This will be a step towards community genomics, which adds an ecological flavour to metagenomics.

Convergence between the processes that shape genetic diversity and community diversity–drift, selection, mutation/speciation and migration–has been noted for decades and is now a paradigm, establishing a continuous scale between levels of diversity patterns, beyond classical approaches based on iconic levels like species and populations. We will aim at deciphering diversity pattern along these gradients, connecting population and community genetics. Therefore, some key points must be adressed on reliability of tools.

Next-generation sequencing technologies are now an essential tool in population and community genomics, either for making evolutionary inferences or for developing SNPs for population genotyping analyses. Two problems are highlighted in the literature related to the use of those technologies for population genomics: variable sequence coverage and higher sequencing error in comparison to the Sanger sequencing technology. Methods are developed to develop unbiased estimates of key parameters, especially integrating sequencing errors [20]. 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 [18]. Several approaches were proposed to correct for paralogy, either by working directly on the sequences issued from mapped reads [18] 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 [12]. Workflows to implement statistical methods that correct for diversity biases estimates now need an implementation for biologists.

SISTM Project-Team

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" [35], "Systems vaccinology" [32], "Systems medicine" [24]. 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 [28]. 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) [23]. However, the implementation of such strategy is difficult especially in developing countries. Some HIV infected individuals do not tolerate antiretroviral regimen or did not reconstitute their immune system. Therefore, vaccine and other immune interventions are required. Many vaccine candidates as well as other immune interventions (IL7, IL15) are currently evaluated. The challenges here are multiple because the effects of these interventions on the immune system are not fully understood, there are no good surrogate markers although the number of measured markers has exponentially increased. Hence, HIV clinical epidemiology has also entered in the era of Big Data because of the very deep evaluation at individual level leading to a huge amount of complex data, repeated over time, even in clinical trials that includes a small number of subjects.

HIEPACS Project-Team

4. Application Domains

4.1. Material physics

Participants: Pierre Blanchard, Olivier Coulaud, Arnaud Etcheverry.

Due to the increase of available computer power, new applications in nano science and physics appear such as study of properties of new materials (photovoltaic materials, bio- and environmental sensors, ...), failure in materials, nano-indentation. Chemists, physicists now commonly perform simulations in these fields. These computations simulate systems up to billion of atoms in materials, for large time scales up to several nanoseconds. The larger the simulation, the smaller the computational cost of the potential driving the phenomena, resulting in low precision results. So, if we need to increase the precision, there are two ways to decrease the computational cost. In the first approach, we improve algorithms and their parallelization and in the second way, we will consider a multiscale approach.

A domain of interest is the material aging for the nuclear industry. The materials are exposed to complex conditions due to the combination of thermo-mechanical loading, the effects of irradiation and the harsh operating environment. This operating regime makes experimentation extremely difficult and we must rely on multi-physics and multi-scale modeling for our understanding of how these materials behave in service. This fundamental understanding helps not only to ensure the longevity of existing nuclear reactors, but also to guide the development of new materials for 4th generation reactor programs and dedicated fusion reactors. For the study of crystalline materials, an important tool is dislocation dynamics (DD) modeling. This multiscale simulation method predicts the plastic response of a material from the underlying physics of dislocation motion. DD serves as a crucial link between the scale of molecular dynamics and macroscopic methods based on finite elements; it can be used to accurately describe the interactions of a small handful of dislocations, or equally well to investigate the global behavior of a massive collection of interacting defects.

To explore i.e. to simulate these new areas, we need to develop and/or to improve significantly models, schemes and solvers used in the classical codes. In the project, we want to accelerate algorithms arising in those fields. We will focus on the following topics (in particular in the currently under definition OPTIDIS project in collaboration with CEA Saclay, CEA Ile-de-france and SIMaP Laboratory in Grenoble) in connection with research described at Sections 3.4 and 3.5 .

- The interaction between dislocations is long ranged ($O(1/r)$) and anisotropic, leading to severe computational challenges for large-scale simulations. In dislocation codes, the computation of interaction forces between dislocations is still the most CPU time consuming and has to be improved to obtain faster and more accurate simulations.
- In such simulations, the number of dislocations grows while the phenomenon occurs and these dislocations are not uniformly distributed in the domain. This means that strategies to dynamically construct a good load balancing are crucial to acheive high performance.
- From a physical and a simulation point of view, it will be interesting to couple a molecular dynamics model (atomistic model) with a dislocation one (mesoscale model). In such three-dimensional coupling, the main difficulties are firstly to find and characterize a dislocation in the atomistic region, secondly to understand how we can transmit with consistency the information between the two micro and meso scales.

