



Activity Report 2015

Team CARDAMOM

Certified Adaptive discRete moDels for robust simulATIons of CoMplex fLOws with Moving fronts

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

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Numerical schemes and simulations

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Team CARDAMOM

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Keywords:

Computer Science and Digital Science:

- 3. - Data and knowledge
 - 3.1. - Data
 - 3.1.4. - Uncertain data
 - 3.4. - Machine learning and statistics
 - 3.4.5. - Bayesian methods
- 6. - Modeling, simulation and control
 - 6.1. - Mathematical Modeling
 - 6.1.1. - Continuous Modeling (PDE, ODE)
 - 6.1.2. - Stochastic Modeling (SPDE, SDE)
 - 6.1.4. - Multiscale modeling
 - 6.1.5. - Multiphysics modeling
 - 6.2. - Scientific Computing, Numerical Analysis & Optimization
 - 6.2.1. - Numerical analysis of PDE and ODE
 - 6.2.2. - Numerical probability
 - 6.2.3. - Probabilistic methods
 - 6.2.4. - Statistical methods
 - 6.2.6. - Optimization
 - 6.2.7. - High performance computing
 - 6.2.8. - Computational geometry and meshes
 - 6.3.1. - Inverse problems
 - 6.3.2. - Data assimilation
 - 6.3.4. - Model reduction

Other Research Topics and Application Domains:

- 3.3. - Geosciences
 - 3.3.2. - Water: sea & ocean, lake & river
 - 3.3.3. - Littoral
- 3.4.1. - Natural risks
- 3.4.2. - Industrial risks and waste
- 4.1. - Fossile energy production
- 4.2. - Renewable energy production
 - 4.2.1. - Biofuels
 - 4.2.2. - Hydro-energy
- 5.2. - Design and manufacturing
 - 5.2.3. - Aviation
 - 5.2.4. - Aerospace
- 5.5. - Materials

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2. Overall Objectives

2.1. Overall Objectives

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

2.2. Scientific context and challenges

The objective of this project is to provide improved analysis and design tools for engineering applications involving fluid flows, and in particular flows with moving fronts. In our applications *a front is either an actual material interface, or a well identified and delimited transition region in which the flow undergoes a change in its dominant macroscopic character*. One example is the certification of wing de anti-icing systems, involving the predictions of ice formation and detachment, and of ice debris trajectories to evaluate the risk of downstream impact on aircraft components [138], [74]. Another application, relevant for space reentry, is the study of transitional regimes in high altitude gas dynamics in which extremely thin layers appear in the flow which cannot be analysed with classical continuous models (Navier-Stokes equations) used by engineers [80], [106]. An important example in coastal engineering is the transition between propagating and breaking waves, characterized by a strong local production of vorticity and by dissipative effects absent when waves propagates [82]. Similar examples in energy and material engineering provide the motivation of this project.

All these application fields involve either the study of new technologies (e.g. new design/certification tools for aeronautics [88], [101], [119], [74] or for wave energy conversion [98]), or parametric studies of complex environments (e.g. harbour dynamics [108], or estuarine hydrodynamics [69]), or hazard assessment and prevention [103]. In all cases, computationally affordable, quick, and accurate numerical modelling is essential to improve the quality of (or to shorten) design cycles and allow performance level enhancements in early stages of development [143]. The goal is to afford simulations over very long times with many parameters or to embed a model in an alert system.

In addition to this, even in the best of circumstances, the reliability of numerical predictions is limited by the intrinsic randomness of the data used in practice to define boundary conditions, initial conditions, geometry, etc. This uncertainty, related to the measurement errors, is defined as *aleatory*, and cannot be removed, nor reduced. In addition, physical models and the related Partial Differential Equations (PDEs), feature a structural uncertainty, since they are derived with assumptions of limited validity and calibrated with manipulated experimental data (filtering, averaging, etc ..). These uncertainties are defined as *epistemic*, as they are a deficiency due to a lack of knowledge [64], [131]. Unfortunately, measurements in fluids are delicate and expensive. In complex flows, especially in flows involving interfaces and moving fronts, they are sometimes impossible to carry out, due to scaling problems, repeatability issues (e.g. tsunami events), technical issues (different physics in the different flow regions) or dangerousness (e.g. high temperature reentry flows, or combustion). Frequently, they are impractical, due to the time scales involved (e.g. characterisation of oxidation processes related to a new material micro-/meso- structure [90]). This increases the amount of uncertainties associated to measurements and reduces the amount of information available to construct physical/PDE models. These uncertainties play also a crucial role when one wants to deal with numerical certification or optimization of a fluid based device. However, this makes the required number of flow simulations grow as high as hundreds or even thousands of times. The associated costs are usually prohibitive. So the real challenge is to be able to construct an accurate and computationally affordable numerical model handling efficiently uncertainties. In particular, this model should be able to take into account the variability due to uncertainties, those coming from the certification/optimization parameters as well as those coming from modelling choices.

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

2.3. Our approach

The schematic of figure 1 shows the standard way a certification study may be conducted. The red box is the main robust certification loop which contains separate boxes involving the evaluation of the physical model, the post-processing of the output, and the exploration of the spaces of physical and stochastic parameters (uncertainties). The physical model itself, is composed of the 3 main elements: PDE system, mesh generation/adaptation, and discretization of the PDE (numerical scheme). There are some known interactions taking place in the loop which are a necessary to exploit as much as possible the potential of high order methods [112] such as e.g. $h-p-r$ adaptation in the physical model w.r.t. some post-processed output value, or w.r.t. some sort of adjoint sensitivity coming from the physical parameter evolution box, etc.

As things stand today, we will not be able to take advantage of the potential of new high order numerical techniques and of hierarchical (multi-fidelity) robust certification approaches without some very aggressive adaptive methodology. Such a methodology, will require interactions between e.g. the uncertainty quantification methods and the adaptive spatial discretization, as well as with the PDE modelling part. Such a strategy cannot be developed, let alone implemented in an operational context, without completely disassembling the scheme of the figure, and letting all the parts of the interact as in figure 2. This is what we want to do in CAR-DAMOM . We have the unique combination of skills which allows to explore such an avenue: PDE analysis, high order numerical discretizations, mesh generation and adaptation, optimization and uncertainty quantification, specific issues related to the applications considered.

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

- What are the relations between PDE model accuracy (asymptotic error) and scheme accuracy, and how to control, en possibly exploit these relations to minimize the error for a given computational effort ;
- How to devise and implement adaptation techniques ($r-$, $h-$, and $p-$) for time dependent problems while guaranteeing an efficient time marching procedure (minimize CPU time at constant error) ;

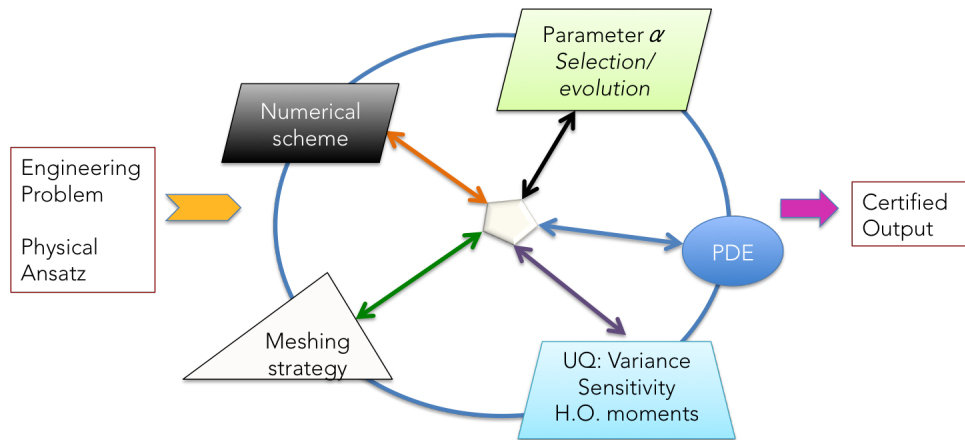


Figure 1. CARDAMOM unified strategy

- How to exploit the wide amount of information made available from the optimization *and* uncertainty quantification process to construct a more aggressive adaptation strategy in physical, parameter, and stochastic space, and in the physical model itself ;

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

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

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

3. Research Program

3.1. Variational discrete asymptotic modelling

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

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

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

In parallel to these developments, we will make an effort in to gain a better understanding of continuous asymptotic PDE models. We will in particular work on improving, and possibly, simplifying their numerical approximation. An effort will be done in trying to embed in these more complex nonlinear PDE models discrete analogs of operator identities necessary for stability (see e.g. the recent work of [115], [118] and references therein).

3.2. High order discretizations on moving adaptive meshes

We will work on both the improvement of high order mesh generation and adaptation techniques, and the construction of more efficient, adaptive high order discretisation methods.

