Activity Report 2018

Project-Team CARDAMOM

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

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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 [116], [50]. 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 [57], [83]. 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 [60]. 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 [67], [78], [97], [50] or for wave energy conversion [76]), or parametric studies of complex environments (e.g. harbour dynamics [85], or estuarine hydrodynamics [49]), or hazard assessment and prevention [80]. 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 [120]. 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 [65], [109]. 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 [69]). This increases the amount of uncertainties associated to measurements and reduces the amount of information available to construct physical/PDE models. These uncertainties play also a crucial role when one wants to deal with numerical certification or optimization of a fluid based device. However, this makes the required number of flow simulations grow as high as hundreds or even thousands of times. The associated costs are usually prohibitive. So the real challenge is to be able to construct an accurate and computationally affordable numerical model handling efficiently uncertainties. In particular, this model should be able to take into account the variability due to uncertainties, those coming from the certification/optimization parameters as well as those coming from modelling choices.

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

2.3. Our approach

A standar way a certification study may be contacted can be described as two box modelling. The first box is the physical model itself, which is composed of the 3 main elements: PDE system, mesh generation/adaptation, and discretization of the PDE (numerical scheme). The second box is the main robust certification loop which contains separate boxes involving the evaluation of the physical model, the post-processing of the output, and the exploration of the spaces of physical and stochastic parameters (uncertainties). There are some known interactions taking place in the loop which are a necessary to exploit as much as possible the potential of high order methods [88] such as e.g. $h-/p-/r-$ adaptation in the physical model w.r.t. some post-processed output value, or w.r.t. some sort of adjoint sensitivity coming from the physical parameter evolution box, etc.

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

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

- What are the relations between PDE model accuracy (asymptotic error) and scheme accuracy, and how to control, en possibly exploit these relations to minimize the error for a given computational effort ;

- How to devise and implement adaptation techniques ($r-$, $h-$, and $p-$) for time dependent problems while guaranteeing an efficient time marching procedure (minimize CPU time at constant error) ;

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

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

- Aeronautics and aerospace engineering (de-anti icing systems, space re-entry) ;

- Energy engineering (organic Rankine cycles and wave energy conversion) ;

- Material engineering (self healing composite materials) ;

- Coastal engineering (coastal protection, hazard assessment etc.).

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

3. Research Program

3.1. Variational discrete asymptotic modelling

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

- comparing the asymptotic limits of discretized forms of the relevant scale resolving equations with the discretization of the analogous continuous asymptotic PDEs. Can we discretize a well understood system of PDEs instead of a less understood and more complex one ? ;

- study the asymptotic behaviour of error terms generated by coarse one-dimensional discretization in the direction of the "small scale". What is the influence of the number of cells along the vertical direction, and of their clustering ? ;

- derive equivalent continuous equations (modified equations) for anisotropic discretizations in which the direction is direction of the "small scale" is approximated with a small number of cells. What is the relation with known asymptotic PDE systems ?

Our objective is to gain sufficient control of the interaction between discretization and asymptotics to be able to replace the coupling of several complex PDE systems by adaptive strongly anisotrotropic finite 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 [91], [96] 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 [47] to hybrid meshes (prism/tetra).

For time dependent adaptation we will try to exploit as much as possible the use of $r-$adaptation techniques based on the solution of some PDE system for the mesh. We will work on enhancing the results of [3] by developing more robust nonlinear variants allowing to embed rapidly moving objects. For this the use of non-linear mesh PDEs (cf e.g. [106], [112], [61]), combined with Bezier type approximations for the mesh displacements to accommodate high order curved meshes [47], 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 [94], [99], [98] 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. [72], [118], [117] 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. [48], [81], [119], [70] 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 [3]. This balance is certainly dependent on the nature of the PDEs, on the accuracy level sought, on the cost of the scheme, and on the time stepping technique. All these elements will be taken into account to try to provide the most efficient formulation ;

- the conservation of volume, and the subsequent preservation of constant mass-momentum-energy states on deforming domains is one of the most primordial elements of Arbitrary Lagrangian-Eulerian formulations. For complex PDEs as the ones considered here, of especially for some applications, there may be a competition between the conservation of e.g. mass, an the conservation of other constant states, as important as mass. This is typically the case for free surface flows, in which mass preservation is in competitions with the preservation of constant free surface levels [3]. 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. [90]). The use of penalization will also provide a natural setting to compute immediate approximations of the forces on the immersed body [97], [100]. 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 [82], or on some iterative Defect Correction method (see e.g. [63]) ;

- 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 [77] in which we have shown how to use a standard continuous Galerkin method for the elliptic equation/variable representative of the dispersive effects, while the underlying hyperbolic system is evolved using a (discontinuous) third order finite volume method. This technique will be generalized to other classes of discontinuous methods, and similar ideas will be used in other context to provide a flexible approximation. Such mathods have clear advantages in multiphase flows but not only. A typical example where such mixed methods are beneficial are flows involving different species and tracer equations, which are typically better treated with a discontinuous approximation. Another example is the use of this mixed approximation to describe the topography with a high order continuous polynomial even in discontinuous method. This allows to greatly simplify the numerical treatment of the bathymetric source terms ;

- the enhancement of stabilized methods based on some continuous finite element approximation will remain a main topic. We will further pursue the study on the construction of simplified stabilization operators which do not involve any contributions to the mass matrix. We will in particular generalize our initial results to higher order spatial approximations using cubature points, or Bezier polynomials, or also hierarchical approximations. This will also be combined with time dependent variants of the reconstruction techniques initially proposed by D. Caraeni [62], allowing to have a more flexible approach similar to the so-called $P^n P^m$ method [75], [111]. 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 [79] ;

- 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 [59], as well as spatial partitioning techniques [87]. A major challenge will be to be able to guarantee sufficient locality to the time integration method to allow to efficiently treat highly refined meshes, especially for viscous reactive flows. Another challenge will be to embed these methods in the stabilized methods we will develop.

