Activity Report 2013

Team BACCHUS

Parallel tools for Numerical Algorithms and Resolution of essentially Hyperbolic problems

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Numerical schemes and simulations

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Team BACCHUS

Keywords: High Performance Computing, Fluid Dynamics, Numerical Methods, Stochastic Methods, Parallel Solver

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2. Overall Objectives

2.1. Overall Objectives

BACCHUS is a joint team of Inria Bordeaux - Sud-Ouest, LaBRI (Laboratoire Bordelais de Recherche en Informatique – CNRS UMR 5800, University of Bordeaux and IPB) and IMB (Institut de Mathématiques de Bordeaux – CNRS UMR 5251, University of Bordeaux). BACCHUS has been created on January 1st, 2009 (http://bacchus.bordeaux.inria.fr).

The purpose of the BACCHUS project is to analyze and solve efficiently scientific computation problems that arise in complex research and industrial applications and that involve scaling. By scaling we mean that the applications considered require an enormous computational power, of the order of tens or hundreds of teraflops, and that they handle huge amounts of data. Solving these kinds of problems requires a multidisciplinary approach involving both applied mathematics and computer science.

Our major focus are fluid problems, and especially the simulation of *physical wave propagation problems* including fluid mechanics, inert and reactive flows, multimaterial and multiphase flows, acoustics, real-gas effects, etc. BACCHUS intends to contribute to the solution of these problems by bringing contributions to all steps of the development chain that goes from the design of new high-performance, more robust and more precise numerical schemes, to the creation and implementation of optimized parallel algorithms and high-performance codes.

By taking into account architectural and performance concerns from the early stages of design and implementation, the high-performance software which will implement our numerical schemes will be able to run efficiently on most of today's major parallel computing platforms (UMA and NUMA machines, large networks of nodes, production GRIDs).

2.2. Highlights of the Year

- In the context of the first contract supported by European Space Agency on uncertainty quantification (UQ), we applied some innovative UQ techniques in the challenging issue of predicting phenomena associated to the atmospheric reentry. In particular, we focused on the characterization of free-stream conditions in flight experiments, and the prediction of the radiative heat flux in high enthalpy facilities.
- In 2013 we have organized or contributed to the organization of three international conferences held at Inria or on the applied science campus of the Université de Bordeaux I : the Second ECCOMAS Young Investigators Conference (http://yic2013.sciencesconf.org), the EUROPEAN WORKSHOP on High Order Nonlinear Numerical Methods for Evolutionary PDEs (http://honom2013.bordeaux.inria.fr/), and the International Workshop on Uncertainty Quantification in fluids Simulation (http://boquse2013.bordeaux.inria.fr/) ;
- We have finally succeded in proposing Residual Distribution schemes that are *uniformly* accurate independently of the Reynolds number laminar, and turbulent compressible flow equations, with a stunning convergence to steady state down to machine zero ;
- We have shown the applicability of stabilized finite elements to the simulation of free surface water waves described by Boussinesq modes. We have demonstrated that residual based stabilization operators do not degrade the accuracy of the underlying finite element scheme, and used this to construct non oscillatory schemes for wave propagation, breaking, and runup ;

- We have developed an algorithm for the robust construction of curved simplicial meshes in two and three dimensions. Starting from a classical (straight) mesh, we are able to curve the boundary elements then the volumic ones and keep the boundary layer structures, even for meshes designed for turbulent simulations ;
- We developed a multiresolution strategy applied to a semi-intrusive scheme recently introduced in the context of uncertainty quantification (UQ) analysis for compressible fluids problems. This is one of the first global schemes in literature permitting an adaptive refinement in the coupled physical/stochastic space .
- `PaMPA` remeshed a coarse mesh of 27 millions of elements up to a fine mesh comprising more than 600 millions of elements, in 34 minutes, on 240 processors of the Avakas cluster at MCIA Bordeaux.
- François Pellegrini published a book on software law ; co-authored with Sébastien Canevet, associate professor at Université de Poitiers.

3. Research Program

3.1. Numerical schemes for fluid mechanics

Participants: Rémi Abgrall, Mario Ricchiuto, Dante de Santis, Pietro Marco Congedo, Cécile Dobrzynzki, Héloïse Beaugendre, Pierre-Henri Maire, Luc Mieussens, Philippe Bonneton, Gérard Vignoles.

A large number of engineering problems involve fluid mechanics. They may involve the coupling of one or more physical models. An example is provided by aeroelastic problems, which have been studied in details by other Inria teams. Another example is given by flows in pipelines where the fluid (a mixture of air–water–gas) does not have well-known physical properties, and there are even more exotic situations. In some occasions, one needs specific numerical tools to take into account *e.g.* a fluids' exotic equation of state, or a the influence of small flow scales in a macro-/meso-scopic flow model, etc. Efficient schemes are needed in unsteady flows where the amount of required computational resources becomes huge. Another situation where specific tools are needed is when one is interested in very specific physical quantities, such as *e.g.* the lift and drag of an airfoil, or the boundary of the area flooded by a Tsunami.

In these situations, commercial tools can only provide a crude answer. These codes, while allowing users to simulate a lot of different flow types, and "always" providing an answer, give results often of poor quality. This is mainly due to their general purpose character, and on the fact that the numerical technology implemented in these codes is not the most recent. To give a few examples, consider the noise generated by wake vortices in supersonic flows (external aerodynamics/aeroacoustics), or the direct simulation of a 3D compressible mixing layer in a complex geometry (as in combustion chambers). Up to our knowledge, due to the very different temporal and physical scales that need to be captured, a direct simulation of these phenomena is not in the reach of the most recent technologies because the numerical resources required are currently unavailable. *We need to invent specific algorithms for this purpose.*

Our goal is to develop more accurate and more efficient schemes that can adapt to modern computer architectures, and allow the efficient simulation of complex real life flows.

We develop a class of numerical schemes, known in literature as Residual Distribution schemes, *specifically tailored to unstructured and hybrid meshes*. They have the most possible compact stencil that is compatible with the expected order of accuracy. This *accuracy is at least of second order, and it can go up to any order of accuracy, even though fourth order is considered for practical applications.* Since the stencil is compact, the implementation on parallel machines becomes simple. These schemes are very flexible in nature, which is so far one of the most important advantage over other techniques. This feature has allowed us to adapt the schemes to the requirements of different physical situations (*e.g.* different formulations allow either en efficient explicit time advancement for problems involving small time-scales, or a fully implicit space-time variant which is unconditionally stable and allows to handle stiff problems where only the large time scales are relevant). This flexibility has also enabled to devise a variant using the same data structure of the popular Discontinuous Galerkin schemes, which are also part of our scientific focus.

The compactness of the second order version of the schemes enables us to use efficiently the high performance parallel linear algebra tools developed by the team. However, the high order versions of these schemes, which are under development, require modifications to these tools taking into account the nature of the data structure used to reach higher orders of accuracy. This leads to new scientific problems at the border between numerical analysis and computer science. In parallel to these fundamental aspects, we also work on adapting more classical numerical tools to complex physical problems such as those encountered in interface flows, turbulent or multiphase flows, geophysical flows, and material science. A particular attention has been devoted to the implementation of complex thermodynamic models permitting to simulate several classes of fluids and to take into account real-gas effects and some exotic phenomenon, such as rarefaction shock waves.
Within these applications, a strong effort has been made in developing more predictive tools for both multiphase compressible flows and non-hydrostatic free surface flows.

Concerning multiphase flows, several advancements have been performed, i.e. considering a more complete systems of equations including viscosity, working on the thermodynamic modeling of complex fluids, and developing stochastic methods for uncertainty quantification in compressible flows. Concerning depth averaged free surface flow modeling, on one hand we have shown the advantages of the use of the compact schemes we develop for hydrostatic shallow water models. On the other, we have shown ho to extend our approach to non-hydrostatic Boussinesq modeling, including wave dispersion, and wave breaking effects.
We expect to be able to demonstrate the potential of our developments on applications ranging from the the reproduction of the complex multidimensional interactions between tidal waves and estuaries, to the unsteady aerodynamics and aeroacoustics associated to both external and internal compressible flows, and the behavior of complex materials. This will be achieved by means of a multi-disciplinary effort involving our research on residual discretizations schemes, the parallel advances in algebraic solvers and partitioners, and the strong interactions with specialists in computer science, scientific computing, physics, mechanics, and mathematical modeling.
Concerning the software platforms, our research in numerical algorithms has led to the development of the `RealfluiDS` platform which is described in section 5.3, and to the `SLOWS` (Shallow-water fLOWS) code for free surface flows, described in sections 5.9 . Simultaneously, we have contributed to the advancement of the new, object oriented, parallel finite elements library `AeroSol`, described in section 5.1, which is destined to replace the existing codes and become the team's CFD kernel.

New software developments are under way in the field of complex materials modeling. These developments are performed in the code in the solver `COCA` (CodeOxydationCompositesAutocicatrisants) for the simulation of the self-healing process in composite materials. These developments will be described in section 5.2.

This work is supported by the EU-Strep IDIHOM, various research contracts and in part by the `ANEMOS` project and the ANR-Emergence `RealFluids` grant. A large part of the team also profited of the `ADDECCO` ERC grant.

3.2. Numerical schemes for Uncertainty quantification and robust optimization

Participants: Rémi Abgrall, Pietro Marco Congedo, Gianluca Geraci, Mario Ricchiuto, Maria Giovanna Rodio, Francesca Fusi, Julie Tryoen, Kunkun Tang.

Another topic of interest is the quantification of uncertainties in non linear problems. In many applications, the physical model is not known accurately. The typical example is that of turbulence models in aeronautics. These models all depend on a number of parameters which can radically change the output of the simulation. Being impossible to lump the large number of temporal and spatial scales of a turbulent flow in a few model parameters, these values are often calibrated to quantitatively reproduce a certain range of effects observed experimentally. A similar situation is encountered in many applications such as real gas or multiphase flows, where the equation of state form suffer from uncertainties, and free surface flows with sediment transport, where often both the hydrodynamic model and the sediment transport model depend on several parameters, and my have more than one formal expression.

This type of uncertainty, called *epistemic*, is associated with a lack of knowledge and could be reduced by further experiments and investigation. Instead, another type of uncertainty, called *aleatory*, is related to the intrinsec aleatory quality of a physical measure and can not be reduced. The dependency of the numerical simulation from these uncertainties can be studied by propagation of chaos techniques such as those developed during the recent years via polynomial chaos techniques. Different implementations exists, depending whether the method is intrusive or not. The accuracy of these methods is still a matter of research, as well how they can handle an as large as possible number of uncertainties or their versatility with respect to the structure of the random variable pdfs.