Concerning curved mesh generation, we will focus on two points. First propose a robust and automatic method to generate curved simplicial meshes for realistic geometries. The untangling algorithm we plan to develop is a hybrid technique that gathers a local mesh optimization applied on the surface of the domain and a linear elasticity analogy applied in its volume. Second we plan to extend the method proposed in [67] to hybrid meshes (prism/tetra).

For time dependent adaptation we will try to exploit as much as possible the use of r -adaptation techniques based on the solution of some PDE system for the mesh. We will work on enhancing the initial results of [71], [73] by developing more robust nonlinear variants allowing to embed rapidly moving objects. For this the use of non-linear mesh PDEs (cf e.g. [127], [134], [83]), combined with Bezier type approximations for the mesh displacements to accommodate high order curved meshes [67], and with improved algorithms to discretize accurately and fast the elliptic equations involved. For this we will explore different type of relaxation methods, including those proposed in [116], [121], [120] allowing to re-use high order discretizations techniques already used for the flow variables. All these modelling approaches for the mesh movement are based on some minimization argument, and do not allow easily to take into account explicitly properties such as e.g. the positivity of nodal volumes. An effort will be made to try to embed these properties, as well as to improve the control on the local mesh sizes obtained. Developments made in numerical methods for Lagrangian hydrodynamics and compressible materials may be a possible path for these objectives (see e.g. [93], [140], [139] and references therein). We will stretch the use of these techniques as much as we can, and couple them with remeshing algorithms based on local modifications plus conservative, high order, and monotone ALE (or other) remaps (cf. [68], [104], [141], [91] and references therein).

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

- the ALE formulation is well adapted both to handle moving meshes, and to provide conservative, high order, and monotone remaps between different meshes. We want to address the issue of cost-accuracy of adaptive mesh computations by exploring different degrees of coupling between the flow and the mesh PDEs. Initial experience has indicated that a clever coupling may lead to a considerable CPU time reduction for a given resolution [73], [71]. This balance is certainly dependent on the nature of the PDEs, on the accuracy level sought, on the cost of the scheme, and on the time stepping technique. All these elements will be taken into account to try to provide the most efficient formulation ;
- the conservation of volume, and the subsequent preservation of constant mass-momentum-energy states on deforming domains is one of the most primordial elements of Arbitrary Lagrangian-Eulerian formulations. For complex PDEs as the ones considered here, of especially for some applications, there may be a competition between the conservation of e.g. mass, and the conservation of other constant states, as important as mass. This is typically the case for free surface flows, in which mass preservation is in competitions with the preservation of constant free surface levels [72]. Similar problems may arise in other applications. Possible solutions to this competition may come from super-approximation (use of higher order polynomials) of some of the data allowing to reduce (e.g. bathymetry) the error in the preservation of one of the competing quantities. This is similar to what is done in super-parametric approximations of the boundaries of an object immersed in the flow, except that in our case the data may enter the PDE explicitly and not only through the boundary conditions. Several efficient solutions for this issue will be investigated to obtain fully conservative moving mesh approaches:
- an issue related to the previous one is the accurate treatment of wall boundaries. It is known that even for standard lower order (second) methods, a higher order, curved, approximation of the boundaries may be beneficial. This, however, may become difficult when considering moving objects, as in the case e.g. of the study of the impact of ice debris in the flow. To alleviate this issue, we plan to follow on with our initial work on the combined use of immersed boundaries techniques with high order, anisotropic (curved) mesh adaptation. In particular, we will develop combined approaches involving high order hybrid meshes on fixed boundaries with the use of penalization techniques and immersed boundaries for moving objects. We plan to study the accuracy obtainable across discontinuous functions with r -adaptive techniques, and otherwise use whenever necessary anisotropic meshes to be able to provide a simplified high order description of the wall boundary (cf. [114]). The use of penalization will also provide a natural setting to compute immediate approximations of the forces on the immersed body [119], [122]. An effort will be also made on improving the accuracy of these techniques using e.g. higher order approaches, either based on generalizations of classical splitting methods [105], or on some iterative Defect Correction method (see e.g. [85]) ;
- the proper treatment of different physics may be addressed by using mixed/hybrid schemes in which different variables/equations are approximated using a different polynomial expansion. A typical example is our work on the discretization of highly non-linear wave models [100] in which we have shown how to use a standard continuous Galerkin method for the elliptic equation/variable representative of the dispersive effects, while the underlying hyperbolic system is evolved using a (discontinuous) third order finite volume method. This technique will be generalized to other classes of discontinuous methods, and similar ideas will be used in other context to provide a flexible approximation. Such methods have clear advantages in multiphase flows but not only. A typical example where such mixed methods are beneficial are flows involving different species and tracer equations, which are typically better treated with a discontinuous approximation. Another example is the use of this mixed approximation to describe the topography with a high order continuous polynomial even in discontinuous method. This allows to greatly simplify the numerical treatment of the bathymetric source terms ;

- the enhancement of stabilized methods based on some continuous finite element approximation will remain a main topic. We will further pursue the study on the construction of simplified stabilization operators which do not involve any contributions to the mass matrix. We will in particular generalize our initial results [129], [70], [130] to higher order spatial approximations using cubature points, or Bezier polynomials, or also hierarchical approximations. This will also be combined with time dependent variants of the reconstruction techniques initially proposed by D. Caraeni [84], allowing to have a more flexible approach similar to the so-called P^hP^m method [96], [133]. How to localize these enhancements, and to efficiently perform local reconstructions/enrichment, as well as p -adaptation, and handling hanging nodes will also be a main line of work. A clever combination of hierarchical enrichment of the polynomials, with a constrained approximation will be investigated. All these developments will be combined with the shock capturing/positivity preserving construction we developed in the past. Other discontinuity resolving techniques will be investigated as well, such as face limiting techniques as those partially studied in [102];
- time stepping is an important issue, especially in presence of local mesh adaptation. The techniques we use will force us to investigate local and multilevel techniques. We will study the possibility constructing semi-implicit methods combining extrapolation techniques with space-time variational approaches. Other techniques will be considered, as multi-stage type methods obtained using Defect-Correction, Multi-step Runge-Kutta methods [81], as well as spatial partitioning techniques [111]. A major challenge will be to be able to guarantee sufficient locality to the time integration method to allow to efficiently treat highly refined meshes, especially for viscous reactive flows. Another challenge will be to embed these methods in the stabilized methods we will develop.

3.3. Coupled approximation/adaptation in parameter and physical space

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

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

Despite the coupling between stochastic and physical space, this approach can be made massively parallel by means of extrapolation/interpolation techniques for the high order moments, in time and on a reference mesh, guaranteeing the complete independence of deterministic simulations. This approach has the additional advantage of being feasible for several different application codes due to its non-intrusive character.

To improve on the accuracy of the above methods, intrusive approaches will also be studied. To propagate uncertainties in stochastic differential equations, we will use Harten's multiresolution framework, following [66]. This framework allows a reduction of the dimensionality of the discrete space of function representation, defined in a proper stochastic space. This reduction allows a reduction of the number of explicit evaluations required to represent the function, and thus a gain in efficiency. Moreover, multiresolution analysis offers a natural tool to investigate the local regularity of a function and can be employed to build an efficient refinement strategy, and also provides a procedure to refine/coarsen the stochastic space for unsteady problems. This strategy should allow to capture and follow all types of flow structures, and, as proposed in [66], allows to formulate a non-linear scheme in terms of compression capabilities, which should allow to handle non-smooth problems. The potential of the method also relies on its moderate intrusive behaviour, compared to e.g. spectral Galerkin projection, where a theoretical manipulation of the original system is needed.

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

The first is the improvement of the efficiency. This may be achieved by means of anisotropic mesh refinement, and by experimenting with a strong parallelization of the method. Concerning the first point, we will investigate several anisotropic refinement criteria existing in literature (also in the UQ framework), starting with those already used in the team to adapt the physical grid. Concerning the implementation, the scheme formulated in [66] is conceived to be highly parallel due to the external cycle on the number of dimensions in the space of uncertain parameters. In principle, a number of parallel threads equal to the number of spatial cells could be employed. The scheme should be developed and tested for treating unsteady and discontinuous probability density function, and correlated random variables. Both the compression capabilities and the accuracy of the scheme (in the stochastic space) should be enhanced with a high-order multidimensional conservative and non-oscillatory polynomial reconstruction (ENO/WENO).

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

3.4. Robust multi-fidelity modelling for optimization and certification

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

1. a robust strategy using the statistics evaluation will be applied separately, *i.e.* using only low or high-fidelity evaluations. Some classical optimization algorithms will be used in this case. Influence of high-order statistics and model reduction in the robust design optimization will be explored, also by further developing some low-cost methods for robust design optimization working on the so-called Simplex² method [89] ;
2. a multi-fidelity strategy by using in an efficient way low fidelity and high-fidelity estimators both in physical and stochastic space will be conceived, by using a Bayesian framework for taking into account model discrepancy and a PC expansion model for building a surrogate model ;
3. develop advanced methods for robust optimization. In particular, the Simplex² method will be modified for introducing a hierarchical refinement with the aim to reduce the number of stochastic samples according to a given design in an adaptive way.