3.3. Coupled approximation/adaptation in parameter and physical space

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

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

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

To improve on the accuracy of the above methods, intrusive approaches will also be studied. To propagate uncertainties in stochastic differential equations, we will use Harten's multiresolution framework, following [46]. 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 [46], 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 [46] is conceived to be highly parallel due to the external cycle on the number of dimensions in the space of uncertain parameters. In principle, a number of parallel threads equal to the number of spatial cells could be employed. The scheme should be developed and tested for treating unsteady and discontinuous probability density function, and correlated random variables. Both the compression capabilities and the accuracy of the

scheme (in the stochastic space) should be enhanced with a high-order multidimensional conservative and non-oscillatory polynomial reconstruction (ENO/WENO).

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

3.4. Robust multi-fidelity modelling for optimization and certification

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

1. a robust strategy using the statistics evaluation will be applied separately, *i.e.* using only low or high-fidelity evaluations. Some classical optimization algorithms will be used in this case. Influence of high-order statistics and model reduction in the robust design optimization will be explored, also by further developing some low-cost methods for robust design optimization working on the so-called Simplex^2 method [68] ;

2. a multi-fidelity strategy by using in an efficient way low fidelity and high-fidelity estimators both in physical and stochastic space will be conceived, by using a Bayesian framework for taking into account model discrepancy and a PC expansion model for building a surrogate model ;

3. develop advanced methods for robust optimization. In particular, the Simplex^2 method will be modified for introducing a hierarchical refinement with the aim to reduce the number of stochastic samples according to a given design in an adaptive way.

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

4. Application Domains

4.1. De-anti icing systems

Impact of large ice debris on downstream aerodynamic surfaces and ingestion by aft mounted engines must be considered during the aircraft certification process. It is typically the result of ice accumulation on unprotected surfaces, ice accretions downstream of ice protected areas, or ice growth on surfaces due to delayed activation of ice protection systems (IPS) or IPS failure. This raises the need for accurate ice trajectory simulation tools to support pre-design, design and certification phases while improving cost efficiency. Present ice trajectory simulation tools have limited capabilities due to the lack of appropriate experimental aerodynamic force and moment data for ice fragments and the large number of variables that can affect the trajectories of ice particles in the aircraft flow field like the shape, size, mass, initial velocity, shedding location, etc... There are generally two types of model used to track shed ice pieces. The first type of model makes the assumption that ice

pieces do not significantly affect the flow. The second type of model intends to take into account ice pieces interacting with the flow. We are concerned with the second type of models, involving fully coupled time-accurate aerodynamic and flight mechanics simulations, and thus requiring the use of high efficiency adaptive tools, and possibly tools allowing to easily track moving objects in the flow. We will in particular pursue and enhance our initial work based on adaptive immerse boundary capturing of moving ice debris, whose movements are computed using basic mechanical laws.

In [51] 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 [45], [100]. In these methods we compensate for the error at solid walls introduced by the penalization by using anisotropic mesh adaptation [73], [89], [90]. 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 [53]. 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 [56], [50] 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 [104], 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 [121], state of the art techniques for freestream characterization rely on several approximations, such as e.g. using an equivalent calorically perfect gas formulas instead of taking into account the complex aero-thermo-chemical behaviour of the fluid. These techniques do not integrate measurement errors nor the heat flux contribution, for which a correct knowledge drives more complex models such as gas surface interaction. In this context, CFD supplied with UQ tools permits to take into account chemical effects and to include both measurement errors and epistemic uncertainties, e.g. those due to the fluid approximation, on the chemical model parameters in the bulk and at the wall (surface catalysis).

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

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

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

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

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

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

These modelling capabilities will be coupled to high order adaptive discretizations to provide high fidelity flow models. One of the most challenging problems is the minimization of the influence of mesh and scheme on the wall conditions on the re-entry module. To reduce this influence, we will investigate both high order adaptation across the bow shock, and possibly adaptation based on uncertainty quantification high order moments related to the heat flux estimation, or shock fitting techniques [54], [95]. 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 [103] for providing an estimation of the numerical errors/uncertainties. We will use some metamodels for solving the inverse problem, by considering all sources of uncertainty, including those on physical models. We will validate the framework sing the experimental data available in strong collaboration with the von Karman Institute for Fluid dynamics (VKI). In particular, data coming from the VKI Longshot facility will be used. We will show application of the developed numerical tool for the prediction in flight conditions.