Our objective is to develop some non-intrusive and semi-intrusive methods, trying to define an unified framework for obtained a reliable and accurate numerical solution at a moderate computational cost. This work have produced a large number of publications on peer-reviewed journal. Concerning the class of intrusive methods, we are developing an unified scheme in the coupled physical/stochastic space based on a multi-resolution framework. Here, the idea is to build a framework for being capable to refine a discontinuity in both stochastic and deterministic mesh. We are extending this class of methods to complex models in CFD, such as in multiphase flows. Concerning the non-intrusive methods, we are working on several methods for treating the following problems : handling a large number of uncertainties, treating high-order statistical decomposition (variance, skewness and kurtosis), and solving efficiently inverse problems.

We have used these methods to several ends : either to have highly accurate quantitative reconstruction of a simulation output's variation over a complex space of parameter variations to study a given model (uncertainty propagation), or as a means of comparing different model's variability to certain parameters thus assessing their robustness (model robustness), or as a tool to compare different numerical implementation (schemes and codes) of a similar model to assess simultaneously the robustness of the numerics and the universality of the trends of the statistics and of the sensitivity measures (robust cross-validation). Moreover, we rebuild statistically some input parameters relying on some experimental measures of the output, thus solving an inverse problem.

The developed methods and tools have been applied to several applications of interest : real-gas effects, multi-phase flows, cavitation, aerospace applications and geophysical flows.

Concerning robust optimization, we focus on problems with high dimensional representation of stochastic inputs, that can be computationally prohibitive. In fact, for a robust design, statistics of the fitness functions are also important, then uncertainty quantification (UQ) becomes the predom- inant issue to handle if a large number of uncertainties is taken into account. Several methods are proposed in literature to consider high dimension stochastic problem but their accuracy on realistic problems where highly non-linear effects could exist is not proven at all. We developed several efficient global strategies for robust optimization: the first class of method is based on the extension of simplex stochastic collocation to the optimization space, the second one consists in hybrid strategies using ANOVA decomposition.

These developments and computations are performed in the platform `RobUQ`, which includes the most part of methods developed in the Team.

This part of our activities is supported by the ERC grant `ADDECCO`, the ANR-MN project `UFO` and the associated team `AQUARIUS`.

3.3. Meshes and scalable discrete data structures

Participants: Cécile Dobrzynski, Sébastien Fourestier, Algiane Froehly, Cédric Lachat, François Pellegrini.

3.3.1. Adaptive dynamic mesh partitioning

Many simulations which model the evolution of a given phenomenon along with time (turbulence and unsteady flows, for instance) need to re-mesh some portions of the problem graph in order to capture more accurately the properties of the phenomenon in areas of interest. This re-meshing is performed according to criteria which are closely linked to the undergoing computation and can involve large mesh modifications: while elements are created in critical areas, some may be merged in areas where the phenomenon is no longer critical.

Performing such re-meshing in parallel creates additional problems. In particular, splitting an element which is located on the frontier between several processors is not an easy task, because deciding when splitting some element, and defining the direction along which to split it so as to preserve numerical stability most, require shared knowledge which is not available in distributed memory architectures. Ad-hoc data structures and algorithms have to be devised so as to achieve these goals without resorting to extra communication and synchronization which would impact the running speed of the simulation.

Most of the works on parallel mesh adaptation attempt to parallelize in some way all the mesh operations: edge swap, edge split, point insertion, etc. It implies deep modifications in the (re)mesher and often leads to bad performance in term of CPU time. An other work [74] proposes to base the parallel re-meshing on existing mesher and load balancing to be able to modify the elements located on the frontier between several processors.

In addition, the preservation of load balance in the re-meshed simulation requires dynamic redistribution of mesh data across processing elements. Several dynamic repartitioning methods have been proposed in the literature [75], [73], which rely on diffusion-like algorithms and the solving of flow problems to minimize the amount of data to be exchanged between processors. However, integrating such algorithms into a global framework for handling adaptive meshes in parallel has yet to be done.

The path that we are following bases on the decomposition of the areas to remesh into boules that can be processed concurrently, each by a sequential remesher. It requires to devise scalable algorithms for building such boules, scheduling them on as many processors as possible, reconstructing the remeshed mesh and redistributing its data. This research started within the context of the PhD of Cédric Lachat, funded by a CORDI grant of EPI PUMAS and is continued thanks to a funding by ADT grant El Gaucho.

3.3.2. Graph partitioning and static mapping

Unlike their predecessors of two decades ago, today's very large parallel architectures can no longer implement a uniform memory model. They are based on a hierarchical structure, in which cores are assembled into chips, chips are assembled into boards, boards are assembled into cabinets and cabinets are interconnected through high speed, low latency communication networks. On these systems, communication is non uniform: communicating with cores located on the same chip is cheaper than with cores on other boards, and much cheaper than with cores located in other cabinets. The advent of these massively parallel, non uniform machines impacts the design of the software to be executed on them, both for applications and for service tools. It is in particular the case for the software whose task is to balance workload across the cores of these architectures.

A common method for task allocation is to use graph partitioning tools. The elementary computations to perform are represented by vertices and their dependencies by edges linking two vertices that need to share some piece of data. Finding good solutions to the workload distribution problem amounts to computing partitions with small vertex or edge cuts and that balance evenly the weights of the graph parts. Yet, computing efficient partitions for non uniform architectures requires to take into account the topology of the target architecture. When processes are assumed to coexist simultaneously for all the duration of the program, this generalized optimization problem is called mapping. In this problem, the communication cost function to minimize incorporates architecture-dependent, locality improving terms, such as the dilation of each edge (that is, by how much it is "stretched" across the graph representing the target architecture), which is sometimes also expressed as some "hop metric". A mapping is called static if it is computed prior to the execution of the program and is never modified at run-time.

The sequential Scotch tool being developed within the BACCHUS team (see Section 5.8) was able to perform static mapping since its first version, in 1994, but this feature was not widely known nor used by the community. With the increasing need to map very large problem graphs onto very large and strongly non uniform parallel machines, there is an increasing demand for parallel static mapping tools. Since, in the context of dynamic repartitioning, parallel mapping software will have to run on their target architectures, parallel mapping and remapping algorithms suitable for efficient execution on such heterogeneous architectures have to be investigated. This leads to solve three interwoven challenges:

- scalability: such algorithms must be able to map graphs of more than a billion vertices onto target architectures comprising millions of cores;
- heterogeneity: not only do these algorithms must take into account the topology of the target architecture they map graphs onto, but they also have themselves to run efficiently on these very architectures;
- asynchronicity: most parallel partitioning algorithms use collective communication primitives, that is, some form of heavy synchronization. With the advent of machines having several millions of cores, and in spite of the continuous improvement of communication subsystems, the demand for more asynchronicity in parallel algorithms is likely to increase.

This research was mainly carried out within the context of the PhD of Sébastien Fourestier, who defended on June.

4. Application Domains

4.1. Introduction

We are working on problems that can be written in the following form

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F}_e(\mathbf{U}) - \nabla \cdot \mathbf{F}_v(\mathbf{U}, \nabla \mathbf{U}) = 0 \tag{1}$$

in a domain $\Omega \subset \mathbb{R}^d$, $d = 1, 2, 3$, subjected to initial and boundary conditions. The variable $\mathbf{U}$ is a vector in general, the flux $\mathbf{F}_e$ is a tensor, as well as $\mathbf{F}_v$ which also depends on the gradient of $\mathbf{U}$. The subsystem

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F}_e(\mathbf{U}) = 0$$

is assumed to be hyperbolic, the subsystem

$$\frac{\partial \mathbf{U}}{\partial t} - \nabla \cdot \mathbf{F}_v(\mathbf{U}, \nabla \mathbf{U}) = 0$$

is assumed to be elliptic. Last, (1) is supposed to satisfy an entropy inequality. The coefficients or models that define the flux and the boundary conditions can be deterministic or random.

The systems (1) are discretised mesh made of conformal elements. The tessalation is denoted by $\mathcal{T}_h$. The simplicies are denoted by K_j, $j = 1, n_e$, and $\cup_j K_j = \Omega_h$, an approximation of Ω. The mesh is assumed to be adapted to the boundary conditions. In our methods, we assume a globaly continuous approximation of $\mathbf{U}$ such that $\mathbf{U}_{|K_j}$ is either a polynomial of degree k or a more complex approximation such as a Nurbs. For now k is uniform over the mesh, and let us denote by V_h the vector space spanned by these functions, taking into account the boundary conditions.

The schemes we are working on have a variational formulation: find $\mathbf{U} \in V_h$ such that for any $\mathbf{V} \in V_h$,

$$a(\mathbf{U}, \mathbf{V}; \mathbf{U}) = 0.$$

The variational operator $a(\mathbf{U}, \mathbf{V}; \mathbf{W})$ is a sum of local operator that use onlty data within elements and boundary elements: it is very local. Boundary conditions can be implemented in a variational formulation or using a penalisation techbnique, see figure 1. The third argument $\mathbf{W}$ stands for the way are implemented the non oscillatory properties of the method.

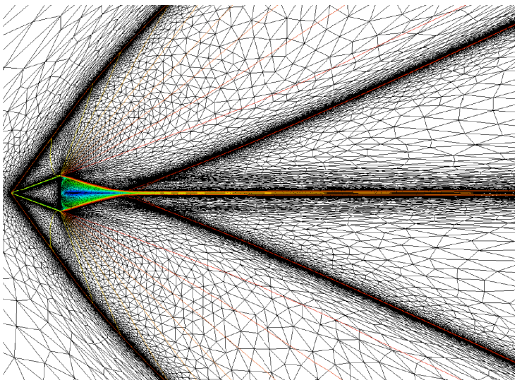

Figure 1. Adapted mesh for a viscous flow over a triangular wedge.