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

4. Application Domains

4.1. De-anti icing systems

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

In [75] it has been proposed to model ice shedding trajectories by an innovative paradigm that is based on Cartesian grids, Penalization and Level Sets (LESCAPE code). Our objective is to use the potential of high order unstructured mesh adaptation and immersed boundary techniques to provide a geometrically flexible extension of this idea. These activities will be linked to the development of efficient mesh adaptation and time stepping techniques for time dependent flows, and their coupling with the immersed boundary methods we started developing in the FP7 EU project STORM [65], [122]. In these methods we compensate for the error at solid walls introduced by the penalization by using anisotropic mesh adaptation [94], [113], [114]. From the numerical point of view one of the major challenges is to guarantee efficiency and accuracy of the time stepping in presence of highly stretched adaptive and moving meshes. Semi-implicit, locally implicit, multi-level, and split discretizations will be explored to this end.

Besides the numerical aspects, we will deal with modelling challenges. One source of complexity is the initial conditions which are essential to compute ice shedding trajectories. It is thus extremely important to understand the mechanisms of ice release. With the development of next generations of engines and aircraft, there is a crucial need to better assess and predict icing aspects early in design phases and identify breakthrough technologies for ice protection systems compatible with future architectures. When a thermal ice protection system is activated, it melts a part of the ice in contact with the surface, creating a liquid water film and therefore lowering ability of the ice block to adhere to the surface. The aerodynamic forces are then able to detach the ice block from the surface [77]. In order to assess the performance of such a system, it is essential to understand the mechanisms by which the aerodynamic forces manage to detach the ice. The current state of the art in icing codes is an empirical criterion. However such an empirical criterion is unsatisfactory. Following the early work of [79], [74] we will develop appropriate asymptotic PDE approximations allowing to describe the ice formation and detachment, trying to embed in this description elements from damage/fracture mechanics. These models will constitute closures for aerodynamics/RANS and URANS simulations in the form of PDE wall models, or modified boundary conditions.

In addition to this, several sources of uncertainties are associated to the ice geometry, size, orientation and the shedding location. In very few papers [125], some sensitivity analysis based on Monte Carlo method have been conducted to take into account the uncertainties of the initial conditions and the chaotic nature of the ice particle motion. We aim to propose some systematic approach to handle every source of uncertainty in an efficient way relying on some state-of-art techniques developed in the Team. In particular, we will perform an uncertainty propagation of some uncertainties on the initial conditions (position, orientation, velocity,...) through a low-fidelity model in order to get statistics of a multitude of particle tracks. This study will be done in collaboration with ETS (Ecole de Technologies Supérieure, Canada). The longterm objective is to produce footprint maps and to analyse the sensitivity of the models developed.

4.2. Space re-entry

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

One of the applications we will consider is the so-called post-flight analysis of a space mission. This involves reconstructing the history of the re-entry module (trajectory and flow) from data measured on the spacecraft by means of a Flush Air Data System (FADS), a set of sensors flush mounted in the thermal protection system to measure the static pressure (pressure taps) and heat flux (calorimeters). This study involves the accurate determination of the freestream conditions during the trajectory. In practice this means determining temperature, pressure, and Mach number in front of the bow shock forming during re-entry. As shown by zur Nieden and Olivier [144], state of the art techniques for freestream characterization rely on several approximations, such as e.g. using an equivalent calorically perfect gas formulas instead of taking into account the complex aero-thermo-chemical behaviour of the fluid. These techniques do not integrate measurement errors nor the heat flux contribution, for which a correct knowledge drives more complex models such as gas surface interaction. In this context, CFD supplied with UQ tools permits to take into account chemical effects and to include both measurement errors and epistemic uncertainties, e.g. those due to the fluid approximation, on the chemical model parameters in the bulk and at the wall (surface catalysis).

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

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

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

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

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

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

These modelling capabilities will be coupled to high order adaptive discretizations to provide high fidelity flow models. One of the most challenging problems is the minimization of the influence of mesh and scheme on the wall conditions on the re-entry module. To reduce this influence, we will investigate both high order adaptation across the bow shock, and possibly adaptation based on uncertainty quantification high order moments related to the heat flux estimation, or shock fitting techniques [78], [117]. These tools will be coupled to our robust inverse techniques. One of our objectives is to development of a low-cost strategy for improving the numerical prediction by taking into account experimental data. Some methods have been recently introduced [124] for providing an estimation of the numerical errors/uncertainties. We will use some metamodels for solving the inverse problem, by considering all sources of uncertainty, including those on physical models. We will validate the framework using the experimental data available in strong collaboration with the von Karman Institute for Fluid dynamics (VKI). In particular, data coming from the VKI Longshot facility will be used. We will show application of the developed numerical tool for the prediction in flight conditions.

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

4.3. Energy

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

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

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

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

The simulation of these gases requires accurate thermodynamic models, such as Span-Wagner or Peng-Robinson (see [87]). The data to build these models is scarce due to the difficulty of performing reliable experiments. The related uncertainty is thus very high. Our work will go in the following directions:

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

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

Wave energy conversion is an emerging sector in energy engineering. The design of new and efficient Wave Energy Converters (WECs) is thus a crucial activity. As pointed out by Weber [143], it is more economical to raise the technology performance level (TPL) of a wave energy converter concept at low technology readiness level (TRL). Such a development path puts a greater demand on the numerical methods used. The findings of Weber also tell us that important design decisions as well as optimization should be performed as early in the development process as possible. However, as already mentioned, today the wave energy sector relies heavily on the use of tools based on simplified linear hydrodynamic models for the prediction of motions, loads, and power production. Our objective is to provide this sector, and especially SMEs, with robust design tools to minimize the uncertainties in predicted power production, loads, and costs of wave energy.

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

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

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

4.4. Materials engineering

Because of their high strength and low weight, ceramic-matrix composite materials (CMCs) are the focus of active research for aerospace and energy applications involving high temperatures, either military or civil. Though based on brittle ceramic components, these composites are not brittle due to the use of a fibre/matrix interphase that preserves the fibres from cracks appearing in the matrix. Recent developments aim at implementing also in civil aero engines a specific class of Ceramic Matrix Composite materials (CMCs) that show a self-healing behaviour. Self-healing consists in filling cracks appearing in the material with a dense fluid formed in-situ by oxidation of part of the matrix components. Self-healing (SH) CMCs are composed of a complex three-dimensional topology of woven fabrics containing fibre bundles immersed in a matrix coating of different phases. The oxide seal protects the fibres which are sensitive to oxidation, thus delaying failure. The obtained lifetimes reach hundreds of thousands of hours [128].

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

In collaboration with the LCTS laboratory (a joint CNRS-CEA-SAFRAN-Bordeaux University lab devoted to the study of thermo-structural materials in Bordeaux), we are developing a multi-scale model in which a structural mechanics solver is coupled with a closure model for the crack physico chemistry. This model is obtained as a multi-dimensional asymptotic crack averaged approximation for the transport equations (Fick's laws) with chemical reactions sources, plus a potential model for the flow of oxide [90], [95], [126]. We have demonstrated the potential of this model in showing the importance of taking into account the multi-dimensional topology of a fibre bundle (distribution of fibres) in the rupture mechanism. This means that the 0-dimensional model used in most of the studies (see e.g. [86]) will underestimate appreciably the lifetime of the material. Based on these recent advances, we will further pursue the development of multi-scale multi-dimensional asymptotic closure models for the parametric design of self healing CMCs. Our objectives are to provide: (i) new, non-linear multi-dimensional mathematical model of CMCs, in which the physico-chemistry of the self-healing process is more strongly coupled to the two-phase (liquid gas) hydro-dynamics of the healing oxide ; (ii) a model to represent and couple crack networks ; (iii) a robust and efficient coupling with the structural mechanics code ; (iv) validate this platform with experimental data obtained at the LCTS laboratory. The final objective is to set up a multi-scale platform for the robust prediction of lifetime of SH-CMCs, which will be a helpful tool for the tailoring of the next generation of these materials.

4.5. Coastal and civil engineering

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

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

Another important aspect which is not understood well enough at the moment is the role of dissipation in wave breaking regions. There are several examples of breaking closure, going from algebraic and PDE-based eddy viscosity methods [110], [132], [123], [92], to hybrid methods coupling dispersive PDEs with hyperbolic ones, and trying to mimic wave breaking with travelling bores [136], [137], [135], [107], [100]. In both cases, numerical dissipation plays an important role and the activation or not of the breaking closure, as the quantitative contribution of numerical dissipation to the flow has not been properly investigated. These elements must be clarified to allow full control of adaptive techniques for the models used in this type of applications.