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

4.3. Energy

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

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

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

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

The simulation of these gases requires accurate thermodynamic models, such as Span-Wagner or Peng-Robinson (see [66]). 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 [120], 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 [76], we will develop, analyse, compare, and use for multi-fidelity optimization,non-linear models of different scales (fidelity) ranging from simple linear hydrodynamics over asymptotic discrete nonlinear wave models, to non-hydrostatic anisoptropic Euler free surface solvers. We will not work on the development of small scale models (VOF-RANS or LES) but may use such models, developed by our collaborators, for validation purposes. These developments will benefit from all our methodological work on asymptotic modelling and high order discretizations. As shown in [76], asymptotic models foe WECs involve an equation for the pressure on the body inducing a PDE structure similar to that of incompressible flow equations. The study of appropriate stable and efficient high order approximations (coupling velocity-pressure, efficient time stepping) will be an important part of this activity. Moreover, the flow-floating body interaction formulation introduces time stepping issues similar to those encountered in fluid structure interaction problems, and require a clever handling of complex floater geometries based on adaptive and ALE techniques. For this application, the derivation of fully discrete asymptotics may actually simplify our task.

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

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

4.4. Materials engineering

Because of their high strength and low weight, ceramic-matrix composite materials (CMCs) are the focus of active research for aerospace and energy applications involving high temperatures, either military or civil. Though based on brittle ceramic components, these composites are not brittle due to the use of a fibre/matrix interphase that preserves the fibres from cracks appearing in the matrix. Recent developments aim at implementing also in civil aero engines a specific class of Ceramic Matrix Composite materials (CMCs) that show a self-healing behaviour. Self-healing consists in filling cracks appearing in the material with a dense fluid formed in-situ by oxidation of part of the matrix components. Self-healing (SH) CMCs are composed of a complex three-dimensional topology of woven fabrics containing fibre bundles immersed in a matrix coating of different phases. The oxide seal protects the fibres which are sensitive to oxidation, thus delaying failure. The obtained lifetimes reach hundreds of thousands of hours [108].

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

In collaboration wit the LCTS laboratory (a joint CNRS-CEA-SAFRAN-Bordeaux University lab devoted to the study of thermo-structural materials in Bordeaux), we are developing a multi-scale model in which a structural mechanics solver is coupled with a closure model for the crack physico chemistry. This model is obtained as a multi-dimensional asymptotic crack averaged approximation fo the transport equations (Fick's laws) with chemical reactions sources, plus a potential model for the flow of oxide [69], [74], [105]. We have demonstrated the potential of this model in showing the importance of taking into account the multi-dimensional topology of a fibre bundle (distribution of fibres) in the rupture mechanism. This means that the 0-dimensional model used in most of the studies (se e.g. [64]) 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 [86], [110], [102], [71], to hybrid methods coupling dispersive PDEs with hyperbolic ones, and trying to mimic wave breaking with travelling bores [114], [115], [113], [84], [77]. In both cases, numerical dissipation plays an important role and the activation or not of the breaking closure, as the quantitative contribution of numerical dissipation to the flow has not been properly investigated. These elements must be clarified to allow full control of adaptive techniques for the models used in this type of applications.

Another point we want to clarify is how to optimize the discretization of asymptotic PDE models. In particular, when adding mesh size(s) and time step, we are in presence of at least 3 (or even more) small parameters. The relations between physical ones have been more or less investigates, as have been the ones between purely numerical ones. We plan to study the impact of numerics on asymptotic PDE modelling by reverting the usual process and studying asymptotic limits of finite element discretizations of the Euler equations. Preliminary results show that this does allow to provide some understanding of this interaction and to possibly propose considerably improved numerical methods [52].

5. Highlights of the Year

5.1. Highlights of the Year

5.1.1. Awards

- On Tuesday, 19 June, the Project AMDECC (Adaptation de Maillage Dynamique et massivement parallèle pour la simulation aux grandes Echelles des Chambres de Combustion aéronautiques), launched 5 years ago within a partnership with Safran Tech and the CORIA (UMR6614 CNRS Université de Rouen and INSA Rouen), received the Award for Best Collaborative Project, one of the Digital Simulation Trophies awarded by Teratec and Usine Digitale. The aim of this project is to design helicopter engines that afford better, and cleaner, performance. To achieve this, the team uses large-scale simulations of engine combustion chambers with a view to improving quality-to-cost ratio. Optimising the simulations is key to the project's success since this approach requires intensive use of high-performance computing. Adaptation is performed with the MMG platform developed by C. Dobrzynski. For more information see `https://www.inria.fr/en/centre/bordeaux/news/amdecc-project-wins-award-at-teratec-forum` and `https://www.mmgtools.org`.

- One of the articles of M. Colin, 'Standing waves for the nonlinear Schrödinger equation coupled with the Maxwell equation', published in Nonlinearity, has been selected for the journal's 2017 Highlights Collection<http://iopscience.iop.org/journal/0951-7715/page/Highlights-of-2017>.

6. New Software and Platforms

6.1. AeroSol

KEYWORD: Finite element modelling

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

NEWS OF THE YEAR: In 2018, the following points were addressed in AeroSol

* A 6 month CNRS contract, led by Vincent Perrier was obtained in the team Cagire, concentrated on the quality of the code. A two-year Inria Hub, led by Héloïse Beaugendre was obtained in the team Cardamom. On both of these contracts, Benjamin Lux was hired (January-June in Cagire team, and since October in Cardamom team). The library has kept on benefiting from the work of Florent Pruvost (Inria Hub HPCLib), on the continuous integration and packaging aspects.