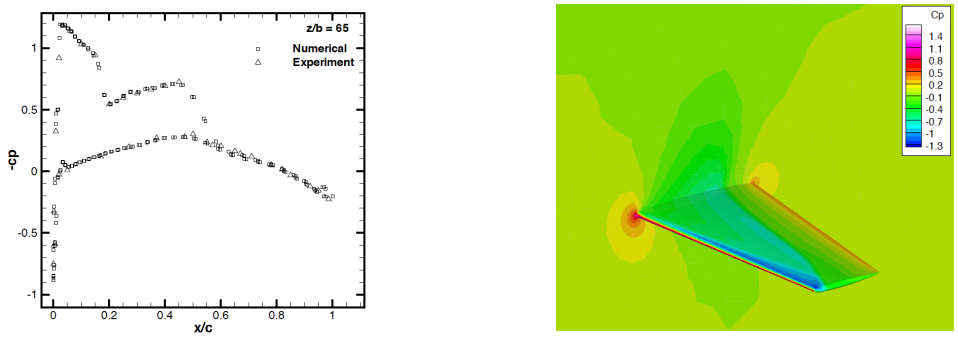

Figure 2. Turbulent flow over a M6 wing (pressure coefficient, mesh by Dassault Aviation).

This leads to highly non linear systems to solve, we use typicaly non linear Krylov space techniques. The cost is reduced thanks to a parallel implementation, the domain is partionnned via `Scotch`. Mesh balancing, after mesh refinement, is handled via `PaMPA`. These schemes are implemented in `RealfluiDS` and, partialy, `AeroSol`. An example of such a simulation is given by Figure 2.

In case of non determistic problems, we have a semi-intrusive strategy. The randomness is expressed via N scalar random parameters (that might be correlated), $X = (x_1, ..., x_N)$ with probability measure $d\mu$ which support is in a subset of $\mathbb{R}^N$. The idea of non intrusive methods is to approximate $d\mu$ either by $d\mu \approx \sum_j \omega_l \delta_{X_l}$ for $\omega_l \geq 0$ that sum up to unity, for "well chosen" samples X_l or by $d\mu \approx \sum_l \mu(\Omega_l) 1_{X_j} dX$ where the sets Ω_j covers the support of $d\mu$ and are non overlapping.

Staring from a discrete approximation of (1), we can implement randomess in the scheme. An example is given on figure 3 applied to the shallow water equations with dry shores, when the amplitude of the incoming tsunami wave is not known.

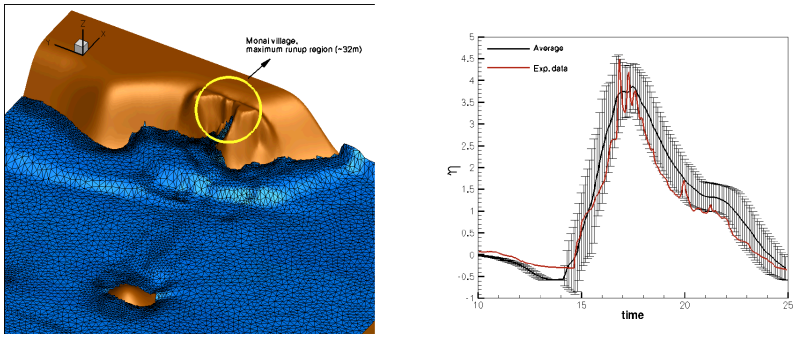

Figure 3. Okushiri tsunami experiment. Left : deterministic computation. Right : mean and variance of the wave height in one of the gauges

4.2. External and internal Aerodynamics

A classical application is the simulation of internal and external flows, with perfect or real gas equation of states, in complex geometries, such as for example the organic dense flows in a turbine cascade. This requires often the use of meshes having heterogeneous structures. We are working with unstructured meshes, either with simplicial elements or mixtures of hex, tets, pyramids and prisms. Mesh refinement can be enable in order to better resolve either the discontinuous flow structures or the capture of boundary layers.

4.3. Multiphase flows with mass transfer

Another domain of application is the simuation of multiphase flows. Here, the system (1) need to be supplemented by at least a PDE describing the phase volume changes, and the equation of states of the phases. The system is in most case written in a non-conservative form, so that additional difficulties need to be handled.

Multiphase fows occur in many applications: for petroleum industry, nuclear industry (accident management), engines, pipes, etc.

An adding difficulty is given by the presence of mass transfer between the phases. Cavitation consists in a local pressure drop below the vapor pressure at the liquid temperature, thus creating a phase change and vapor bubbles formation. Their collapse in high-pressure region can dramatically lead to failure, erosion and other undesirable effects. For this reason, there is a strong effort devoted to develop predictive numerical tools for cavitating flows in industrial applications. Unfortunately, an accurate description of interactions between the

vapour and liquid phases requires accurate physical models and a way to take into account the dynamics of the interface. Moreover, multiscale effects, turbulence and thermodynamics should be also considered. Cavitation models are typically dependent on two types of parameters: first, on some physical parameters, such as for example the number of bubbles, that is not usually well measured; secondly, on some empiric parameters, useful for fitting and calibration procedures with respect to the experimental data. Therefore, model parameters represent an important source of uncertainty. Moreover, it is not an easy task to well define boundary and initial conditions, because of difficulties encountered in order to control accurately experiments in cavitating flows. As a result, conditions imposed for the setting of a numerical simulation, are affected by a dramatic randomness.

We performed a systematic study for considering the probabilistic properties of the input parameters permitting to capture non-linearities in uncertainty propagation. Moreover, the DEM method has been modified to take into account exotic phenomena with real-gas effects.

4.4. Inflight icing and ice shedding

Actual concerns about greenhouse gases lead to changes in aircraft design with an increased use of composite materials. This offers new possibilities for the design of ice protection systems. These systems remove ice formed on the protected surfaces following a periodic cycle. One of their drawbacks of de-icing device is that ice pieces shed into the flow and may cause impact/ingestion on/in aircraft components located downstream. Aircraft manufacturers rely mainly on flight tests to evaluate the potential negative effects of ice shedding because of the lack of appropriate numerical tools. The random shape and size taken by ice shed particles together with their rotation as they move make it difficult for classical CFD tools to predict trajectories. The numerical simulation of a full unsteady viscous flow, with a set of moving bodies immersed within, shows several difficulties for grid based methods. Drawbacks income from the meshing procedure for complex geometries and the re-griding procedure in tracing the body motion. A new approach that take into account the effect of ice accretion on flow field is used to solve the ice trajectory problem. The approach is based on mesh adaptation, penalization method and level sets.

4.5. ORCs cycles

ORCs are Rankine cycles that use properly chosen low-boiling molecularly heavy organic compounds to drive the turbine in place of steam. This makes them suitable for the exploitation of low grade heat sources like biomass combustion, geothermal reservoirs and heat recovery from industrial processes. ORC turbines mainly use a single (less frequently, two) stage to expand the fluid. Up till present, no experimental data are available for flows of heavy fluids in the dense gas region. Experiments are difficult be cause of high temperature and pressure conditions, and fluid decomposition or inflammability in presence of air. This has motivated the use of numerical simulation as a preferential tool for dense gas flow analysis, but only a limited number of papers have been devoted to the computation of dense gas flows. With no experimental validation yet available for any of these configurations, care must be taken in the analysis of the computed flow fields because of their sensitivity to the thermodynamic model and to the numerical ingredients of the discretization scheme. Since no comparison with experimental data is possible, particular attention is devoted to code validation and model assessment. We created the plateform `ORComp`, for computing some global performance metrics, and we applied some UQ and numerical methods for taking into account the sun variability in the design of ORCs cycles, by using the platform `RobUQ`.

4.6. Atmospheric entries of spacecraft

Simulation of atmospheric entries of spacecraft is a challenging problem involving many complex physical phenomena, including rarefied gas effects, aerothermochemistry, radiation, and the response of thermal protection materials to extreme conditions. The post-flight analysis of a space mission requires accurate determination of the freestream conditions for the trajectory, that is, temperature and pressure conditions and the Mach number in front of the shock. The latters can be rebuilt from the pressure and heat flux measured

on the spacecraft by means of a Flush Air Data System (FADS). This instrumentation comprises a set of sensors flush mounted in the thermal protection system to measure the static pressure (pressure taps) and heat flux (calorimeters). In this context, Computational Fluid Dynamics (CFD) supplied with UQ tools permits to take into account chemical effects and to include both measurement errors and epistemic uncertainties on the chemical model parameters in the bulk and at the wall (surface catalysis). Rebuilding the freestream conditions from the FADS data therefore amounts to solving a stochastic inverse problem. In this context, we proposed a new methodology for solving the inverse problem based on a Bayesian setting, that is, probability densities of possible values of freestream conditions are rebuilt from stagnation-point pressure and heat flux measurements. A Bayesian setting offers a rigorous foundation for inferring input parameters from noisy data and uncertain forward models, a natural mechanism for incorporating prior information, and a quantitative assessment of uncertainty on the inferred results.

4.7. Free surface hydrodynamics

Prediction of free surface flow hydrodynamics can be of extreme importance in many applications such as , e.g. protection of coastal environments, design of coastal structures, etc. We have developed simulation tools for the prediction of both hydrostatic and non-hydrostatic free surface flows, including also wave breaking effects. We have also started work on the improvement of the asymptotic modeling of the dispersive wave behavior which controls strongly the heights and position of the waves. These models are discretized by appropriate generalizations of the residual based techniques we propose.

In addition to the basic modeling activity, we have started to study the output dependence on the variability of input data depending on the model (such as for example, for the friction coefficient), and on environmental conditions (topography, incoming wave description etc). These quantities often involve a certain degree of uncertainty. By coupling a robust shallow-water solver based on a residual distribution scheme with some stochastic methods to show the large variability of important physical outputs (e.g. wave runup, flooded area, etc) due to input uncertainties.

4.8. Self healing composite materials

In a collaboration with the UMR LCTS we are studying the influence of the in-crack physico-chemistry on the lifetimes of self healing composite materials. The self healing character of these materials is given by the presence of a reactive phase in the composite matrix which reacts with oxygen and yields a liquid oxide with a very high specific volume (compared to the reactive). The extra volume occupied by the oxide gives a protecting layer shielding the composite fibers from farther oxidation. The failure mechanism of these materials is thus strongly dependent on the evolution of this oxide.

Our objective is to develop a simplified asymptotic model of the physics and chemistry of a single crack, to be used as a numerical closure model for structural mechanics computations. This model as to provide time integrated values of oxygen concentrations at fibers, which can be used to infer fiber weakening and rupture, thus to change the crack topology. This process can be iterated until failure is obtained. Our contribution consists in developing the chemistry and flow models, related discretization, and implementation in an ad-hoc module which will be coupled with the structural solver of LCTS.