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

5. Highlights of the Year

5.1. Highlights of the Year

- A whole new release of the mesh adaptation platform MMG is available, with a brand new looking website : <http://www.mmgttools.org/> ;
- We have solved the conflict between the conservation of either mass and steady equilibria relevant in applications (lake at rest state) when performing mesh-adaptive computations of shallow water flows. This algorithm will be embedded in the FMG adaptation library which will be part of the MMG tools ;
- We have shown the potential of Boussinesq-type depth averaged codes for the simulation of Wave Energy Converters [97], [98]. This result paves the way to the construction of new medium fidelity models to be used in the optimization of converters. This will be achieved in the framework of the MIDWEST project funded this year (EU OCEANERanet call) ;
- We have finally proven that fully discrete asymptotic approaches allow to construct new discretizations of depth averaged weakly nonlinear Boussinesq models with greatly improved phase and linear shoaling. We are now working on the construction of improved genuinely nonlinear models ;

6. New Software and Platforms

6.1. AeroSol

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

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

The generic features of the library are

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

We would like to emphasize three assets of this library:

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

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

At the end of 2014, AeroSol had the following features:

- **Development environment** Use of CMake for compilation (gcc, icc and xlc), CTest for automatic tests and memory checking, lcov and gcov for code coverage reports. Development of a CDash server for collecting the unitary tests and the memory checking. Beginning of the development of an interface for functional tests. Optional linking with HDF5, PAPI, with dense small matrices libraries (BLAS, Eigen)
- **In/Out** Link with the XML library for handling with parameter files. Parallel reader for GMSH, with an embedded geometrical pre-partitioner. Writer on the VTK-ASCII legacy format (cell and point centered). Parallel output in vtU and pvtU (Paraview) for cell-centered visualization, and XDMF/HDF5 format for both cell and point centered visualization. Ability of saving the high

order solution and restarting from it. Computation of volumic and probe statistics. Ability of saving averaged layer data in quad and hexa meshes. Ability of defining user defined output visualization variables.

- **Quadrature formula** up to 11th or
- April-June 2015: A. Javadi (PhD student) from Chalmers University, Gothenburg, Sweden (3 months).der for Lines, Quadrangles, Hexaedra, Pyramids, Prisms, up to 14th order for tetrahedron, up to 21st order for triangles. Gauss-Lobatto type quadrature formula for lines, triangles, quadrangles and hexaedra.
- **Finite elements** up to fourth degree for Lagrange finite elements and hierarchical orthogonal finite element basis (with Dubiner transform on simplices) on lines, triangles, quadrangles, tetrahedra, prisms, hexaedra and pyramids. Finite element basis that are interpolation basis on Gauss-Legendre points for lines, quadrangles, and hexaedra, and triangle (only 1st and 2nd order)
- **Geometry** Elementary geometrical functions for first order lines, triangles, quadrangles, prisms, tetrahedra, hexaedra and pyramids. Handling of high order meshes.
- **Time iteration** explicit Runge-Kutta up to fourth order, explicit Strong Stability Preserving schemes up to third order. Optimized CFL time schemes: SSP(2,3) and SSP(3,4). CFL time stepping. Implicit integration with BDF schemes from 2nd to 6th order Newton method for stationary problems. Implicit unstationary time iterator non consistent in time for stationary problems. Implementation of in house GMRES and conjugate gradient based on Jacobian free iterations.
- **Linear Solvers** Link with the external linear solver UMFPack, PETSc and MUMPS. Internal solver for diagonal and block-diagonal matrices.
- **Memory handling** discontinuous and continuous, sequential and parallel discretizations based on PaMPA for generic meshes, including hybrid meshes.
- **Models** Perfect gas Euler system, real gas Euler system (template based abstraction for a generic equation of state), scalar advection, Waves equation in first order formulation, generic interface for defining space-time models from space models. Diffusive models: isotropic and anisotropic diffusion, compressible Navier-Stokes. Scalar advection-diffusion model.
- **Numerical schemes** Continuous Galerkin method for the Laplace problem (up to fifth order) with non consistent time iteration or with direct matrix inversion. Explicit and implicit discontinuous Galerkin methods for hyperbolic systems, diffusive and advection-diffusion problems. Beginning of optimization by stocking the geometry for advection problems. SUPG and Residual distribution schemes. Optimization of DG schemes for advection-diffusion problems: stocking of the geometry and use of BLAS for all the linear phases of the scheme.
- **Numerical fluxes** Centered fluxes, exact Godunov' flux for linear hyperbolic systems, and Lax-Friedrich flux. Riemann solvers for Low Mach flows. Numerical flux accurate for steady and unsteady computations.
- **Boundary conditions** Periodic boundary conditions, time-dependent inlet and outlet boundary conditions. Adiabatic wall and isothermal wall. Steger-Warming based boundary condition.
- **Parallel computing** Mesh redistribution, computation of Overlap with PaMPA. Collective asynchronous communications (PaMPA based). Asynchronous point to point communications. Tests on the cluster Avakas from MCIA, and on Mésocentre de Marseille, and PlaFRIM. Tier-1 Turing (Blue-Gene).
- **C++/Fortran interface** Tests for binding fortran with C++.
- **Instrumentation** Aerosol can give some traces on memory consumption/problems with an interfacing with the PAPI library. Tests have also been performed with VTUNE and TAU. Tests with Maqao and Scalasca (VIHPS workshop).
- **Validation** Poiseuille, Taylor-Green vortex. Laplace equation on a ring and Poiseuille flow on a ring. Implementation of volumic forcing based on wall dissipation.

In 2015, N. Pattakos was hired in the team Cardamom, in order to improve the code architecture and for easing the installation of the library. The following features were added or improved:

- **Development environment** The use of CMake was strongly improved, which induced also easier test launching. Documentation, code cleaning and refactorization have also been led. The shared project of Plafrim was updated, and so was the joint Aerosol/Scotch/PaMPA project on the continuous integration platform. Integration of SPack for handling dependencies has begun. Interface with ESSL was fixed.
- **Multigrid** Development of p -multigrid methods. This includes also the possibility of beginning a computation with an order and to decrease or increase the order of approximation when restarting. For the p multigrid methods, V and W cycle have been developed, and restriction and prolongation operators have also been developed. Implementation of h -multigrid has started, with the development of tests of the aggregation methods of PaMPA, and the definition of finite element basis on arbitrary cells.
- **Boundary conditions** Development of the Synthetic Eddy Method boundary condition.
- **Models** Linearized Euler equations, and Sutherland model for non isothermal diffusive flows. Shallow-water model.
- **Parallel computing** Weighted load balancing for hybrid meshes.
- **Validation** Turbulent channel flow.
- **Postprocessing** Development of high order projections over line postprocessing, possibility of stocking averaged data, such as the average flow and the Reynolds stresses.

6.2. Cut-ANOVA

Participants: Pietro Marco Congedo, Kunkun Tang [Corresponding member].

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

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

6.3. Sparse-PDD

Participants: Pietro Marco Congedo, Kunkun Tang [Corresponding member].

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

6.4. RobUQ

Participants: Pietro Marco Congedo [Corresponding member], Maria Giovanna Rodio, Kunkun Tang.

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 UF0.

6.5. ORComp

Participants: Pietro Marco Congedo [Corresponding member], Nassim Razaaly, Maria-Giovanna Rodio.

The ORComp platform is a simulation tool permitting to design an ORC cycle. Starting from the solar radiation, this platform 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 fluidbox code 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.

6.6. sDEM

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

The sDEM platform is a simulation tool permitting to simulate multiphase flows with transition modelling. In particular, the code relies on the formulation of a DEM method, the use of a complex thermodynamics, the possibility to model cavitating phenomena. Moreover, the method has been generalized in order to take into account directly uncertainty, thus proposing the so-called Stochastic DEM (sDEM) method. This is one of the first stochastic semi-intrusive scheme, permitting to consider uncertainties in multiphase flows including heat and mass transfer terms. This software is developed together with the University of Zurich.

6.7. SLOWS

Participants: Luca Arpaia, Andrea Filippini, Maria Kazolea, Mario Ricchiuto [Corresponding member].

SLOWS is a C-platform allowing the simulation of free surface shallow water flows with friction. It can be used to simulate near shore hydrodynamics, wave transformations processes, etc. Both hydrostatic (shallow water) and non-hydrostatic (Boussinesq-type) versions exist. The latter are currently based on the dispersive model of Madsen and Sorensen (1992). A fully nonlinear (Green-Naghdi) version is under development based on the one dimensional prototype discussed in [99]. Three different approaches are available, based on conditionally depth-positivity preserving implicit schemes, or on conditionally depth-positivity preserving genuinely explicit discretizations, or on an unconditionally depth-positivity preserving space-time approach. Newton and frozen Newton loops are used to solve the implicit nonlinear equations. The linear algebraic systems arising in the discretization are solved with the MUMPS library. This year implicit and explicit (extrapolated) multistep higher order time integration methods have been implemented, and a mesh adaptation technique based on mesh deformation (r -adaptation) has been also included. A node-centred high order MUSCL finite volume discretisation has also been added to benchmark the mesh adaptation strategies, and compare with the residual based method constituting the kernel of the code. To date, SLOWS is the only existing near shore code allowing to choose between a classical finite volume approximation, and the more recent non-linear residual distribution methods developed in CARDAMOM. It allows an accurate simulation of free surface flows on arbitrary topographies with both static and time dependent unstructured mesh adaptation, accounting for both hydrostatic and non-hydrostatic effects.