4.2. Co-design for scalable numerical algorithms in scientific applications

Participants: Pierre Brenner, Jean-Marie Couteyen, Mathieu Faverge, Xavier Lacoste, Guillaume Latu, Salli Moustafa, Pierre Ramet, Fabien Rozar, Jean Roman.

The research activities concerning the ITER challenge are involved in the Inria Project Lab (IPL) C2S@EXA.

4.2.1. MHD instabilities edge localized modes

The numerical simulations tools designed for ITER challenges aim at making a significant progress in understanding 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. Project is focused in particular on the numerical modeling 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 the related physics and propose possible new strategies to improve effectiveness of ELM control techniques. The tool for the nonlinear MHD modeling (code 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 in order to progress in urgently needed solutions for ITER.

The fully implicit time evolution scheme in the JOREK code leads to large sparse linear systems that have to be solved at every time step. The MHD model leads to very badly conditioned matrices. In principle the PaStiX library can solve these large sparse problems using a direct method. However, for large 3D problems the CPU time for the direct solver becomes too large. Iterative solution methods require a preconditioner adapted to the problem. Many of the commonly used preconditioners have been tested but no satisfactory solution has been found. The research activities presented in Section 3.3 will contribute to design new solution techniques best suited for this context.

4.2.2. Turbulence of plasma particules inside a tokamak

In the context of the ITER challenge, the GYSELA project aims at simulating the turbulence of plasma particules inside a tokamak. Thanks to a better comprehension of this phenomenon, it would be possible to design a new kind of source of energy based of nuclear fusion. Currently, GYSELA is parallalized in a 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. In fact, the memory consumption is a bottleneck on very large simulations (449 K cores). 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.

The scientific objectives of these research activities are first the design of advanced generic tools to manage and to better predict and limit the memory consumption peak in order to reduce the memory footprint of GYSELA, and second to design a set of tools that analyses the performance and the topology of the targeted architecture to optimize the deployment of Gysela runs. This will allow the design of new advanced numerical methods (for the gyroaverage operator, for the source and collision operators) and efficient scalable parallel algorithms in order to be able to deal with new physics in GYSELA. In particular the objective is to tackle kinetic electron configurations for more realistic simulations.

4.2.3. 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.

4.2.4. 3D aerodynamics for unsteady problems with moving bodies

Aribus Defence and Space has developped 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, zero being the level with the slowest cells and each level being twice as fast as the previous one. 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 research is to design a new scalable version of FLUSEPA from a task-based parallelization over a runtime system in order to run efficiently on modern multicore parallel architectures very large 3D simulations (for example ARIANE 5 and 6 booster separation).

PHOENIX Project-Team

4. Application Domains

4.1. Introduction

Building on our previous work, we are studying software development in the context of communication services, in their most general forms. That is, going beyond human-to-human interactions, and covering human-to-machine and machine-to-machine interactions. Software systems revolving around such forms of communications can be found in a number of areas, including telephony, pervasive computing, and assisted living; we view these software systems as coordinating the communication between networked entities, regardless of their nature: human, hardware or software. In this context, our three main application domains are pervasive computing, internet of things and assistive computing.

4.2. Pervasive Computing

Pervasive computing systems are being deployed in a rapidly increasing number of areas, including building automation and supply chain management. Regardless of their target area, pervasive computing systems have a typical architectural pattern. They aggregate data from a variety of distributed sources, whether sensing devices or software components, analyze a context to make decisions, and carry out decisions by invoking a range of actuators. Because pervasive computing systems are standing at the crossroads of several domains (e.g., distributed systems, multimedia, and embedded systems), they raise a number of challenges in software development:

Heterogeneity. Pervasive computing systems are made of off-the-shelf entities, that is, hardware and software building blocks. These entities run on specific platforms, feature various interaction models, and provide non-standard interfaces. This heterogeneity tends to percolate in the application code, preventing its portability and reusability, and cluttering it with low-level details.