* The CNRS contract, aiming at improving the code resulted in the successful porting from the inria gforge to the inria gitlab, with a functional pipeline of code assessment (based on Jenkins) and code quality assessment (based on sonarqube).

* Installation was simplified. A fully automatic installation script based on spack was developed.

* Development of a true documentation policy, based on a wiki. About half of the functional tests were documented and updated. Doxygen documentation was improved.

* An API was developed for the AeroSol library. The mesh reading, and parallel distribution was refactored.

* Update of the test case interface was updated by using this APIfor being more convenient. About half of the functional tests are now using this interface.

* Refactoring of the xml parameter file.

* Hyperbolized models, based on the hyperbolization of advection-diffusion models were added.

* Handling of nonconservative hyperbolic models.

* Improvement of mesh adaptation

* Beginning of implementation of droplet model for icing.

* Add the possibility of using several matrices, with a different number of variables

- Participants: Benjamin Lux, Damien Genet, Dragan Amenga Mbengoue, Hamza Belkhayat Zougari, Mario Ricchiuto, Maxime Mogé, Simon Delmas and Vincent Perrier
- Contact: Vincent Perrier

6.2. Crysa

KEYWORDS: Image analysis - 2D
FUNCTIONAL DESCRIPTION: Analyzes the organization of objects placed in a hexagonal grid in an image and the crystalline structure induced in this image.

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

6.3. Cut-ANOVA

Cut-ANOVA Global Sensitivity Analysis
KEYWORDS: Stochastic models - Uncertainty quantification

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

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

- Participants: Kunkun Tang and Pietro-Marco Congedo
- Contact: Kunkun Tang

6.4. Fmg

KEYWORD: Mesh adaptation

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

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

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

6.5. Mmg

Mmg Platform

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

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

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

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

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

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

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

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

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

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

6.6. MMG3D

Mmg3d

KEYWORDS: Mesh - Anisotropic - Mesh adaptation

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

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

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

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

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

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

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

6.7. NOMESH

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

- Participants: Algiane Froehly, Ghina El Jannoun and Cécile Dobrzynski
- Partners: Université de Bordeaux - CNRS - IPB
- Contact: Cécile Dobrzynski

6.8. ORComp

FUNCTIONAL DESCRIPTION: The ORComp platform is a simulation tool permitting to design an ORC cycle. Starting from the solar radiation, this plateform computes the cycle providing the best performance with optimal choices of the fluid and the operating conditions. It includes RobUQ , a simulation block of the ORC cycles, the RealfluiDS 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.

- Participants: Maria-Giovanna Rodio and Pietro-Marco Congedo
- Contact: Maria-Giovanna Rodio
- URL: https://github.com/Orcomp/Orcomp

6.9. RealfluiDS

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

- Participants: Cécile Dobrzynski, Héloïse Beaugendre, Leo Nouveau, Pietro-Marco Congedo and Quentin Viville
- Contact: Héloïse Beaugendre

6.10. SH-COMP

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

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

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

6.11. SLOWS

Shallow-water fLOWS

KEYWORDS: Simulation - Free surface flows - Unstructured meshes

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

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

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

6.12. Sparse-PDD

Adaptive sparse polynomial dimensional decomposition for global sensitivity analysis

KEYWORDS: Stochastic models - Uncertainty quantification

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

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

- Participants: Kunkun Tang and Pietro-Marco Congedo
- Contact: Kunkun Tang

6.13. TUCWave

KEYWORD: Physical simulation

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

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

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

7. New Results

7.1. Modelling of free surface flows

- Participants: Umberto Bosi, Mathieu Colin, Maria Kazolea, and Mario Ricchiuto
- Corresponding member: Mario Ricchiuto

This year we have continued our work on Boussinesq-type models. We have focused on the enhanced equations of Nwogu [101], and on a frequency enhanced version of the Green-Naghdi system as proposed in [55], [77]. These models allow to account for weak dispersive effects which become relevant in the near shore region. Two papers on the topic are published. The first one [9] compares two popular wave breaking closures. We perform a study of the behaviour of the two closures for different mesh sizes, with attention to the possibility of obtaining grid independent results. Based on a classical shallow water theory, we also suggest some monitors to quantify the different contributions to the dissipation mechanism, differentiating those associated to the scheme from those of the partial differential equation. Our main results show that numerical dissipation contributes very little to the the results obtained when using eddy viscosity method. This closure shows little sensitivity to the grid, and may lend itself to the development and use of non-dissipative/energy conserving numerical methods. The opposite is observed for the hybrid approach, for which numerical dissipation plays a key role, and unfortunately is sensitive to the size of the mesh. The second paper [8] presents the application and validation, with respect to the transformation, breaking and run-up of irregular waves, of an unstructured high-resolution finite volume (FV) numerical solver for the 2D extended BT equations of [101].

The extension of these techniques to also account for the presence of floating structures is ongoing [34].