5. Software and Platforms

5.1. AeroSol

Participants: Dragan Amenga-Mbengoué [Bacchus], Simon Delmas [Cagire], Damien Genet [Bacchus], Maxime Mogé [Cagire], Yann Moguen [Cagire], Francois Pellegrini [Bacchus], Vincent Perrier [Corresponding member], Francois Rué [Bacchus], Mario Ricchiuto [Bacchus].

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

This year some important features were added including : definition of CMake options for optimization and for using different compilers (GNU gcc, Intel icc, and IBM xlc) ; new element classes (lagrange and hierarchical orthogonal finite element basis for pyramids, Gauss Lagrange elements) ; implicit time integrators (backward Euler, Crank-Nicolson, and BDF from 2nd to 6th order) ; anisotropic diffusion models and (compressible) Navier-Stokes models ; debuggin by looging at memory traces with an interfacing with the PAPI library (tests have also been performed with VTUNE and TAU) ; improvements in schemes robustness and efficiency (Galerkin discretization of advection optimized by stocking most of the geometrical functions and finite elements computations, explicit and implicit version of the DG discretization of diffusion problems, implementation of Taylor-Galerkin stabilization and simplified SUPG stabilization) ; boundary conditions (time dependent, periodic, non reflecting) ; low Mach numerical fluxes for DG ; development of steady and unsteady tests related to all these new features.

5.2. COCA

Participants: Mario Ricchiuto [corresponding member], Gérard Vignoles, Gregory Perrot.

COCA(CodeOxydationCompositesAutocicatrisants) is a Fortran 90 code for the simulation of the oxidation process in self-healing composites COCA solves the discrete finite element equations relative to the oxidation (chemistry) and flow (potential) models. Time integration is performed with an implicit approach (Backward Euler or second order backward differencing). The linear algebraic systems arising in the discretization are solved with the MUMPSlibrary.

5.3. RealfluiDS

Participants: Dante de Santis, Gianluca Geraci, Pietro Marco Congedo, Rémi Abgrall [corresponding member].

RealfluiDS is a software dedicated to the simulation of inert or reactive flows. It is also able to simulate multiphase, multimaterial, MHD flows and turbulent flows (using the SA model). There exist 2D and 3D dimensional versions. The 2D version is used to test new ideas that are later implemented in the 3D one. This software implements the more recent residual distribution schemes. The code has been parallelized with and without overlap of the domains. The uncertainty quantification library RobUQhas been coupled to the software. A partitioning tool exists in the package, which uses Scotch. Recently, the code has been developed for taking into account real-gas effects, in order to use a whatever complex equation of state. Further developments concerning multiphase effects are under way.

5.4. MMG3D

Participants: Cécile Dobrzynski [corresponding member], Algiane Froehly.

MMG3D is a tetrahedral fully automatic remesher. Starting from a tetrahedral mesh, it produces quasi-uniform meshes with respect to a metric tensor field. This tensor prescribes a length and a direction for the edges, so that the resulting meshes will be anisotropic. The software is based on local mesh modifications and an anisotropic version of Delaunay kernel is implemented to insert vertices in the mesh. Moreover, MMG3D allows one to deal with rigid body motion and moving meshes. When a displacement is prescribed on a part of the boundary, a final mesh is generated such that the surface points will be moved according this displacement. MMG3D is used in particular in GAMMA for their mesh adaptation developments, but also at EPFL (maths department), Dassault Aviation, Lemma (a french SME), etc. MMG3D can be used in FreeFem++ (http://www.freefem.org), a free software which eases the solving of PDEs and in Gmsh (http://geuz.org/gmsh/). More details can be found on http://www.math.u-bordeaux1.fr/~dobj/logiciels/mmg3d.php.

A new version of MMG3D is under development. The big novelty of this version is the modification of the surface triangulation. A. Froehly, ingenieer in the FUI Rodin, is working on this new version.

5.5. ORComp

Participants: Pietro Marco Congedo [Corresponding member], Rémi Abgrall, Dante de Santis, Maria-Giovanna Rodio.

The ORComp platform is a simulation tool permitting to design an ORC cycle. Starting from the solar radiation, this plateform computes the cycle providing the best performance with optimal choices of the fluid and the operating conditions. It includes RobUQ, a simulation block of the ORC cycles, the RealfluiDScode for the simulation of the turbine and of the heat exchanger, the software FluidProp (developed at the University of Delft) for computing the fluid thermodynamic properties.

5.6. PaMPA

Participants: Cédric Lachat, François Pellegrini [Corresponding member], Cécile Dobrzynski, Hervé Guillard [PUMAS], Laurent Hascoët [Tropics].

PaMPA ("Parallel Mesh Partitioning and Adaptation") is a middleware library dedicated to the management of distributed meshes. Its purpose is to relieve solver writers from the tedious and error prone task of writing again and again service routines for mesh handling, data communication and exchange, remeshing, and data redistribution. It is based on a distributed data structure that represents meshes as a set of *entities* (elements, faces, edges, nodes, etc.), linked by *relations* (that is, computation dependencies).

PaMPA interfaces with Scotch for mesh redistribution, and with MMG3D for parallel remeshing of tetrahedral elements. Other sequential remeshers can be plugged-in, in order to handle other types of elements.

Following the PhD defense of Cédric Lachat last December, version 1.0 is about to be released publicly under the GPL license. This version allows users to declare distributed meshes, to declare values attached to the entities of the meshes (e.g. temperature attached to elements, pressures to the faces, etc.), to exchange values between overlapping entities located at the boundaries of subdomains assigned to different processors, to iterate over the relations of entities (e.g. iterate over the faces of elements), to remesh in parallel the areas of a mesh that need to be emeshed, and to redistribute evenly the remeshed mesh across the processors of the parallel architecture.

PaMPA is already used as the data structure manager for two solvers being developed at Inria: Plato (team PUMAS) and AeroSol(teams BACCHUS and CAGIRE).

5.7. RobUQ

Participants: Pietro Marco Congedo [Corresponding member], Rémi Abgrall, Gianluca Geraci, Maria Giovanna Rodio, Kunkun Tang, Julie Tryoen.

The RobUQ platform has been conceived to solve problems in uncertainty quantification and robust design. It includes the optimization code ALGEN, and the uncertainty quantification code NISP. It includes also some methods for the computation of high-order statistics, efficient strategies for robust optimization, the Simplex2 method. Some methods are developed in partnership with the Stanford University (in the framework of the associated team AQUARIUS). Other methods are developed in the context of ANR UFO.

5.8. Scotch

Participants: François Pellegrini [corresponding member], Sébastien Fourestier.

parallel graph partitioning, parallel static mapping, parallel sparse matrix block ordering, graph repartitioning, mesh partitioning.

Scotch (http://www.labri.fr/~pelegrin/scotch/) is a software package for parallel and sequential sparse matrix ordering, parallel and sequential graph partitioning, as well as sequential static mapping and remapping, without and with fixed vertices, and mesh and hypergraph partitioning.

The initial purpose of Scotch was to compute high-quality static mappings of valuated graphs representing parallel computations onto target architectures of arbitrary topologies. This allows the mapper to take into account the topology and heterogeneity of the target architecture in terms of processor speed and link bandwidth. This feature, which was meant for the NUMA machines of the 1980's, has not been widely used in the past because machines in the 1990's became UMA again thanks to hardware advances. Now, architectures become NUMA again, and these features are regaining popularity.

The Scotch package consists of two libraries: the sequential Scotch library, and the parallel PT-Scotch library (for "*Parallel Threaded Scotch*") that operates according to the distributed memory paradigm, using MPI. Scotch was the first full 64-bit implementation of a general purpose graph partitioner.

Version 6.0, released on December 2012, corresponding to the 20th anniversary of Scotch, offers many new features: static mapping with fixed vertices, static remapping, and static remapping with fixed vertices. Several critical algorithms of the formerly strictly sequential Scotch library can now run in a multi-threaded way. All of these features, which exist only in the sequential version, will be available to the parallel PT-Scotch library in the upcoming release 6.1.

Scotch has been integrated in numerous third-party software, which indirectly contribute to its diffusion. It is natively available in several Linux and Unix distributions, as well as on some vendors platforms (SGI, etc).

5.9. SLOWS

Participants: Mario Ricchiuto [corresponding member], Andrea Filippini.

SLOWS ("*Shallow-water fLOWS*") is a C-platform allowing the simulation of free surface shallow water flows with friction. Arbitrary bathymetries are allowed, defined either by some complex piecewise analytical expression, or by xyz data files, the classical Manning model for friction is used, and an Exner model is implemented for sediment transport. For non-hydrostatic propagation the enhanced Boussinesq equations of Madsen and Sorensen are used. The equations are discretized with a residual based approach which is an adaptation of the schemes developed for aeronautics applications. Due to the inherent unsteadiness of these flows, the time discretization plays an important role. Three different approaches are available, based on conditionally depth-positivity preserving implicit schemes, or on conditionally depth-positivity preserving genuinely explicit discretizations, or on an unconditionally depth-positivity preserving space-time approach. Newton and frozen Newton loops are used to solve the implicit nonlinear equations. The linear algebraic systems arising in the discretization are solved with the MUMPSlibrary.

5.10. Nomesh

Participants: Cécile Dobrzynski [corresponding member], Algiane Froehly.

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

6. New Results

6.1. Residual distribution schemes for steady problems

Participants: Rémi Abgrall [Corresponding member], Mario Ricchiuto, Dante de Santis, Algiane Froehly, Cécile Dobrzynski, Pietro Marco Congedo.

We have understood how to approximate the advection diffusion problem in the context of residual distribution schemes. The third order version of the schemes has been validated for both laminar and turbulent flows. It is uniformly accurate with respect to the local Reynolds number. The turbulent version makes used of extension to the Spalart Allmaras model. We have studied the (iterative) convergence issues using Jacobian Free techniques or the LUSGS algorithm. Tests in two and three dimensions have been carried out. This work is submitted to J.Comput.Phys. We are now able to handle two and three dimensional laminar and turbulent flows on hybrid and high order (curved boundaries) meshes. Moreover, we have extended the scheme to the use of complex equations of state, and we perform high-order computations with real-gas effects. This work is submitted to Computers&Fluids.

6.2. Curved meshes

Participants: Rémi Abgrall, Cécile Dobrzynski [Corresponding member], Algiane Frohely.