6.8. TUCWave

Participant: Maria Kazolea [Corresponding member].

TUCWave, developed within the PhD of M. Kazolea, is a high-order well-balanced unstructured finite volume (FV) solver for weakly nonlinear and weakly dispersive water waves over varying bathymetries, as described by the 2D depth-integrated extended Boussinesq equations of Nwogu (1993). The FV scheme numerically solves the conservative form of the equations following the median dual node-centered approach, for both the advective and dispersive part of the equations. The code uses an efficient edge based structure. For the advective fluxes Roe's approximate Riemann solver is used along with a well-balanced treatment of the topography source. Higher order accuracy is achieved through a MUSCL-type reconstruction technique, and via a strong stability preserving explicit Runge-Kutta time stepping. The numerical techniques implemented in TUCWave are being imported in SLOWS.

6.9. Realfluids

Participants: Héloïse Beaugendre [Corresponding member], Pietro Marco Congedo, Andrea Cortesi, Léo Nouveau, Quentin Viville.

RealFluids (developed in the BACCHUS team) solves compressible viscous turbulent flow equations, with real-gas effects and arbitrarily complex equations of state, with the most recent residual distribution schemes. It is currently used for simulating turbines in ORC optimization, and for the immersed boundary simulations for de-anti icing applications. It is being coupled to the Mutation library to be able to perform some CFD simulations of low-altitude re-entry flows.

6.10. FMG

Participants: Luca Arpaia, Cécile Dobrzynski [Corresponding member], Andrea Cortesi, Léo Nouveau, Mario Ricchiuto.

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

6.11. MMG platform

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

MMG is an open source software for surface and volume remeshing. It provides three applications : 1) mmg2d: generation of a triangular mesh , adaptation and optimization of a triangular mesh 2) mmgs: adaptation and optimization of a surface triangulation representing a piecewise linear approximation of an underlying surface geometry 3) mmg3d: adaptation and optimization of a tetrahedral mesh and implicit domain meshing

URL : <http://www.mmgtools.org>

6.12. Nomesh

Participants: Cécile Dobrzynski [Corresponding member], Ghina El Jannoun.

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.

7. New Results

7.1. High order discretizations on unstructured meshes

Participants: Héloïse Beaugendre [Corresponding member], Cécile Dobrzynski, Léo Nouveau, Mario Ricchiuto, Quentin Viville.

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

- We have extended the team's previous work on the consistent residual based approximation of viscous flow equations to the framework of Immersed Boundary Methods (IBM). This is an increasingly popular approach in Computational Fluid Dynamics as it simplifies the mesh generation problem. In our work, we consider a technique based on the addition of a penalty term to the Navier-Stokes equations to account for the wall boundary conditions. To adapt the residual distribution method to the IBM, we developed a new formulation based on a Strang splitting approach in time. This approach, couples in a fully consistent manner an implicit asymptotically exact integration procedure of the penalization ODE, with the explicit residual distribution discretization for the Navier-Stokes equations, based on the method proposed in (Ricchiuto and Abgrall, *J.Comput.Phys* 229, 2010). The ODE integrator provides an operator which is exact up to orders η^2 , with η the penalty parameter assuming values of the order of 10^{-10} . To preserve the accuracy of the spatial discretization in the Navier-Stokes step, we have introduced, in vicinity of the penalised region, a modification of the solution gradient reconstruction required for the evaluation of the viscous fluxes. We have shown formally and numerically that the approach proposed is second order accurate for smooth solutions, and shown its potential when combined with unstructured mesh adaptation strategies w.r.t. the (implicitly described) solid walls. This work has been accepted on *Comp.Meth.Appl.Mech.Eng.* ;
- Another research axis consists in proposing a novel approach that allows to use p-adaptation with continuous finite elements. Under certain conditions, primarily the use of a residual distribution scheme, it is possible to avoid the continuity constraint imposed to the approximate solution, while still retaining the advantages of a method using continuous finite elements. The theoretical material, the complete numerical method and practical results show as a proof of concept that p-adaptation is possible with continuous finite elements. Its extension to penalized Navier-Stokes equations are under progress ;

- We have continued the study of the properties of residual based methods in the time dependent case. We have been able to further characterize one of the variants of the approach proposed in (Ricchiuto and Abgrall, *J.Comput.Phys* 229, 2010) in terms of preservation of the positivity of the density showing this property in practical applications involving the shallow water equations [130]. The impact of the simplified construction leading to these schemes has also been investigated. In particular, we have shown that despite the additional complexity associated to the inversion of the mass matrix, non-linear methods providing monotone solution and yet featuring linear mass matrices can be constructed [142]. These methods, have been shown to have some potential w.r.t. fully diagonal approaches as those used in (Ricchiuto and Abgrall, *J.Comput.Phys* 229, 2010), in terms of error as function of CPU time : the non-diagonal schemes showing error reductions up to one order of magnitude. Current work is devoted to the use of other multistage (defect correction type) and multistep (extrapolated methods) techniques, comparing them to space time approaches.

7.2. Modelling of free surface flows

Participants: Luca Arpaia, Stevan Bellec, Mathieu Colin, Sebastien de Brye, Andrea Filippini, Maria Kazolea, Mario Ricchiuto [Corresponding member].

We have introduced a new systematic method to obtain discrete numerical models for incompressible free-surface flows. The method consists in first discretizing the Euler equations with respect to the horizontal variables, keeping the vertical z variable and time continuous. We have focused so far on (continuous) Galerkin finite element discretizations in the horizontal. We then perform an asymptotic analysis on the resulting semi-discrete system. Our initial result, has led to a new discrete approximation, which we have shown to be consistent with the Boussinesq system known as Peregrine model. We have proven that the method obtained by means of this discrete asymptotic method, has phase and linear shoaling errors far lower than those obtained by discretizing the continuous model directly by means of the Galerkin method. Extensions to other weakly non-linear models have been obtained, and the study of fully nonlinear variants is under way.

We have also investigated the relations between some of the most common weakly nonlinear Boussinesq models. It is known since many years that, for given phase linear shoaling relations, two families of models exist depending on whether the dispersive terms are evaluated using derivatives of the speed, or of the flux (depth times speed). We have shown both analytically and numerically, that, independently on the phase and linear shoaling relations, these two families provide (quantitatively *and* qualitatively) only two distinct behaviours when approaching the nonlinear regime. Models based on velocity derivatives, provide taller more asymmetric waves, all models of the same family produce stunningly similar results, even when the linear relations differ considerably.

To extend our initial work on unstructured solvers for dispersive wave models to the fully nonlinear case we have proposed a new framework to approximate the so-called Green-Naghdi equations [99]. The method proposed, while remaining unsplit in time, is based on a separation of the elliptic and hyperbolic components of the equations. This separation is designed to recover the standard shallow water equations in the hyperbolic step, so that the method can be written as an *algebraic* correction to an existing shallow water code. In particular, in our approach we fix the method used for the elliptic component (a continuous Galerkin method), and couple it to different hyperbolic shallow water solvers. As long as the hyperbolic step is more than second order accurate, the approach proposed allows accuracies comparable to those of a fourth order finite difference method, with a natural potential for h and p - adaptation on unstructured grids. The two-dimensional extension is in the testing phase.

The tools developed have been also used intensively in funded research programs. Within the TANDEM project, several benchmarks relevant to tsunami modelling have been performed and several common publications with the project partners are in preparation. Independently on this activity, this year we used our codes to investigate two case studies. The first is the study of the wave conditions for the old Venetian harbour of Chania in Crete [109]. The study compares fully nonlinear-weakly dispersive COULWAVE code, developed at the University of South California, and TUCWave. The models are used to explore the appearance of resonance, eventually determining the resonant frequencies for the entire basin. The second study concerns the

conditions for tidal bore formation in convergent alluvial estuaries [69]. A new set of dimensionless parameters has been introduced to describe the problem, and the code SLOWS has been used to explore the space of these parameters allowing to determine a critical curve allowing to characterize an estuary as "bore forming" or not. Surprising physical behaviours, in terms of dissipation and nonlinearity of the tides, have been highlighted. Part of this work has been accepted on *Estuarine, Coastal and Shelf Science*, with a manuscript on the numerical aspects in review on *Ocean Modelling*.

7.3. Wave energy conversion hydrodynamics

Participants: Umberto Bosi, Mario Ricchiuto [Corresponding member].