The methods and models developed have also led to physical studies and applications. In particular, in collaboration with the EPOC laboratory in Bordeaux, we are conducting a parametric study of bore propagation in estuaries. In particular, Three types of bores are observed in nature long wavelength undulating, short wavelength undulating, and breaking. The first kind is invisible to the eye, but measurable. The other two can be seen during mascarets. Understanding the mechanisms ruling the

transition from one to the other has tremendous impact on human activities in estuarine areas. We introduced a new set of dimensionless parameters to characterize the transition to breaking bores. We have shown that they allow to determine if the transition is dominated by friction or nonlinearity (wave amplitude). The work discussed in [7] somewhat represents an accomplishment of our activity, combining simulations using fully non-linear unstructured grid dispersive models, an exploration of parameter space based on adaptive sampling, locally enriched using a smoothness indicator related to the onset of wave breaking. Further extensions of this work are ongoing, and aim at proposing some mechanism for the first transition (see the preprint [35]).

7.2. Modelling of icing and de-icing of aircrafts

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

Flying debris is generated in several situations: when a roof is exposed to a storm, when ice accretes on rotating wind turbines, or during inflight aircraft deicing. Four dimensionless parameters play a role in the motion of flying debris. The goal of our work was to investigate the relative importance of four dimensionless parameters: the Reynolds number, the Froude number, the Tachikawa number, and the mass moment of inertia parameters. Flying debris trajectories have been computed with a fluid-solid interaction model formulated for an incompressible 2D laminar flow. The rigid moving solid effects are modelled in the Navier-Stokes equations using penalization. A VIC scheme was used to solve the flow equations. The aerodynamic forces and moments are used to compute the acceleration and the velocity of the solid. A database of 64 trajectories has been built using a two-level full factorial design for the four factors. The dispersion of the plate position at a given horizontal position decreases with the Froude number. Moreover, the Tachikawa number has a significant effect on the median plate position.

Ice release is of concern to aircraft manufacturers due to the potential damage that the ice debris can cause on aircraft components. This raises the need for accurate ice trajectory simulation tools to support pre-design, design and certification phases while improving cost efficiency. High-fidelity models involve fully coupled time-accurate aerodynamic and flight mechanics simulations and thus require the use of emerging simulation tools, such as approaches based on immersed boundary methods or chimera grids. The developments of current simulations tools for ice block trajectories performed in the scope of the recently completed research project STORM have been described and validated against a STORM experimental data base of trajectories created by the German Aerospace Center (DLR) in collaboration with the German-Dutch Wind Tunnel foundation.

Immersed boundary methods (IBM) are alternative methods to simulate fluid flows around complex geometries. The grid generation is fast as it does not need to conform to the fluid-solid interface. However, special treatments are needed in the flow equations to properly take into account the wall proximity. The penalization method is a particular case of the IBM in which the wall boundary conditions are imposed via continuous forcing terms into the governing equations. Reynolds Averaged NavierâStokes (RANS) equations completed with a turbulence model are still the most common way to model turbulence in engineering applications. However, RANS turbulence model implementation with penalization into a vortex formulation is not straight forward, in part because of the variable turbulent viscosity and partly because of the boundary conditions. Our work extends the penalization technique to turbulent flows. The objective is to validate the use of the SpalartâAllmaras turbulence model in the context of penalization and vortex formulation. Details of the resolution using a Vortex In Cell (VIC) numerical scheme are given. The proposed scheme is based on the advection of particles of vorticity and particles of turbulent viscosity. A Lagrangian framework is chosen to solve the advection part. The remaining parts of the system of equations are solved with an Eulerian framework using a Cartesian uniform grid. To avoid fine meshes near the wall, a wall function compatible with the penalization method and the vortex formulation is proposed. The formulation and the coding are validated against the wellknown periodic channel flow. Velocity profiles are computed without

and with the wall function. Results agree with analytic law of the wall solutions, showing that RANS simulations can be conducted with VIC schemes and penalization.

Ice formation can reduce the efficiency of aircraft lifting surfaces. Experiments proved that even the onset of icing (increased roughness) could cause an increase of 63% on the minimum drag coefficient of a NACA0015 airfoil when compared to a smooth airfoil. To investigate stall behavior due to ice formation, a roughness wall extension for the Spalart-Allmaras turbulence model was implemented in the open-source code SU2 so that the onset of ice formation could also be evaluated.

7.3. High order embedded and immersed boundary methods

- Participants: Heloise Beaugendre and Mario Ricchiuto
- Corresponding member: Heloise Beaugendre

Immersed and embedded methods are a flexible and efficient approach to handle complex, and moving geometries. In these techniques, domain boundaries are not meshed exactly, but are embedded/immersed in the grid. Ad-hoc techniques are then required to account for the effect of the coupling/boundary conditions defined on the domain boundaries on the nodes in the computational domain. This year we have made some progress on these methods on two aspects.

Preliminary results on the use of higher order schemes with penalization have been obtained. As in [100], the main idea is to combine a simple penalization technique to impose the no-slip condition with mesh adaptation to control the error. In the work done this year we have looked into the possibility of exploiting curved meshes and higher order schemes to further improve the accuracy in laminar flow computations [20], [21].