One of the main open problems in high order schemes is the design of meshes that fit with enough accuracy the boundary of the computational domain. If this curve/surface is not locally straight/planar, the elements must be curved near the boundary, and their curvature need to be propagated to the interior of the domain to have valid elements. When the mesh is very stretched, this can be quite challenging since, in addition, we want that the mesh keep a structure, in particular for boundary layers. Using tools explored in iso-geometrical analysis, we have been able to construct a software computing curved meshes (in 2D and 3D), while keeping as much as possible the structure of the mesh and guaranteeing that the generated mesh is suitable to CFD simulation (all elements have a positive Jacobian). This software is being used for high order computations with the IDIHOM project. The full paper has been accepted in IJNMF and will be published in 2014.

6.3. Hypoelastic models

Participants: Rémi Abgrall [Corresponding member], Pierre-Henri Maire.

In collaboration with CEA (P.H. Maire), we have developed and tested a new finite volume like algorithm able to simulate hypo-elastic and plastics problems on unstructured meshes. This has been published in [19].

6.4. Penalisation methods using unstructured meshes

Participants: Rémi Abgrall, Heloise Beaugendre [Corresponding member], Cécile Dobrzynski, Leo Nouveau, Quentin Viville.

In Computational Fluid Dynamics the interest on embedded boundary methods for Navier-Stokes equations increases because they simplify the meshing issue, the simulation of multi-physics flows and the coupling of fluid-solid interactions in situation of large motions or deformations. Nevertheless an accurate treatment of the wall boundary conditions remains an issue of these methods. In this work we develop an immersed boundary method for unstructured meshes based on a penalization technique and we use mesh adaption to improve the accuracy of the method close to the boundary. The idea is to combine the strength of mesh adaptation, that is to provide an accurate flow description especially when dealing with wall boundary conditions, to the simplicity of embedded grids techniques, that is to simplify the meshing issue and the wall boundary treatment when combined with a penalization term to enforce boundary conditions. The bodies are described using a level-set method and are embedded in an unstructured grid. Once a first numerical solution is computed mesh adaptation based on two criteria the level-set and the quality of the solution is performed. The full paper will be published in the Journal of Computational Physics in january 2014.

6.5. Unsteady problem

Participants: Rémi Abgrall, Mario Ricchiuto [Corresponding member].

A higher order version of the explicit multi-stage RD schemes we have designed has been obtained in one dimension, and its extension to two space dimensions is in the works. A moving mesh ALE formulation of the multistage explicit schemes developed [58] (paper submitted to J.Sci.Comp.) as a basis for adaptive mesh movement, in development in collaboration with Pr. A. Guardone. We have also started work on new formulations based on different time stepping schemes of the multi-step type.

Concerning implicit schemes, the work on higher order space time formulations in collaboration with the Leeds university and with A. Larat of Ecole Centrale Paris. The advantage of this formulation in terms of efficiency has been shown for shallow water problems [24], while the extension to higher than second order is still in development (Inria RR-7843).

6.6. Uncertainty Quantification

Participants: Rémi Abgrall, Pietro Congedo [Corresponding member], Gianluca Geraci, Maria Giovanna Rodio, Kunkun Tang, Julie Tryoen, Mario Ricchiuto, Thierry Magin.

We developed an unified scheme in the coupled physical/stochastic space. Basing on the Harten multiresolution framework in the stochastic space, we proposed a method allowing an adaptive refinement/derefinement in both physical and stochastic space for time dependent problems (aSI scheme). As a consequence, an higher accuracy is obtained with a lower computational cost with respect to classical non-intrusive approaches, where the adaptivity is performed in the stochastic space only. Performances of this algorithm are tested on scalar Burgers equation and Euler system of equations, comparing with the classical Monte Carlo and Polynomial Chaos techniques [6], [7]. We have also coupled the aSI scheme withe the DEM method for building an accurate stochastic scheme for multiphase flows. A paper is submitted to the Journal of Computational Physics on this topic.

Concerning non-intrusive methods, we proposed a formulation in order to compute the decomposition of high-order statistics. The idea is to compute the most influential parameters for high orders permitting to improve the sensitivity analysis. Second objective is to illustrate the correlation between the high-order functional decomposition and the PC-based techniques, thus displaying how to compute each term from a numerical point of view. This method has been proposed in both classical and Anchored ANOVA representation. Two papers are actually under revision on this topic. Moreover, a bayesian-based method has been used within a Polynomial Chaos framework for rebuilding the freestream conditions, starting from wall measurements during the atmospheric reentry of a space vehicle. See [16] for more details. Moreover, an uncertainty propagation method has been applied to the robust analysis of cavitating flows in a Venturi tube, displaying very interesting results concerning the influence of inlet conditions and the multiphase model parameters (see[23] for more details).

Uncertainty propagation studies are actually underway for assessing the influence of boundary conditions and model parameters for the simulation of a tsunami.

6.7. Robust Design Optimization

Participants: Pietro Congedo [Corresponding member], Gianluca Geraci, Gianluca Iaccarino.

The Simplex-Simplex approach, that has been proposed in 2011, has been further developed. In particular, the algorithm has been improved yielding an evolved version of the Simplex2 approach, and the formulation has been extended to treat mixed aleatory/epistemic uncertainty. The resulting SSC/NM (Simplex Stochastic Collocation/Nelder-Mead) method, called Simplex2, is based on i) a coupled stopping criterion and ii) the use of an high-degree polynomial interpolation of the optimization space. Numerical results show that this method is very efficient for mono-objective optimization and minimizes the global number of deterministic evaluations to determine a robust design. This method is applied to some analytical test cases and to a realistic problem of robust optimization of a multi-component airfoil (see [17] for more details).

Morevoer, we proposed a strategy for multi-objective robust design optimization, with a stochastic dimension reduction based on ANOVA analysis. The developed strategy has been applied to the robust optimization of dense-gas turbines (see [15] for more details).

6.8. Multiphase flows

Participants: Rémi Abgrall [Corresponding member], Pietro Congedo, Maria-Giovanna Rodio.

We developed the numerical solver based on a DEM formulation modified for including viscous effects and a more complex equation of state for the vapor region. The method used is the DEM for the resolution of a reduced five equation model with the hypothesis of pressure and velocity equilibrium , without mass and heat transfer. This method results in a well-posed hyperbolic systems, allowing an explicit treatment of non conservative terms, without conservation error (see [8] for more details). The DEM method directly obtains a well-posed discrete equation system from the single-phase conservation laws, producing a numerical scheme which accurately computes fluxes for arbitrary number of phases. We considered two thermodynamic models , i.e. the SG EOS and the Peng-Robinson (PR) EOS. While SG allows preserving the hyperbolicity of the system also in spinodal zone, real-gas effects are taken into account by using the more complex PR equation. The higher robustness of the PR equation when coupled with CFD solvers with respect to more complex and potentially more accurate multi-parameter equations of state has been recently discussed. In this paper, no mass transfer effect is taken into account, thus the PR equation can be used only to describe the vapor behavior, while only the SG model is used for describing the liquid [22].

Another topic covered by Bacchus is about the numerical approximation of non conservative systems. One very interesting example is obtained by the Kapila model, for which shock relations can be found from physical principles. Most, if not all, the know discretisation are at best stable, but do not converge under mesh refinement. We have proposed a way to do so by using some modifications of a Roe-like solver.

6.9. Depth averaged free surface modeling

Participants: Mario Ricchiuto [Corresponding member], Philippe Bonneton, Andrea Filippini, Stevan Bellec.

We have improved the modeling capabilities of our codes by an efficient implementation of residual based dicretizations of a non-hydrostatic enhanced Boussinesq system [21]. in particular, we have demonstrated how residual based stabilization terms do not pollute the accuracy of the underlying centered discretization, and lead very low dispersion error, while allowing to handle in a stable manner the hyperbolic (hydrostatic) limit. In the framework of the internship of P. Bagicaluppi, this has been used to construct a non-oscillatory model including wave breaking effects (paper in preparation).

In parallel, we have started an in depth study of the improvement of the dispersion operators, which control the position and height of the waves. This has allowed to highlight the existence of new form of weakly nonlinear models [62]. A paper is in preparation.

6.10. Self healing composites modeling

Participants: Mario Ricchiuto [Corresponding member], Gérard Vignoles, Gregory Perrot.

This year we have started the coupling between COCA and the structural solver of the LCTS lab. The coupling is done for the moment using simple scripting, and providing the structural solver with an equivalent fiber-surface in contact with oxygen at a given time. A simplified potential flow model (classical source potential) for the oxide has also been developed and is being tested.

6.11. Parallel remeshing

Participants: Cécile Dobrzynski, Cédric Lachat, François Pellegrini [Corresponding member].

All the work of the elapsed year on PaMPA concentrated on the design and implementation of parallel remeshing algorithms (see Section 5.6 for more details about the software itself). These algorithms are based on several steps: (i) identification of the areas to remesh; (ii) splitting of these areas into zones of prescribed size and/or estimated workload; (iii) redistribution and centralization of as many zones as possible on the processors; (iv) sequential remeshing of the zones; (v) reintegration of the zones to their original locations; (vi) identification of the remaining areas and loop to step (ii) when work remains.

Several splitting algorithms have been designed and evaluated, so as to provide zones with adequate aspect ratios to the sequential partitioners. Load imbalance is still a concern, since zones must not be too small, while they must be numerous enough so as to maximize concurrency across all of the available processors.

As of December, PaMPA has been able to remesh a coarse mesh of 27 millions of tetraedra up to a fine mesh comprising more than 600 millions of tetraedra, in 34 minutes, on 240 processors of the Avakas cluster at MCIA Bordeaux, using the MMG3D sequential remesher. Remeshing up to a finer mesh of above one billion of elements is the next milestone to reach, to evidence the capabilities of the software.

Cédric Lachat defended his PhD last December. A first abstract has been submitted, and two more journal papers are in preparation.

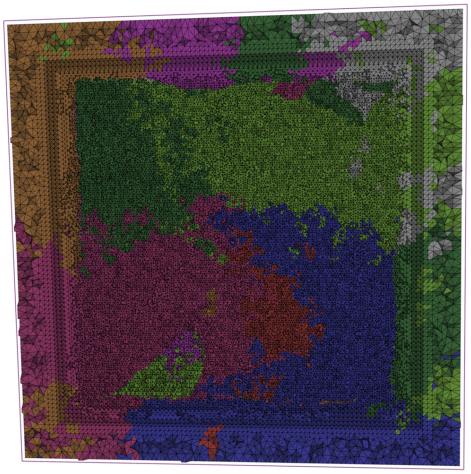

Figure 4. Cut of a 3D cube made of tetrahedra showing the effect of parallel remeshing by PaMPA.