We have developed a prototype spectral element solver for a coupled set of differential equations modelling wave propagation (so-called outer domain), and the submerged flow under a floating body (inner domain). Both systems of equations are depth-averaged (Boussinesq type) systems involving some dispersive terms. They are further coupled to a force balance providing a (system of) ODE(s) for the floater. This model constitutes an intermediate fidelity approximation for the hydrodynamics of a wave energy converter. Differently from all industrial state of the art, it is a (fully) nonlinear model. However, its cost is extremely low when compared to full three-dimensional CFD analyses, due to the dimensional reduction brought from the depth averaged modelling. This year we have shown the potential of this Boussinesq-type model to predict the hydrodynamics of a floater in a simplified case [97], [98] (journal version to appear on *J. Ocean Eng. and Marine Energy*). This result paves the way to the construction of new medium fidelity models to be used in the optimization of converters. This will be achieved in the framework of the MIDWEST project funded this year under the EU OCEANERanet call.

7.4. Two-phase flow numerical simulation with real-gas effects and occurrence of rarefaction shock waves

Participants: Maria Giovanna Rodio, Pietro Marco Congedo [Corresponding member].

We have studied the prediction in numerical simulation of turbulent cavitating flows, which could be strongly influenced by the presence of several empirical coefficients. The aim of this work is to explore the interaction between the cavitation model and turbulence in terms of uncertainty propagation through an unsteady numerical solver, for assessing the robustness and the accuracy of the physical models at different times. Furthermore, the influence of experimental data in the setting of some turbulence and cavitation model coefficients is investigated by means of a Bayesian approach. Finally, the interest is to provide some innovative insights for improving the understanding of these models for cavitating flows.

7.5. Formulation of stochastic methods for CFD

Participants: Maria Giovanna Rodio, Pietro Marco Congedo [Corresponding member].

We have worked on the extension of the Truncate and Encode (TE) approach, previously proposed by some of the authors (Abgrall et al. in *J Comput Phys* 257:19?56, 2014. doi:10.1016/j.jcp.2013.08.006), for taking into account uncertainty in partial differential equations (PDEs). Innovative ingredients are given by an algorithm permitting to recover the multiresolution representation without requiring the fully resolved solution, the possibility to treat a whatever form of pdf and the use of high-order (even non-linear, i.e. data-dependent) reconstruction in the stochastic space. Moreover, the spatial-TE method is introduced, which is a weakly intrusive scheme for uncertainty quantification (UQ), that couples the physical and stochastic spaces by minimizing the computational cost for PDEs. The proposed scheme is particularly attractive when treating moving discontinuities (such as shock waves in compressible flows), even if they appear during the simulations as it is common in unsteady aerodynamics applications. The proposed method is very flexible since it can easily be coupled with different deterministic schemes, even with high-resolution features. Flexibility and performances of the present method are demonstrated on various numerical test cases (algebraic functions and ordinary differential equations), including partial differential equations, both linear and non-linear, in presence of randomness. The efficiency of the proposed strategy for solving stochastic linear advection and Burgers equation is shown by comparison with some classical techniques for UQ, namely Monte Carlo or the non-intrusive polynomial chaos methods.

A new scheme for the numerical approximation of a five-equation model taking into account Uncertainty Quantification (UQ) is also presented. In particular, the Discrete Equation Method (DEM) for the discretization of the five-equation model is modified for including a formulation based on the adaptive Semi-Intrusive (aSI) scheme, thus yielding a new intrusive scheme (sDEM) for simulating stochastic two-phase flows. Some reference test-cases are performed in order to demonstrate the convergence properties and the efficiency of the overall scheme. The propagation of initial conditions uncertainties is evaluated in terms of mean and variance of several thermodynamic properties of the two phases.

7.6. Sensitivity analysis, metamodelling, and and robust optimization

Participants: Kunkun Tang, Francesca Fusi, Pietro Marco Congedo [Corresponding member].

We have worked on two different formulations for sensitivity analysis. Moreover, we have proposed a new metamodelling technique and an innovative method for performing robust optimization.

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

A sensitivity analysis method is extended in order to compute third and fourth-order statistic moments, i.e. skewness and kurtosis, respectively. It is shown that this decomposition is correlated to a Polynomial Chaos (PC) expansion, permitting to easily compute each term. Then, new sensitivity indexes are proposed basing on the computation of skewness and kurtosis. PC-based numerical technique is used in order to compute the convergence of the sensitivity indexes according to the polynomial order by using the exact solution as the reference one. The interest of the proposed analysis is first depicted by considering several test-functions. In particular, a functional decomposition based on variance, skewness and kurtosis is computed, displaying how sensitivity indexes vary according to the order of the statistical moment. Then, the problem of how reducing the complexity of a stochastic problem is treated by proposing two strategies: i) the reduction of the number of dimensions, the reduction of the order of interaction. In both cases, the impact on the statistics of the reduced function is then assessed. Feasibility of the proposed analysis in a real-case is then demonstrated by presenting a stochastic study about the uncertainty propagation in a challenging engineering simulation: the numerical prediction of a turbine cascade in an Organic Rankine Cycles (ORCs), with the use of complex thermodynamic models and the presence of multiple sources of uncertainty. Basing on high-order statistics decomposition and physical remarks, it is shown how the analysis proposed in this work can help to drive the design process in a real-engineering problem.

For the metamodelling technique, a polynomial dimensional decomposition (PDD) method is proposed for the global sensitivity analysis and uncertainty quantification (UQ) of stochastic systems subject to a moderate to large number of input random variables. Due to the intimate structure between the PDD and the Analysis of Variance (ANOVA) approach, PDD is able to provide a simpler and more direct evaluation of the Sobol' sensitivity indices, when compared to the Polynomial Chaos expansion (PC). Unfortunately, the number

of PDD terms grows exponentially with respect to the size of the input random vector, which makes the computational cost of standard methods unaffordable for real engineering applications. In order to address the problem of the curse of dimensionality, this work proposes essentially variance-based adaptive strategies aiming to build a cheap meta-model (i.e. surrogate model) by employing the sparse PDD approach with its coefficients computed by regression. Three levels of adaptivity are carried out in this paper: 1) the truncated dimensionality for ANOVA component functions, 2) the active dimension technique especially for second- and higher-order parameter interactions, and 3) the stepwise regression approach designed to retain only the most influential polynomials in the PDD expansion. During this adaptive procedure featuring stepwise regressions, the surrogate model representation keeps containing few terms, so that the cost to resolve repeatedly the linear systems of the least-squares regression problem is negligible. The size of the finally obtained sparse PDD representation is much smaller than the one of the full expansion, since only significant terms are eventually retained. Consequently, a much less number of calls to the deterministic model is required to compute the final PDD coefficients.

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

7.7. High order mesh generation and mesh adaptation

Participants: Luca Arpaia, Cécile Dobrzynski [Corresponding member], Ghina El Jannoun, Mario Ricchiuto.

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

- We have enhanced our work on r -adaptation techniques for time dependent equations. These techniques are based on mesh deformations obtained by solving continuous differential equations for the local displacements. These equations are controlled by an error monitor. Several improvements have been made. We have studied in depth the formulation of the coupling of the mesh movement with the flow solver. We have found that for both finite volume and residual distribution methods, a coupling of mesh and solution evolution (by means of an ALE method) provides accuracy enhancements, and is to be preferred to a simpler adapt-project-evolve approach. The method has been fully tested in two space dimensions. The adaptation library has been extended to three dimensions, and benchmarking is under way. We have improved the definition of the error monitor, and we are now able to prescribe directly the local mesh size. For problems with source terms, and in particular problems admitting some important physical invariants as the shallow water equations, we have solved the conflict between the conservation of either mass or the invariant, allowing for the conservation of both quantities up to machine accuracy;
- We upgrade our technique for generating high order curved meshes: starting from a straight mesh with a curved boundary, a new smoothing and untangling approach is proposed to ensure a final

valid mesh. The untangling algorithm is a hybrid technique that gathers a local mesh optimization applied on the surface of the domain and a linear elasticity analogy applied in its volume. On the one hand, the local topological optimization consists in simultaneously relocating the vertices and control points of a local patch around the invalid element in order to optimize the quality and validity of the elements inside the patch. The elements' validity problem is formulated as an unconstrained optimization problem using a log-barriers that is solved progressively using the conjugate gradient method. On the other hand, the linear elasticity analogy permits the propagation of the curvature to the volume of the domain hence untangling volume mesh elements.

7.8. Virtual self-healing composite for aeronautic propulsion

Participants: Mathieu Colin [Corresponding member], Xi Lin, Gregory Perrot, Mario Ricchiuto.

As a composite material having excellent properties, Ceramic-matrix composites (CMCs) comprise a ceramic matrix reinforced by a refractory fiber such as silicon carbide fiber. Due to the self-healing process (which consists in filling cracks produced by oxydation by an oxide formed in-situ), CMCs have extremely long lifetimes even under severe mechanical and chemical solicitations. These time spans make most full-scale experimental investigations impractical : laboratory tests have necessarily to be replaced by predictions based on numerical models. Initial results have already been obtained by in the past with simplified crack averaged models based on simple potential approximations of the flow field of the oxide. In this direction, Xi Lin has developed new asymptotic models by creating a hierarchy inside two different families : the Saint-Venant equations and the thin film equations. The hierarchy is based on the use of several different boundary conditions. The main goal is to obtain more accurate hydrodynamic models accounting for surface tension and viscous effects which may be very important for the oxide evolution.