Lack of structuring. Pervasive computing systems coordinate numerous, interrelated components. A lack of global structuring makes the development and evolution of such systems error-prone: component interactions may be invalid or missing.

Combination of technologies. Pervasive computing systems involve a variety of technological issues, including device intricacies, complex APIs of distributed systems technologies and middleware-specific features. Coping with this range of issues results in code bloated with special cases to glue technologies together.

Dynamicity. In a pervasive computing system, devices may either become available as they get deployed, or unavailable due to malfunction or network failure. Dealing with these issues explicitly in the implementation can quickly make the code cumbersome.

Testing. Pervasive computing systems are complicated to test. Doing so requires equipments to be acquired, tested, configured and deployed. Furthermore, some scenarios cannot be tested because of the nature of the situations involved (e.g., fire and smoke). As a result, the programmer must resort to writing specific code to achieve ad hoc testing.

4.3. 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.

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.

4.4. Assistive Computing

Cognitive impairments (memory, attention, time and space orientation, *etc.*) affect a large part of the population, including older adults, patients with brain injuries (traumatic brain injury, stroke, etc), and people exhibiting cognitive incapacities, such as Down syndrome.

The emerging industry of assistive technologies provide hardware devices dedicated to specific tasks, such as a telephone set with a keyboard picturing relatives (http://www.doro.fr), or a device for audio and video communication over the web (http://www.technosens.fr). These assistive technologies apply a traditional approach to personal assistance by providing an equipment dedicated to a single task (or a limited set of tasks), without leveraging surrounding devices. This traditional approach has fundamental limitations that must be overcome to significantly improve assistive technologies:

- They are not adaptable to one's needs. They are generally dedicated to a task and have very limited functionalities: no networking, limited computing capabilities, a limited screen and rudimentary interaction modalities. This lack of functionality may cause a proliferation of devices, complicating the end-user life. Moreover, they are rarely designed to adapt to the cognitive changes of the user. When the requirements evolve, the person must acquire a new device.
- They are often proprietary, limiting innovation. As a result, they cannot cope with the evolution of users' needs.
- They have limited or no interoperability. As a result, they cannot rely on other devices and software services to offer richer applications.

To break this model, we propose to offer an assistive platform that is open-ended in terms of applications and entities. (1) An online catalog of available applications enables every user and caregiver to define personalized assistance in the form of an evolving and adapted set of applications; this catalog provides a community of developers with a mechanism to publish applications for specific daily-activity needs. (2) New types of entities (whether hardware or software) can be added to a platform description to enhance its functionalities and extend the scope of future applications.

STORM Team

4. Application Domains

4.1. Supporting Numeric Libraries and Scientific Simulation Applications

The application of our work covers linear algebra, solvers, fast-multipole methods, in collaboration with other Inria teams and with industry. This allows the scientific development of new techniques adapted to these applications, and opens its use in a large variety of physic simulations in high performance computing.

In terms of direct application, the software developped in the team have allowed applications in various physics fields, ranging from sismic, 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.

TADAAM Team

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.

[0] http://www.prace-ri.eu/prace-9th-regular-call/

FLOWERS Project-Team

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 developped in coordination with experimental evidence and investigation, see https://flowers.inria.fr/curiosity-information-seeking-and-attention-in-human-adults-models-and-experiments/.

Personal 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 aging society. For example, UNECE evaluates that the industry of entertainment, personal and service robotics will grow from $5.4Bnto$17.1Bn over 2008-2010. Yet, to realize this vision, important obstacles need to be overcome: these robots will have to evolve in unpredictable homes and learn new skills 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.

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. Video games. In conjunction with entertainment robotics, a new kind of video games are developing in which the player must either take care of a digital creature (e.g. Neopets), or tame it (e.g. Nintendogs), or raise/accompany them (e.g. Sims). The challenges entailed by programming these creatures share many features with programming personal/entertainment robots. Hence, the video game industry is also a natural field of application for FLOWERS.

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

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

MANAO Project-Team

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.

POTIOC Project-Team

4. Application Domains

4.1. Popularization of science, education, 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

- popularization of science
- education
- art
- entertainment

See "Objective 3: Exploring new applications and usages" (3.4) for a detailed description.