6.12. Graph remapping

Participants: Sébastien Fourestier, François Pellegrini [Corresponding member].

The work on remapping mostly took place in the context of the PhD of Sébastien Fourestier, who defended last June. This work concerned the coding and evaluation of the parallel graph repartitioning and remapping algorithms that were designed last year. Indeed, the sequential version of these algorithms had been integrated in version `6.0` of `Scotch`, released in the beginning of December 2012. The implementation of the parallel algorithms, which started last year, took place in the `6.1` branch of `Scotch`, to be released once the `6.0` branch is made stable.

The evaluatin of our algorithms showed that the diffusion-based optimization algorithm, which behaves well in the context of partitioning, exhibits an unwanted behavior when adapted to the repartitioning and remapping cases. Typically, when the mapping changes too much, external constraints to the flows that represent the different parts may prevent them from meeting, thus reducing the quality of the frontier they should create by flooding one against the others. These algorithm have to be improved.

A journal paper summing-up all the work done during the past years in the context of process mapping, within the Joint Laboratory for Petascale Computing (JLPC) between Inria and UIUC, has been submitted.

6.13. Sparse matrix reordering for ILU solvers

Participants: Astrid Casadei [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Sébastien Fourestier, François Pellegrini [Corresponding member].

In the context of ANR `PETALh`, our task is to find ways of reordering sparse matrices so as to improve the robustness of incomplete LU factorization techniques. The path we are following is to favor the diagonal dominance of the matrices corresponding to the subdomains of the Schur complement. Our studies aim at injecting some information regarding off-diagonal numerical values into nested dissection like reordering methods, so as to favor the preservation of high off-diagonal values into either the subdomains or the separators of Schur complement techniques.

The experimental framework had been set-up last year. It consisted in a modified version of the `Scotch` sparse matrix ordering library for computing orderings and of the `HIPS` iterative sparse linear system solver for evaluating them. The text cases used were provided by the industrial partners of the `PETALh` project.

In order to improve diagonal dominance, several cut-off methods have been proposed in order to carve the matrix pattern and speed-up computations towards convergence. These cut-off methods were based on either linear or logarithmic scales, with cut-off values selected according to various distributions.

While some of these methods improve convergence on some restricted classes of matrices, as our first experiments showed last year, no method was able to provide overall improvement on a wide range of matrices. This research path is consequently considered as inefficient. A research report has been written.

6.14. Numerical methods for high altitude aerodynamics and rarefied gas flows

Participants: Luc Mieussens [Corresponding member], Florent Pruvost [IMB, engineer], G. Dechristé [IMB, PhD], N. Hérouard [CEA-CESTA, PhD], Stéphane Brull [IMB], L. Forestier-Coste [IMB, Post Doc].

This activity involves many developments for rarefied gas flow simulations for very different applications, and the design of numerical schemes for high altitude aerodynamics based on some kinetic model :

- the simulation code `CORBIS` (rarefied gases in 2 space dimensions on structured meshes) has been re-engineered : modular form, use of the `git` version control system, modification to use unstructured meshes, MPI/OpenMP hybrid parallelization. Very good performance in terms of scalability and efficiency have been obtained, up to 700 cores.
- a new method to generate locally refined grids in the space of velocities has been proposed and shown to provide CPU time gains of the order of 30 (w.r.t the existing approach). This work has been published in (Baranger *et al., J. Comput. Phys* 257(15), 2014) ;
- the second order Discontinuous Galerkin method has been shown to be more accurate and faster than higher order finite volume methods (up to fourth order) for one-dimensional rarefied gases problems. We have analytically proved that this method is Asymptotic Preserving for the Stokes regime ;

- a new kinetic model for multispecies reacting flows for re-entry applications has been proposed. In this model, the mixture oxygen-nytrogen is described by a kinetic equation, while the minor species (O, NO, N) are described by reaction diffusion equations. The implementation of this model in a full 3D code is under way ;
- we have presented one of the first numerical simulation of the Crookes radiometer ever. This has been obtained with a Cartesian grid approach, with a cut-cell techniques allowing a simplified treatment of moving solid boundaries. This work has been published in the proceedings of the 28th Symposium on rarefied Gas Dynamics ;
- We have proposed a new method to discretize kinetic equations based on a discretization of the velocity variable which is local in time and space. This induces an important gain in term of memory storage and CPU time, at least for 1D problems (this work has been presented in a paper submitted for publication). Two-dimensional extensions are under development ;
- We have shown that the recent method "Unified Gas Kinetic Scheme", proposed by K. Xu to simulate multi-scale rarefied gas flows, can be extended to other fields, like radiative transfer. This approach, based on a simple finite volume technique, is very general and can be easily applied to complex geometries with unstructured meshes. This work has been published in (Mieussens, *et al., J. Comput. Phys* 253(15), 2013).

7. Partnerships and Cooperations

7.1. Regional Initiatives

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

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

Grant: 55Keuros (co-funding PhD A. Filippini)

Coordinator: M. Ricchiuto

Other partners: UMR EPOC (P. Bonneton)

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

7.2. National Initiatives

7.2.1. Inria Project Lab

7.2.1.1. C2S@Exa - Computer and Computational Scienecs at Exascale

Participants: Olivier Aumage [RUNTIME project-team, Inria Bordeaux - Sud-Ouest], Jocelyne Erhel [SAGE project-team, Inria Rennes - Bretagne Atlantique], Philippe Helluy [TONUS project-team, Inria Nancy - Grand-Est], Laura Grigori [ALPINE project-team, Inria Saclay - Île-de-France], Jean-Yves L'excellent [ROMA project-team, Inria Grenoble - Rhône-Alpes], Thierry Gautier [MOAIS project-team, Inria Grenoble - Rhône-Alpes], Luc Giraud [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Michel Kern [POMDAPI project-team, Inria Paris - Rocquencourt], Stéphane Lanteri [Coordinator of the project], François Pellegrini [BACCHUS project-team, Inria Bordeaux - Sud-Ouest], Christian Perez [AVALON project-team, Inria Grenoble - Rhône-Alpes], Frédéric Vivien [ROMA project-team, Inria Grenoble - Rhône-Alpes].

Since January 2013, the team is participating to the C2S@Exa http://www-sop.inria.fr/c2s_at_exa Inria Project Lab (IPL). This national initiative aims at the development of numerical modeling methodologies that fully exploit the processing capabilities of modern massively parallel architectures in the context of a number of selected applications related to important scientific and technological challenges for the quality and the security of life in our society. At the current state of the art in technologies and methodologies, a multidisciplinary approach is required to overcome the challenges raised by the development of highly scalable numerical simulation software that can exploit computing platforms offering several hundreds of thousands of cores. Hence, the main objective of C2S@Exa is the establishment of a continuum of expertise in the computer science and numerical mathematics domains, by gathering researchers from Inria project-teams whose research and development activities are tightly linked to high performance computing issues in these domains. More precisely, this collaborative effort involves computer scientists that are experts of programming models, environments and tools for harnessing massively parallel systems, algorithmists that propose algorithms and contribute to generic libraries and core solvers in order to take benefit from all the parallelism levels with the main goal of optimal scaling on very large numbers of computing entities and, numerical mathematicians that are studying numerical schemes and scalable solvers for systems of partial differential equations in view of the simulation of very large-scale problems.

7.2.1.2. ANR

Title: PETALH: Preconditioning scientific applications on pETascALe Heterogeneuous machines

Type: ANR

Grant: Cosinus 2010

Duration: September 2011 - May 2013

Coordinator: GRIGORI Laura (Inria Saclay-Île de France)

Other partners: Inria Saclay-Île de France (leader of the project), Paris 6, IFP (Rueil-Malmaison), CEA Saclay.

See also: http://petal.saclay.inria.fr/

Abstract: In this collaborative effort, we propose to develop parallel preconditioning techniques for the emergent hierarchical models of clusters of multi-core processors, as used for example in future petascale machines. The preconditioning techniques are based on recent progress obtained in combining the well known incomplete LU (ILU) factorization with tangential filtering.

The track we are following in order to contribute to this goal is to investigate improved graph ordering techniques that would privilege the diagonal dominance of the matrices corresponding to the subdomains of the Schur complement. It amounts to integrating numerical values into the adjacency graph of the matrices, so that the importance of off-diagonal terms is taken into account when computing graph separators. The core of this work is planned to take place at the beginning of next year.

This project is a continuation of `PETAL` project that was funded by ANR Cosinus 2008 call.

7.2.1.3. FUI Rodin

Title: Robust structural Optimization for Design in Industry (Rodin)

Type: FUI

Duration: July 2012 - July 2015

Coordinator: ALBERTELLI Marc (Renault)

Abstract: From the research point of view, the RODIN project will focus on: (1) extending level set methods to nonlinear mechanical or multiphysics models and to complex geometrical constraints, (2) developing algorithms for moving meshes with a possible change of topology, (3) adapting in a level-set framework second-order optimization algorithms having the ability of handling a large number of design variables and constraints.

The project will last 3 years and will be supported by a consortium of 7 partners: (1) 2 significant end-users, Renault and EADS, who will provide use-cases reflecting industrial complexity; (2) 3 academics partners, CMAP, J.-L. Lions laboratory and Inria of Bordeaux, who will bring expertise in applied mathematics, structural optimization and mesh deformation; (3) A software editor, ESI Group, who will provide mechanical software package and will pave the way of an industrialization; (4) A SME, Eurodecision, specialized in large-scale optimization.

7.2.1.3.1. ANR MAIDESC

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

Type: ANR

Duration: 48 months

Starting date : 1st Oct 2013

Coordinator: Dervieux Alain (Inria Sophia)

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

7.2.1.3.2. ANR UFO

Title: Uncertainty quantification For compressible fluid dynamics and Optimisation.

Type: ANR

Duration: 36 months

Starting date : 1st June 2011

Coordinator: Remi Abgrall (Inria Bordeaux Sud-Ouest)

Abstract: This project deals with the simulation and the optimization of stochastic flows where the uncertainties can be both in the data and in the models. The focus will be on handling the uncertainties coming from the turbulence models or thermodynamics models in dense-gas flows. Since the thermodynamic models for dense-gas flows are not well-known, it is mandatory to compute the probability density functions of some quantities of interest by starting from the experimental data. Several methods have been developed for both reducing the global computational cost and increasing the accuracy in the statistics computation.