In parallel, we have worked on a different strategy to achieve higher order in the context of an embedded approach: the shifted boundary method, initially proposed in [92], [93]. We have worked on an extension of this method to hyperbolic problems, which are difficult to treat with penalization. The extension proposed for linear waves, as well as for the nonlinear shallow water equations show that second order results can be easily achieved in this context [15] (see also [27], [26]).

7.4. Adaptation techniques

- Participants: Heloise Beaugendre, Cecile Dobrzynski and Mario Ricchiuto
- Corresponding member: Cecile Dobrzynski

Previous work on interpolation free adaptation for compressible flows [107] has been further extended to account for non-ideal gas effects. Simulations are carried out to assess grid adaptation criteria in presence of these effects [12]. We have found that for some cases, especially in presence of a strong non-ideal dependence of the speed of sound on the density and the temperature, Mach number estimators prove to be more effective.

We have also completed the study of adaptive mesh deformation for shallow water flows, and proposed a comprehensive study of the efficiency of different techniques based on a adapt-project-evolve paradigm, or on a fully coupled ALE approach. The issue of marrying mass conservation and well-balancedness, which is peculiar to shallow water models, has been treated by means of a high order projection of the topography [3]. Preliminary results on the extension of these techniques have also been obtained [16].

7.5. Composites Materials

- Participants: Mathieu Colin, Cecile Dobrzynski and Mario Ricchiuto

- Corresponding member: Mario Ricchuito

We have continued our study on composite materials. We have finalized the phd of Xi Lin. We have finished to write the fluid models describing the propagation of an oxyde in the cracks appearing in self-healing composite materials. More precisely, we obtained two families of models, governed by the boundaries conditions. The first one looks like Shallow Water Equations and the second one comes from Lubrication theory. In order to evaluate the relevance of our models, we investigate the well-posedness of our model. In this direction, in [58] we propose in the full generality a link between the BD entropy introduced by D. Bresch and B. Desjardins for the viscous shallow-water equations and the Bernis-Friedman (called BF) dissipative entropy introduced to study the lubrications equations. Different dissipative entropies are obtained playing with the drag terms on the viscous shallow water equations. It helps for instance to prove global existence of nonnegative weak solutions for the lubrication equations starting from the global existence of nonnegative weak solutions for appropriate viscous shallow-water equations. Two articles are in preparation.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

- BGS IT&E, Flash flood simulations with a coupled model, Coordinator: M. Ricchiuto, 32 keuros total (2 consulting contracts from 2016 to 2019)
- THALES/16-12035, Activity around the numerical certification of debris codes, Coordinator: P.M. Congedo, 23 Keuros ;
- ArianeGroup, Activity around techniques for computing low-probabilities, Coordinator: P.M. Congedo, 20 Keuros ;
- CEA-CESTA, Coordinator: P.M. Congedo, 40 Keuros ;

9. Partnerships and Cooperations

9.1. Regional Initiatives

9.1.1. CRA - Region Nouvelle Aquitaine EVE

Title : Virtual prototyping of EVE engines

Type : Co-funded from Region Aquitaine and Inria

Duration : 36 months

Starting : January 2017

Coordinator : P.M. Congedo

Abstract : The main objective of this thesis is the construction of a numerical platform, for permitting an efficient virtual prototyping of the EVE expander. This will provide EXOES with a numerical tool, that is much more predictive with respect to the tools currently available and used in EXOES, by respecting an optimal trade-off in terms of complexity/cost needed during an industrial design process.i Two research axes will be mainly developed. First, the objective is to perform some high-predictive numerical simulation for reducing the amount of experiments, thanks to a specific development of RANS tools (Reynolds Averaged Navier-Stokes equations) for the fluids of interest for EXOES. These tools would rely on complex thermodynamic models and a turbulence model that should be modified. The second axis is focused on the integration of the solvers of different fidelity in a multi-fidelity platform for performing optimization under uncertainties. The idea is to evaluate the system perfor- mances by using massively the low-fidelity models, and by correcting these estimations via only few calculations with the high-fidelity code.

9.1.2. CRA - Region Nouvelle Aquitaine SANSON

Title : CRA/15-CARDAMOM THESE SANSON-10199

Type : Co-funded from Region Aquitaine and Inria

Duration :

Starting :

Coordinator :

Abstract :

9.1.3. CRA - Region Aquitaine ETRURIA

Title : EvaluaTion des Risques de submersion côtière et Urbaine par Remaillage et déformatIon Adaptative de maillage (ETRURIA)

Type : Co-funded from Region Aquitaine and Inria

Duration : 36 months

Starting : November 2018

Coordinator : M. Ricchiuto

Abstract : the objective of this project is to develop improved tools for the simulation of coastal floods by combining mesh adaptation techniques based on remeshing and deformation, representations of the coastal structures allowing to mix exact meshing and embedded representations, and high order schemes. The tools developed will be used to study inundation of French coasts, and in particular coasts of the Nouvelle Aquitaine Region, in collaboration with BRGM, and the Rivages ProTech Center of SUEZ.