In parallel, we have made great progress in the coupling of the chemistry module with the structural mechanics solver of the LCTS laboratory in Bordeaux. The first fully coupled simulations of a fatigue test for a so-called mini-composite (on single fibre tow). The simulations have allowed to reproduce the gradual breaking mechanism typical of these materials, allowing to reproduce numerically the delayed rupture observed in practice.

7.9. Numerical simulation of the liquid ablation

Participants: Gérard Gallice, Luc Mieussens [Corresponding member], Simon Peluchon.

During the atmospheric re-entry phase, a space vehicle undergoes a heating due to the friction of the atmospheric gases. Conversion of kinetic energy to thermal energy leads to a sudden increase of the temperature of the solid boundary. This leads to a physical-chemical degradation of the thermal protective system, and to a boundary recession. For some materials, this recession occurs with a melting of the materials into a fluid phase. The numerical simulation of this phenomenon requires to take into account a two-phase flow with a compressible gaz (the air flow) and a weakly compressible liquid (the melted material). Numerically, this problem is strongly stiff.

We have proposed a splitting strategy to simulate compressible two-phase flows using the five equation model. The main idea of the splitting is to separate the acoustic and transport phenomena. The acoustic step is solved in Lagrangian coordinates by using a scheme based on an approximate Riemann solver. On the one hand, since the acoustic time step driven by the fast sound velocity is very restrictive, an implicit treatment of the Lagrangian step is performed. On the other hand, we use an explicit scheme for the transport step driven by the slow material waves. The global scheme resulting from this splitting operator strategy is conservative, positive, and preserves contact discontinuities. Numerical simulations of compressible diphasic flows are presented on 2d-structured grids. The implicit-explicit strategy allows large time steps, which do not depend on the fast acoustic waves.

7.10. Boundary conditions for the Navier-Stokes equations in the transitional regime

Participants: Céline Baranger, Pietro Marco Congedo, Giorgio Martalo, Julien Mathiaud, Luc Mieussens [Corresponding member].

In reentry flows at high altitude, the parietal fluxes along the boundary of a space vehicle are computed by solving the Boltzmann equation of the gas kinetic theory. It depends on the way particles are reflected by the solid wall. In this kind of applications, the reflection is usually supposed to be 80% diffuse (the particles are re-emitted in a random direction in thermal equilibrium with the wall), and 20% specular.

In lower altitude, it is possible to use the compressible Navier-Stokes equations, but the standard boundary conditions do not take into account the specular part. These equations are hence not very accurate in the transition regime (in which the Knudsen number is around 0.01).

By using an asymptotic boundary layer analysis, we have derived boundary conditions for the compressible Navier-Stokes equations that formally make the fluid model a second order approximation of the Boltzmann equation of the kinetic gas theory (with respect to the Knudsen number), and that can take into account the effect of the specular reflections. These boundary conditions include a slip velocity at the wall and a temperature jump, with some coefficients that depend on some auxiliary half-space problems. An existing numerical method has been extended to solve these problems and give numerical values for these coefficients. This makes our boundary conditions practically usable into any Navier-Stokes code.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

Participant: Pietro Marco Congedo [Corresponding member].

Several contracts have been realized:

- SAFRAN-HERAKLES, 20Keuros for the in-situ evaluation of the Cut-ANOVA and RobUQ codes.
- EXOES, 8 KEuros, for the analysis of the performances of the EVE engine, produced by EXOES.
- CNES, 15 KEuros, for the robust analysis of the DEBRISK code.

9. Partnerships and Cooperations

9.1. Regional Initiatives

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

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

Coordinator: M. Ricchiuto

Other partners: UMR EPOC (P. Bonneton)

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

9.2. National Initiatives

9.2.1. ANR MAIDESC

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

Type: ANR

Duration: 48 months

Starting date : 1st Oct 2013

Coordinator: Dervieux Alain (Inria Sophia)

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

9.2.2. PIA TANDEM

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

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

Duration: 48 months

Starting date : 1st Jan 2014

Coordinator: H. Hebert (CEA)

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

9.2.3. 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.

9.2.4. APP Bordeaux 1

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

Type : Project Bordeaux 1

Duration : 36 months

Starting : September 2014

Coordinator : M. Colin

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

9.3. European Initiatives

9.3.1. FP7 & H2020 Projects

9.3.1.1. 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), TECHSPACE AERO SA (BE)

Inria contact: Héloïse Beaugendre

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

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

9.3.2. Collaborations in European Programs, except FP7 & H2020

Program: OCEANEraNET

Project acronym: MIDWEST

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

Duration: December 2015 - December 2018

Coordinator: Mario Ricchiuto

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

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

9.4. International Initiatives

9.4.1. Inria International Labs

Inria@SiliconValley

Associate Team involved in the International Lab:

9.4.1.1. AQUARIUS2

Title: Advanced methods for uncertainty quantification in compressible flows

International Partner (Institution - Laboratory - Researcher):

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

Start year: 2014

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

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

9.4.1.2. AMoSS

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

International Partner (Institution - Laboratory - Researcher):

Inria Sophia-Antipolis and University of Nice (France)

Inria Bordeaux and University of Bordeaux (France)

University of Marseille (France)

National Cheng Kung University, Tainan, Taiwan

National Taiwan University and Academia Sinica, Taipei, Taiwan

Duration: 2014 - 2016

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

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

9.4.1.3. Informal International Partners

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

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

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

University of Nottingham, Department of Mathematics : Dr. M.E. Hubbard. 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

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

9.5. International Research Visitors

9.5.1. Visits of International Scientists

From april 2015 (up to april 2016), Tatsuya Watanabe (Department of Mathematics, Faculty of Science, Kyoto Sangyo University Motoyama, Kamigamo, Kita-Ku, Kyoto-City 603-8555, Japan) comes to visit Mathieu Colin. During his stay, T. Watanabe is funded by a JSPS-grant.

From 09/04/2015 to 24/04/2015 F. Morency () has visited us to work with H. Beaugendre on the construction of penalization methods for the analysis of de-anti icing systems.

From 01/06/2015 to 08/06/2015, T. Magin (von Karman Institute for Fluid Dynamics) has visited us to work with P.M. Congedo on the robust analysis of Reentry flows.

From 01/07/2015 to 28/07/2015 Prof. A. Kurganov (Tulane University, New Orleans) has visited us to work with M. Ricchiuto on semi-implicit time integration methods and adaptive mesh deformation techniques.

9.5.2. Visits to International Teams

In May 2015, P.M. Congedo visited the Uncertainty Quantification Laboratory in Stanford University. Andrea Cortesi visited NASA-Ames (California) in November-December 2015.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific events organisation

In collaboration with J.-C. Saut, Mathieu Colin has organized the workshop "Quasilinear and nonlocal nonlinear Schrödinger equations" at the Pauli institute, Vienna. (sept. 28th 2015-oct. 2nd 2015).

Pietro Marco Congedo and Luc Mieussens have contributed to the organisation of the Workshop "Modèles et Méthodes Cinétiques pour la Dynamique des Gaz Raréfiés", Octobre 2015, Bordeaux (with Céline Baranger and Julien Mathiaud).

10.1.1.1. Member of the conference program committees

In collaboration with H. Kalisch (University of Bergen), Mathieu Colin has organized the session "Fully nonlinear Boussinesq models: Theory and practice" to the Ninth IMACS International Conference on Nonlinear Evolution Equation and Wave phenomena : Computation and Theory (April 01-05 2015).

In collaboration with A.-P. Engsig-Karup (DTU Compute), and C. Eskilsson (Chalmers University), Mario Ricchiuto has organized the session "Hydrodynamic modelling of wave energy converters" at the 2nd Frontiers in Computational Physics Conference: Energy Sciences, 3-5 June 2015, Zurich, Switzerland

In collaboration with E. Miglio (MOX Politecnico di Milano), Mario Ricchiuto has organized the session "Robust and Multi Scale Models for Water Wave Propagation" at the 2015 SIAM Conference on Mathematical and Computational Issues in the Geosciences, Stanford, June 29-July 2, 2015

10.1.1.2. Member of the editorial boards

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

Mario Ricchiuto is member of the editorial board of *Computers & Fluids*, Elsevier.