7.3. European Initiatives

7.3.1. FP7 Projects

7.3.1.1. IDIHOM

Title: Industrialisation of High-Order Methods

Type: COOPERATION (TRANSPORTS)

Instrument: Specific Targeted Research Project (STREP)

Duration: October 2010 - September 2013

Coordinator: Deutsches Zentrum fur Luft und Raumfahrt (Germany)

Others partners: DLR (Germany), Dassault Aviation (France), EADS-Cassidian (Germany), Cenaero (Belgium), Numeca (Belgium), ARA (UK), FOI (Sweden), Inria (france), NLR (the Nederlands), ONERA (France), TSAGI (Russia), ENSAM (France), Imperial College (UK), Universities of Bergamo (Italy), Varsaw (Poland), Poznan (Poland), Linköping (Sweden), UniversitĆatholique de Louvain (Belgium).

See also: http://www.dlr.de/as/en/desktopdefault.aspx/tabid-7027/11654_read-27492/

Abstract:The proposed IDIHOM project is motivated by the increasing demand of the European aerospace industries to advance their CFD-aided design procedure and analysis by using accurate and fast numerical methods, so-called high-order methods. They will be assessed and improved in a top-down approach by utilising industrially relevant complex test cases, so-called application challenges in the general area of turbulent steady and unsteady aerodynamic flows, covering external and internal aerodynamics as well as aeroelastic and aeroacoustic applications. Thus, the major aim is to support the European aeronautics industry with proven-track method(s) delivering an increased predictive accuracy for complex flows and (by same accuracy) an alleviation of computational costs which will secure their global leadership. An enhancement of the complete "high-order methods suite" is envisaged, including the most relevant methods, Discontinuous Galerkin and Continuous Residual-Based methods, in combination with underlying technologies as high-order grid generation and adaptation, visualisation, and parallelisation. The IDIHOM project is a key-enabler for meeting the ACARE goals, as higher-order methods offer the potential of more accurate prediction and at the same time faster simulations. Inria is involved in the design of Continuous Residual-Based methods for the simulation of steady trubulent flows.

7.3.1.2. STORM

Type: COOPERATION

Defi: NC

Instrument: Specific Targeted Research Project

Objectif: NC

Duration: October 2013 - September 2016

Coordinator: SNECMA (France)

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

Inria contact: Heloise Beaugendre

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

solutions, and of new regulations adopted that require aero engine manufacturers to address an extended range of icing conditions.

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

7.3.1.3. ADDECCO

Title: ADaptive schemes for DEterministic and stoChastiC Flow PrOblems (ADDECCO)

Type: IDEAS (AdG # 226316)

Instrument: ERC Advanced Grant (Advanced)

Duration: December 2008 - November 2013

Coordinator: Inria (France)

Others partners: none

See also: http://www.math.u-bordeaux.fr/~rabgrall

Abstract: The numerical simulation of complex compressible flow problem is still a challenge nowadays, even for the simplest physical model such as the Euler and Navier Stokes equations for perfect gases. Researchers in scientific computing need to understand how to obtain efficient, stable, very accurate schemes on complex 3D geometries that are easy to code and to maintain, with good scalability on massively parallel machines. Many people work on these topics, but our opinion is that new challenges have to be tackled in order to combine the outcomes of several branches of scientific computing to get simpler algorithms of better quality without sacrificing their efficiency properties. In this proposal, we will tackle several hard points to overcome for the success of this program. We first consider the problem of how to design methods that can handle easily mesh refinement, in particular near the boundary, the locations where the most interesting engineering quantities have to be evaluated. CAD tools enable to describe the geometry, then a mesh is generated which itself is used by a numerical scheme. Hence, any mesh refinement process is not directly connected with the CAD. This situation prevents the spread of mesh adaptation techniques in industry and we propose a method to overcome this even for steep problems. Second, we consider the problem of handling the extremely complex patterns that occur in a flow because of boundary layers: it is not always sufficient to only increase the number of degrees of freedom or the formal accuracy of the scheme. We propose to overcome this with class of very high order numerical schemes that can utilise solution dependant basis functions. Our third item is about handling unsteady uncertainties in the model, for example in the geometry or the boundary conditions. This need to be done efficiently: the amount of computation increases a priori linearly with the number of uncertain parameters. We propose a non–intrusive method that is able to deal with general probability density functions (pdf), and also able to handle pdfs that may evolve during the simulation via a stochastic optimisation algorithm, for example. This will be combined with the first two items of this proposal. Many random variables may be needed, the curse of dimensionality will be dealt thanks to multiresolution method combined with sparse grid methods. The aim of this proposal is to design, develop and evaluate solutions to each of these challenges. Currently, and up to our knowledge, none of these problems have been dealt with for compressible flows with steep patterns as in many moderns aerodynamics industrial problems. We propose a work program that will lead to significant breakthroughs for flow simulations with a clear impact on numerical schemes and industrial applications. Our solutions, though developed and evaluated on flow problems, have a wider potential and could be considered for any physical problem that are essentially hyperbolic.

7.3.2. TRP Contract with European Space Agency

- Contrat ESA AO /1-6938/11/NL/SFE) for uncertainty quantification in aerospace application.
- Starting Date : 1st June 2012
- Coordinator : Thierry Magin (VKI)
- Type : ESA (European Spatial Agency).
- Grant : 250.000 euros
- Abstract: this project deals with the development of uncertainty quantification methods for aerospace applications. This is the first project financed by ESA concerning uncertainty quantification. The approach that we propose to follow will be based on the quantification and reduction of all the uncertainties, thoroughly identified, in a balanced manner. A fundamental characteristic of this integrated simulation strategy must be also the ability to control the numerical errors present in the highly integrated computations.

7.4. International Initiatives

7.4.1. Inria Associate Teams

AQUARIUS associated team is a research project dealing with uncertainty quantification and numerical simulation of high Reynolds number flows. It represents a challenging study demanding accurate and efficient numerical methods. It involves the Inria team BACCHUS and the groups of Pr. Charbel Farhat from the Department of Aeronautics and Astronautics and Pr. G. Iaccarino from the Department of Mechanical Engineering at Stanford University. The first topic concerns the simulation of flows when only partial information about the physics or the simulation conditions (initial conditions, boundary conditions) is available. In particular we are interested in developing methods to be used in complex flows where the uncertainties represented as random variables can have arbitrary probability density functions. The second topic focuses on the accurate and efficient simulation of high Reynolds number flows. Two different approaches are developed (one relying on the XFEM technology, and one on the Discontinuous Enrichment Method (DEM), with the coupling based on Lagrange multipliers). The purpose of the proposed project is twofold : i) to conduct a critical comparison of the approaches of the two groups (Stanford and Inria) on each topic in order to create a synergy which will lead to improving the status of our individual research efforts in these areas ; ii) to apply improved methods to realistic problems in high Reynolds number flow.

A summary of research activities, publications, visits can be found on http://www.stanford.edu/group/uq/aquarius/index3.html

7.4.2. Inria International Partners

7.4.2.1. Informal International Partners

von Karman Institute for Fluid Dynamics (Belgium). With Pr. H. Deconinck we work on the design of high order methods, including goal oriented mesh adaptation strategies

Leeds University, School of Computing : Dr. M.E. Hubbard (as of January 2014 in University of Nottingham, Department of Mathematics). Collaboration on high order schemes for time dependent shallow water flows

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

LEGI, Grenoble : Collaboration with C. Corre, E. Goncalves and G. Balarac on uncertainty quantification methods, multiphase flows, cavitation and turbulence.

CWI, The Netherlands : Collaboration with J. Witteveen about the Simplex2 methods for robust design optimization.

University of Trieste : Collaboration with V. Pediroda and L. Parussini concerning robust optimization methods.

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

7.4.3. Inria International Labs

7.4.3.1. JLPC

In the context of the JLPC (Joint Laboratory for Petascale Computing), people involved in the development of graph partitioning algorithms in `Scotch` collaborate with several US partners (UIUC, Argonne) so as to improve partitioning run time and quality for large scale simulations. Sébastien Fourestier has been attending the Inria-UIUC meeting of last September and has delivered two talks, one regarding `Scotch` and the other regarding `PaMPA`.

7.4.3.2. Inria@SILICONVALLEY

People involved in the development of graph partitioning algorithms in `Scotch` have a loose collaboration with Sherry Li and her team at Berkeley, regarding sparse matrix reordering techniques.

7.4.4. Participation In other International Programs

7.4.4.1. Inria-CNPq

In the context of the `HOSCAR` project jointly funded by Inria and CNPq, coordinated by Stéphane LANTERI on the French side, François Pellegrini and Pierre Ramet have participated in a joint workshop in Petrópolis last September. A collaboration is envisioned regarding parallel graph partitioning algorithms for data placement in the context of big data applications.

7.5. International Research Visitors

7.5.1. Visits of International Scientists

- Kazuo AOKI, Kyoto University (Kyoto, Japan), from August 31st to September 9th ;
- Smadar KARNI, University of Michigan Ann Arbor (Ann Arbor, Michigan, USA), from January 15th to March 23rd ;
- Alexander KURGANOV, Tulane University (New-Orleans, USA), from July 8th to July 13th ;
- Dimitris VALOUGEORGIS, University of Thessaly (Grece), from June 24th to July 5th ;
- Federica VIGNATI, Politecnico di Milano (Italy), from May 6th to May 18th ;
- Bernhard MULLER, NTNU Trondheim (Norway), on sabbatical from October 2013 to May 2014.

We also received a large number of shorter visits (on/two days) from several internationally recognized scientists : M. Pelanti (ENSTA PArisTech, France), S. Takata (Kyito University, Japan), E. Audit (CEA, France), E. Caron (Ecole Nomale Superieur Lyon, France), C. Corre (LEGI Grenoble, France), H. Deconinck (von Karman Institute, Belgium), B. Despres (Université Paris VI, France), M. Giles (Oxford University, UK), D. Lucor (Université Paris VI, France), H. Meyerhenke (KIT, Germany), C. Poloni (Università di Trieste, Italy), P. Sagaut (Université P. et M. Curie, France), P. Siarry (UPEC, France), and many others.