9.2. National Initiatives

9.2.1. ANR VISCAP

Title:

Type: ANR

Duration: 48 months

Starting date : 1st Jan 2018

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

Abstract: Self-healing Ceramic-Matrix Composites (SH-CMCs) have extremely long lifetimes even under severe thermal, mechanical and chemical solicitations. They are made of ceramic fibres embedded in a brittle ceramic matrix subject to multi-cracking, yielding a ?damageable-elastic? mechanical behaviour. The crack network resulting from local damage opens a path to fibre degradation by corrosion and ultimately to failure of the composite, e.g. under static fatigue in high-temperature oxidative conditions. But these materials have the particularity of protecting themselves against corrosion by the formation of a sealing oxide that fills the matrix cracks, delaying considerably the fibres degradation. Applications encompass civil aeronautic propulsion engine hot parts and they represent a considerable market; however this is only possible if the lifetime duration of the materials is fully certified. Numerical modelling is an essential tool for such an aim, and very few mathematical models exist for these materials; fulfilling the needs requires a strong academic-level effort before considering industrial valorisation. Therefore, the ambition of this innovative project is to provide reliable, experimentally validated numerical models able to reproduce the behaviour of SH-CMCs. The starting point is an existing image-based coupled model of progressive oxidative degradation under tensile stress of a mini-composite (i.e. a unidirectional bundle of fibres embedded in multi-layered matrix). Important improvements will be brought to this model in order to better describe several physic-chemical phenomena leading to a non-linear behaviour: this will require an important effort in mathematical analysis and numerical model

building. A systematic benchmarking will allow creating a large database suited for the statistical analysis of the impact of material and environmental parameter variations on lifetime. Experimental verifications of this model with respect to tests carried out on model materials using in-situ X-ray tomography ? in a specially adapted high-temperature environmental & mechanical testing cell ? and other characterizations are proposed. The extension of the modelling procedure to Discrete Crack Networks for the large-scale description of the material life will be the next action; it will require important developments on mesh manipulations and on mathematical model analysis. Finally, experimental validation will be carried out by comparing the results of the newly created software to tests run on 3D composite material samples provided by the industrial partner of the project. The project originality lies in a multidisciplinary character, mixing competences in physico-chemistry, mechanics, numerical and mathematical modelling, software engineering and high-performance computing. It aims creating a true computational platform describing the multi-scale, multidimensional and multi-physics character of the phenomena that determine the material lifetime. Important outcomes in the domain of civil aircraft jet propulsion are expected, that could relate to other materials than those considered in this study.

9.2.2. FUI ICARUS

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

Type: FUI

Duration: January 2017 - December 2019

Coordinator: Turbomeca, Safran group

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

subsectionFUI ICARUS

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

Type: FUI

Duration: January 2017 - December 2019

Coordinator: Turbomeca, Safran group

9.2.3. APP University of Bordeaux

Title : Modélisation d'un système de dégivrage thermique

Type : Project University of Bordeaux

Duration : 36 months

Starting : October 2016

Coordinator : H. Beaugendre and M. Colin

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

9.3. European Initiatives

9.3.1. FP7 & H2020 Projects

Program: FET-Future & emerging technologies

Project acronym: ExaQUte

Project title: EXAscale Quantification of Uncertainties for Technology and Science Simulation

Duration: 2018-2021

Coordinator: Riccardo Rossi (CIMNE, Barcelona)

Other partners: EPFL (Switzerland), UPC (Spain), TUM (Germany), VSB (Czech Republic), str.ucture GmbH (Germany)

The ExaQUte project aims at constructing a framework to enable Uncertainty Quantification (UQ) and Optimization Under Uncertainties (OUU) in complex engineering problems using computational simulations on Exascale systems. The stochastic problem of quantifying uncertainties will be tackled by using a Multi Level MonteCarlo (MLMC) approach that allows a high number of stochastic variables. New theoretical developments will be carried out to enable its combination with adaptive mesh refinement, considering both, octree-based and anisotropic mesh adaptation. Gradient-based optimization techniques will be extended to consider uncertainties by developing methods to compute stochastic sensitivities, This requires new theoretical and computational developments. With a proper definition of risk measures and constraints, these methods allow high-performance robust designs, also maximizing the solution reliability. The description of complex geometries will be possible by employing embedded methods, which guarantee a high robustness in the mesh generation and adaptation steps, while allowing preserving the exact geometry representation. The efficient exploitation of Exascale system will be addressed by combining State-of-the-Art dynamic task-scheduling technologies with space-time accelerated solution methods, where parallelism is harvested both in space and time. The methods and tools developed in ExaQUte will be applicable to many fields of science and technology. The chosen application focuses on wind engineering, a field of notable industrial interest for which currently no reliable solution exists. This will include the quantification of uncertainties in the response of civil engineering structures to the wind action, and the shape optimization taking into account uncertainties related to wind loading, structural shape and material behavior. All developments in ExaQUte will be open-source and will follow a modular approach, thus maximizing future impact.