10.1.1.3. Reviewer - Reviewing activities

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

10.1.2. Invited talks

- 13th US National Congress on Computational Mechanics: H. Beaugendre *et al.*, Unsteady residual distribution schemes adapted to immersed boundary methods on unstructured grids to account for moving bodies, San Diego, CA, July 26-30, 2015.
- Pietro Marco Congedo has been invited as Speaker in three Lectures at the VKI lecture Series 38th Advanced Computational Fluid Dynamics. Adjoint methods and their application in Computational Fluid Dynamics, 2015, Von Karman Institute.
- P.M. Congedo, A phase transition model and scheme for reproducing cavitation, Workshop TOTAL MATHIAS, October 2015, Paris.
- Mario Ricchiuto, Simple conservative Simple and conservative mesh adaptation for shallow water flows, Oberwolfach workshop on “Recent Developments in the Numerics of Nonlinear Hyperbolic Conservation Laws”, Oberwolfach (Germany), September 2015
- Luc Mieussens, SIAM conference on Computational Science & Engineering, 2015, Salt Lake City (Utah, USA)
- Luc Mieussens, Workshop “Kinetic and Related Equations”, 2015, Oaxaca (Mexico), July 2015
- Luc Mieussens, Numerical Simulation of the Crookes Radiometer, 2nd European Conference on Non-equilibrium Gas Flows, University of Technology of Eindhoven (Netherlands), December 2015

10.1.3. Leadership within the scientific community

- As of January 2015, Luc Mieussens is member of the scientific board of CEA ;
- Pietro Marco Congedo is part of the scientific committee of the ARA (Association pour la rentrée atmosphérique) Association;
- Mario Ricchiuto is member of the Industrial CFD committee of the Aristote association ;

10.1.4. Scientific expertise

H. Beaugendre: ANR expertise (programme accompagnement spécifique des travaux de recherches et d’innovation defense).

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

Licence : Mathieu Colin, Analyse Fonctionnelle et Intégration, 54 h, L3, ENSEIRB-MATMÉCA, FRANCE

Licence : Mathieu Colin, TER 32h, L3, ENSEIRB-MATMÉCA, FRANCE

Licence : Mathieu Colin, Analyse, L1, Formation alternée INP, FRANCE

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

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

Licence : Cécile Dobrzynski, Analyse numérique, 24h, L3, ENSEIRB-MATMÉCA, FRANCE

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

Master : Héloïse Beaugendre, Responsable de filière de 3ème année, 15h, M2, ENSEIRB-MATMÉCA, France

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

Master : Héloïse Beaugendre, Encadrement de projets de la filière Calcul Haute Performance, 15h, M2, ENSEIRB-MATMÉCA, France

Master : Héloïse Beaugendre, Calcul Haute Performance et décomposition de domaine, 39h, M2, ENSEIRB-MATMÉCA et Université Bordeaux, France

Master : Héloïse Beaugendre, Projet fin d'études, 4h, M2, ENSEIRB-MATMÉCA, FRANCE

Master : Mathieu Colin, PDE, 30 H, M1, ENSEIRB-MATMÉCA, FRANCE

Master : Mathieu Colin, EDP approfondies, 36 h, M2, Université de Bordeaux, FRANCE

Master : Mathieu Colin, TER, 12h, M1, ENSEIRB-MATMÉCA, FRANCE

Master : Mathieu Colin, Projet fin d'études, 6h, M2, ENSEIRB-MATMÉCA, FRANCE

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

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

Master : Cécile Dobrzynski, TER, 16h, M1, ENSEIRB-MATMÉCA, FRANCE

Master : Cécile Dobrzynski, Théorie du maillage, 12h, M2, formation Structures Composites, ENSCBP, FRANCE

Master : Cécile Dobrzynski, Techniques de maillages, 36h, M2, ENSEIRB-MATMÉCA, FRANCE

Post-graduate: Mario Ricchiuto, 12h, Computational Methods for Compressible Flows, Research Master, von Karman Institute for Fluid Dynamics, BELGIUM

10.2.2. Supervision

PhD in progress : Arpaia Luca, Continuous mesh deformation and coupling with uncertainty quantification for coastal inundation problems, started in March 2014.

PhD in progress : Bosi, Umberto, ALE spectral element Boussinesq modelling of wave energy converters, started in November 2015

PhD in progress : Bellec Stevan, Discrete asymptotic modelling of free surface flows, October 2013.

PhD in progress : Cortesi Andrea, Predictive numerical simulation for rebuilding freestream conditions in atmospheric entry flows, started in October 2014.

PhD in progress : Filippini Andrea, Nonlinear finite element Boussinesq modelling of non-hydrostatic free surface flows, started in February 2014.

PhD in progress: Fusi Francesca, Stochastic robust optimization of a helicopter rotor airfoil, started in October 2013.

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

PhD in progress : Nouveau Léo, Adaptation de maillage non structurés anisotropes pour les méthodes de pénalisation en mécanique des fluides compressibles, started in Oct 2013.

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

PhD in progress : Peluchon Simon, Approximation numérique et modélisation de l'ablation différentielle de deux matériaux: application à l'ablation liquide. Started in December 2014.

PhD in progress : Viville Quentin, Etude sur les méthodes de pénalisation adaptées aux maillages non-structurés fortement anisotropiques et utilisation de l'adaptation de maillage, started in Oct 2013.

10.2.3. Juries

PhD Jury:

- B. Monmarson, Institut National Polytechnique de Grenoble (P. Congedo, rapporteur).
- A. Resmini, UPMC, Paris (P. Congedo).
- L. Margheri, UPMC, Paris (P. Congedo).
- C. Mimeau, LJK, Grenoble (H. Beaugendre).
- R. Chauvin, ONERA ISAE SUPAERO, Toulouse (H. Beaugendre).
- G. Perrot, U. Bordeaux (M. Ricchiuto)

10.3. Popularization

- P.M. Congedo, "Houston, YOU have a problem !", Unithé ou café Seminar, Inria Bordeaux Sud-Ouest, Avril 2015.
- M. Ricchiuto has contributed to the organisation of the Solutions Cop21 ¹, and represented Inria representatives at the research stand on the opening day.

11. Bibliography

Publications of the year

Articles in International Peer-Reviewed Journals

- [1] R. ABGRALL, P. M. CONGEDO, G. GERACI, G. IACCARINO. *An adaptative multiresolution semi-intrusive for UQ in compressible fluid problems*, in "International Journal for Numerical Methods in Fluids", February 2015, 32 p. , <https://hal.inria.fr/hal-01120609>
- [2] L. ARPAIA, M. RICCHIUTO, R. ABGRALL. *An ALE Formulation for Explicit Runge–Kutta Residual Distribution*, in "Journal of Scientific Computing", 2015, forthcoming [DOI : 10.1007/s10915-014-9910-5], <https://hal.inria.fr/hal-01087936>
- [3] P. M. CONGEDO, R. ABGRALL, M. G. RODIO, G. GERACI. *Stochastic Discrete Equation Method (sDEM) for two-phase flows*, in "Journal of Computational Physics", June 2015, pp. 1-40, <https://hal.inria.fr/hal-01166094>
- [4] P. M. CONGEDO, G. GERACI, G. IACCARINO, R. ABGRALL. *High-order statistics in global sensitivity analysis: decomposition and model reduction*, in "Computer Methods in Applied Mechanics and Engineering", January 2016, <https://hal.inria.fr/hal-01247458>
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- [8] F. FUSI, P. M. CONGEDO. *An adaptive strategy on the error of the objective functions for uncertainty-based derivative-free optimization*, in "Journal of Computational Physics", February 2016, vol. 309, pp. 241–266 [DOI : 10.1016/J.JCP.2016.01.004], <https://hal.inria.fr/hal-01251604>
- [9] F. FUSI, A. GUARDONE, G. QUARANTA, P. M. CONGEDO. *Multi-fidelity physics-based method for robust optimization with application to a hovering rotor airfoil*, in "A.I.A.A. Journal", May 2015, 40 p. , <https://hal.inria.fr/hal-01152698>

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- [10] G. GERACI, P. M. CONGEDO, R. ABGRALL, G. IACCARINO. *A novel weakly-intrusive non-linear multiresolution framework for uncertainty quantification in hyperbolic partial differential equations*, in "Journal of Scientific Computing", June 2015, 34 p. , <https://hal.inria.fr/hal-01139813>
- [11] F. MORENCY, H. BEAUGENDRE. *Mathematical model for ice wall interactions within a level set method*, in "International Journal of Engineering Systems Modelling and Simulation", 2016, vol. 8, n^o 2, pp. 125-135, <https://hal.inria.fr/hal-01250169>
- [12] M. RICCHIUTO. *An explicit residual based approach for shallow water flows*, in "Journal of Computational Physics", 2015, vol. 280, n^o 1, pp. 306-344 [DOI : 10.1016/J.JCP.2014.09.027], <https://hal.inria.fr/hal-01087940>
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Invited Conferences

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- [18] P. M. CONGEDO. *Advanced methods for uncertainty quantification and application of adjoints*, in "38th Advanced Computational Fluid Dynamics. Adjoint methods and their application in Computational Fluid Dynamics, September 2015, von Karman Institute", Bruxelles, France, September 2015, <https://hal.inria.fr/hal-01257743>
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