7.5.1.1. Internships

- Paola BACIGALUPPI. From April to October. Subject : Wave breaking modeling in a stabilized finite element code. University : Politecnico di Milano. Supervisor : M. Ricchiuto ;
- Sophie DALLET. From March to August. Subject : Approximation de modèles multiphase par mèthodes aux résidus. Supervisor : R. Abgrall ;
- Marc DUVERNET. From March to June. Subject : Coupler un code numérique qui résout les équations du mélange liquide-vapeur avec un code pour la quantification des incertitudes basé sur un cadre bayésien. Supervisor : P. Congedo ;

- Simon ETTOUATI. From February to August. Subject : Déformation de maillage pour les maillages d'ordre élevé. Supervisor : C. Dobrzynski ;
- Andrea FILIPPINI. From January to April. Subject : Stabilized finite element modeling of non-hydrostatic wave propagation. University : Politecnico di Milano. Supervisor : M. Ricchiuto ;
- Adballa MANSOURI. From March to June. Subject : Génération d'un modèle thermodynamique complexe pour les gaz réels. Supervisor : P. Congedo ;
- Léo NOUVEAU. From February to August. Subject : Etude sur les mèthodes de pénalisation adaptées aux maillages non-structurés fortement anisotropiques et utilisation de l'adaptation de maillage. Supervisor : H. Beaugendre ;
- Nassim RAZAALY. From Ferbuary to July. Subject : Modifier un code de simulation numérique d'ordre élevé pour implémenter des modèles thermodynamiques précis. University : ENSEIRB-MATMECA. Supervisor : P. Congedo.

7.5.2. Visits to International Teams

- P.M. Congedo, Stanford University (USA), two weeks in May 2013.
- P.M. Congedo, University of Salento (Italy), two weeks in August 2013.
- G. Geraci, Stanford University, 1 month in August 2013.

8. Dissemination

8.1. Scientific Animation

R. Abgrall is co-chief editor of the International Journal on Numerical Methods in Fluids, associate editor of the Journal of Computational Physics, mathematics of Computation, Computers and Fluids, the Journal of Scientific Computing, and Advances in Applied Mathematics and Mechanics. He is responsible of the SMAI-GAMNI group, and Treasurer of ECCOMAS. He is member of the Scientific committee of CERFACS. He is scientific advisor at ONERA and William Penny Fellow of the AWE (Atomic Weapon Agency, UK).

Cécile Dobrzynski was one of the organizers of the seminar "Modélisation et Calcul" of the Institut de Mathématiques de Bordeaux. She is member of the board of the GAMNI group of SMAI and she is secretary.

Heloise Beaugendre, Cécile Dobrzynski, and Mario Ricchiuto have participated to the organization of the second ECCOMAS Young Investigators Conference (http://yic2013.sciencesconf.org) in Bordeaux, counting 120 participants attending talks in the domains of modeling and simulation in Mechanics. Cécile Dobrzynski has also been conference chairwoman.

R. Abgrall, C. Dobrzynski, P. Congedo, H. Beaugendre and M Ricchiuto have organized the EUROPEAN WORKSHOP on High Order Nonlinear Numerical Methods for Evolutionary PDEs (HONOM 2013) , March 18-22, 2013, with more than 70 participants and less than a third from France. There was 8 invited speakers. A proceeding is being processed. This has been mainly funded by ADDECCO, see http://honom2013.bordeaux.inria.fr/.

Pietro Congedo and Remi Abgrall have organized the International Workshop on Uncertainty Quantification in fluids Simulation, December 16-18, 2013 http://boquse2013.bordeaux.inria.fr/. This workshop was intended to be an exchange forum for scientists working on innovative and efficient techniques for uncertainty quantification and robust design in Fluid Mechanics.There was 9 invited talks in 3 sessions and more than 70 participants. This workshop has been funded by the CPU center d'excellence de l'Université de Bordeaux, Inria and ADDECCO.

8.2. Teaching - Supervision - Juries

8.2.1. Teaching

Licence : Cécile Dobrzynski, Langages en Fortran 90, 54h, L3, ENSEIRB-MATMÉCA, FRANCE

Licence : Cécile Dobrzynski, Analyse numérique, 24h, M1, ENSEIRB-MATMÉCA, FRANCE

Licence : Cécile Dobrzynski, Outils informatiques pour le calcul scientifique, 65h, formation Structures Composites, ENSCBP, FRANCE

Licence : Mario Ricchiuto, Fundamentals of Numerical Analysis, 24h,ENSEIRB-MATMÉCA, France.

License : Héloïse Beaugendre, Responsable des projets TER de première année, 10h, L3, ENSEIRB-MATMÉCA, FRANCE

License : Héloïse Beaugendre, Encadrement TER, 16h, L3, ENSEIRB-MATMÉCA, FRANCE

Licence : Pietro Marco Congedo, Fundamentals of Numerical Analysis II, 24h, ENSEIRB-MATMÉCA, France.

Licence : Pietro Marco Congedo, Fundamentals of Fluid Mechanics II, 20h, ENSEIRB-MATMÉCA, France.

Master : Pietro Marco Congedo, Simulation Numérique des écoulements fluides, 20h, M2, ENSEIRB-MATMÉCA, France

Master : Cécile Dobrzynski, Projet fin d'études, 6h, M2, ENSEIRB-MATMÉCA, FRANCE

Master : Cécile Dobrzynski, TER, 18h, M1, ENSEIRB-MATMÉCA, FRANCE

Master : Mario Ricchiuto, Simulation Numérique des écoulements fluides, 16h, M3, ENSEIRB-MATMÉCA, France

Master : Mario Ricchiuto, Post-graduate course on introduction to CFD, 18h, M2 IAS (Master Spe´cialisé Inge´nierie Ae´ronautique et Spatiale, http://www.ensam.fr/fr/formation_initiale/masteres_specialises/ingenierie_aeronautique_et_spatiale), ENSAM, France

Master : Héloïse Beaugendre, Approximation numérique et problèmes industriels, 52h, M1, ENSEIRB-MATMÉCA, France

Master : Héloïse Beaugendre, Outils informatiques pour l'insertion professionnelle, 9h, M2, Université de Bordeaux, France

Master : Héloïse Beaugendre, Calcul Parallèle (OpenMP-MPI), 40h, M1, ENSEIRB-MATMÉCAi et Université de Bordeaux, France

Master : Héloïse Beaugendre, Calcul Haute Performance (MPI), 36h, M2, ENSEIRB-MATMÉCA, France

Master : Héloïse Beaugendre, Calcul Haute Performance et décomposition de domaine, 36h, M2, ENSEIRB-MATMÉCA et Université Bordeaux, France

8.2.2. Supervision

HDR: Pietro Congedo, Contributions to the reliability of numerical simulations in fluid mechanics. Application to the flow simulation of thermodynamically complex gases [1], HDR Defense, December 6 2013, Université de Bordeaux I

PhD: Dante De Santis, High order residual distribution methods for turbulent steady flows [2], PhD defense December 3 2013, Université de Bordeaux I (supervisors : Rémi Abgrall and Mario Ricchiuto)

PhD: Gianluca Geraci, Multi-resolution inspired methods for uncertainty quantification, PhD defense December 5 2013, Université de Bordeaux I (supervisors : Rémi Abgrall and Pietro Marco Congedo)

PhD : Sébastien Fourestier, Redistribution dynamique parallèle efficace de la charge pour les problèmes numériques de très grandes tailles [3], PhD defense June 2013, Université de Bordeaux I (supervisor : F. Pellegrini)

PhD: Cédric Lachat, Partitionnement et adaptation parallèles de maillages pour des simulations dans les tokamaks [4], PhD defense December 2013, Université de Nice (supervisors : F. Pellegrini and C. Dobrzynski)

PhD in progress : Damien Genêt, Design of a parallele object oriented platform for computational fluid dynamics (supervisors : F. Pellegrini and M. Ricchiuto)

PhD in progress : Léo Nouveau, Adaptation de maillage non structurés anisotropes pour les méthodes de pénalisation en mécanique des fluides compressibles (supervisors : R. Abgrall, H. Beaugendre and C. Dobrzynski)

PhD in progress : Quentin Viville, Etude sur les méthodes de pénalisation adaptées aux maillages non-structurés fortement anisotropiques et utilisation de l'adaptation de maillx'age (supervisors : R. Abgrall, H. Beaugendre and C. Dobrzynski)

PhD in progress : Stevan Bellec, Discrete asymptotic PDEs for non-hydtrostatic wave propagation (supervisors : M. Colin and M. Ricchiuto)

PhD in progress : Andrea Filippini, Adaptive finite element discretizations of nonlinear non-hydrostatic depth averaged wave models (supervisors : M. Ricchiuto and P. Bonneton)

PhD in progress : Gregory Perrot, Two-dimensional image-based modeling of self-healing ceramic matrix composite materials (supervisors : G. Vignoles and M. Ricchiuto)

PhD in progress : Francesca Fusi, Development of efficient numerical techniques for the optimization under uncertainty of morphing helicopter rotor blade (supervisors : A. Guardone, P.M. Congedo)

8.2.3. Juries

PhD : Emilie Sauvage, Patient-specific blood flow modelling, université catholique de Louvain, Belgique, Cécile Dobrzynski : jury

PhD : Mario Falese, A study of the effects of bifurcations in swirling flows using LES and mesh adaptation, Cerfacs, Cécile Dobrzynski : jury

PhD: Koen Hillewaert, DG methods for industrial CFD, Université Catholique de Louvain, Belgium, R. Abgrall: referee

PhD: H. Lundt, Relaxation models for two-phase flow with applications to CO2 transport, NTNU, Trondheim, Norway, R. Abgrall: referee

PhD: Steven Diot, High order WENO like methods for CFD, Université de Toulouse, R. Abgrall: referee.

HDR: R. Duvigneau, Optimisation methods, Université de Nice, R. Abgrall: referee

PhD: Gauthier Folzan, Modélisation multi-matériaux multi-vitesse en dynamique rapide, Ecole Polytechnique, R. Abgrall: referee.

PhD: Karim Grimish, Méthodes de résidu d<ordre élevé, ENSAM Paris, R. Abgrall: referee.

PhD: Jonathan Jung, Méthodes numériques d'écoulements multiphasiques tridimensionnels sur GPU, Université de Strasbourg, R. Abgrall: referee.

9. Bibliography

Publications of the year

Doctoral Dissertations and Habilitation Theses

[1] P. M. CONGEDO. , *Contributions to the reliability of numerical simulations in fluid mechanics. Application to the flow simulation of thermodynamically complex gases*, Université Sciences et Technologies - Bordeaux I, December 2013, Habilitation à Diriger des Recherches, http://hal.inria.fr/tel-00940088

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