9.3.2. Collaborations in European Programs, Except FP7 & H2020

Program: Ocean ERANET

Project acronym: MIDWEST

Project title: Multi-fidelity decision making tools for wave energy systems

Duration: October 2015- October 2018

Coordinator: Mario Ricchiuto

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

MIDWEST is a project starting in 2016 (kick-off in December 2015) and funded by the EU-OceaneraNET program by the French ADEME, by the Swedish SWEA, and by the Portuguese FCT, aiming at proposing new tools for the wave energy industry. Wave energy converters (WECs) design currently relies on low-fidelity linear hydrodynamic models. While these models disregard fundamental nonlinear and viscous effects â which might lead provide sub-optimal designs â 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 Associate Teams Not Involved in an Inria International Labs

9.4.1.1. HAMster

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

International Partner (Institution - Laboratory - Researcher):

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

Inria Bordeaux Sud-Ouest (France) - CARDAMOM team - Mario Ricchiuto

Start year: 2017

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

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

9.4.2. Inria International Partners

9.4.2.1. Informal International Partners

- We entertain since many years a collaboration with Ecole de Technologie SupÃ©rieure de Mon-trÃ©al (Quebec), and in particular with Prof. Francois Morency, on the modelling of wing icing
- Collaboration with Universitá La Sapienza i (Prof. Renato Paciorri) and Universitá della Basilicata (Prof. Aldo Bonfiglioli) on the development of shock fitting techniques. We have regular exchanges of mutual visits and of students (this year Mirco Ciallella)
- We collaborate with Politecnico di Milano (Prof. Alberto Guardone) on the development of adaptive mesh techniques for time dependent problems. Within this collaboration Luca Cirrottola has spend part of his PhD in CARDAMOM
- We work with DTU Compute in Denmark (Prof. Allan-Peter Engsig Karup) and with and RISE in Sweden (Dr. Claes Eskilsson) on the simulation of free surface flows with floating structures. The PhD of U. Bosi is partially (and informally) co-supervised by Prof. Engsig-Karup and Dr. Eskilsson
- We work with Alireza Mazaheri (NASA LaRC, Virginia) on high order adaptive discretizations for compressible flows. Marco Lorini visited the NASA center in March/April

9.5. International Research Visitors

9.5.1. Visits of International Scientists

- L. Nouveau
- G. Scovazzi, Professor at Duke University (Durham, NC), has visited Mario Ricchiuto in January and in June 2018 to work on high order embedded methods

- Aron Roland, CEO of BGS IT&E (Information Technology & Engineering) has visited Mario Ricchiuto in February 2018 to work on the simulation of flash floods
- Nicolas Perinet, Postdoctoral fellow at University of Chile has visited Mario Ricchiuto to work on the benchmarking of the SLOWS CODE. From Jul 2018 until Sep 2018
- Tatsuya Watanabe, Professor at Kyoto Sangyo University has visited Mathieu Collin to work on Born-Infeld theory in March 2018.
- Francois Morency, Professeur at Ecole de Technologie Supérieure de Montréal has visited Héloïse Beaugendre to work on aircraft icing, roughness modeling and performance degradation, on Jul 2018 and from Sep to Dec 2018

9.5.1.1. Internships

- Agnes Chan (Inria, M. Sc. Student). From Jun 2018 until Sep 2018.
- Beatrice Battisti (Inria, M. Sc. Student). From Apr 2018 until Sep 2018.
- Elie Solai (Inria, M. Sc. Student). From Mar 2018 until Aug 2018.
- Mirco Ciallella (Inria, M. Sc. Student). From Nov 2018.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Selection

10.1.1.1. Member of the Conference Program Committees

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

10.1.2. Journal

10.1.2.1. Member of the Editorial Boards

- Mathieu Colin is a member of the board of the journal Applications and Applied Mathematics: An International Journal (AAM)
- P.M. Congedo is Editor of Mathematics and Computers in Simulation, MATCOM (Elsevier)
- Mario Ricchiuto is member of the editorial board of *Computers & Fluids (Elsevier)*, and of *Water Waves: An interdisciplinary journal (Springer)*

10.1.2.2. Reviewer - Reviewing Activities

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

10.1.3. Invited Talks

Mario Ricchiuto has give a plenary talk at the 2018 edition of the Melosh Medal award, held at Duke University in April 2018.

10.1.4. Research Administration

Mario Ricchiuto is member of the "bureau du comité des projets" of the Inria BSO center, as representative of the theme *Modelling, High-Performance Computing and Parallel Architecture.*

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

- License: Héloïse Beaugendre, Encadrement de projets sur la modélisation de la portance, 20h, L3, ENSEIRB-MATMÉCA, France
- Master : Héloïse Beaugendre, TD C++, 52h, M1, ENSEIRB-MATMÉCA, France
- Master : Héloïse Beaugendre, Calcul Haute Performance (OpenMP-MPI), 40h, M1, ENSEIRB-MATMÉCA et Université de Bordeaux, France
- Master : Héloïse Beaugendre, Responsable de filière de 3ème année, 15h, M2, ENSEIRB-MATMÉCA, France
- Master : Héloïse Beaugendre, Calcul parallèle (MPI), 39h, M2, ENSEIRB-MATMÉCA, France
- Master : Héloïse Beaugendre, Encadrement de projets de la filière Calcul Haute Performance, 14h, M2, ENSEIRB-MATMÉCA, France
- Master : Héloïse Beaugendre, Co-organisatrice du Hackathon, Inria, PlaFRIM et CATIE sont organisateurs sur Bordeaux du Hacakathon GENCI, France
- Master : Héloïse Beaugendre, Encadrement de projets sur la modélisation de la pyrolyse, 20h, M1, ENSEIRB-MATMÉCA, France
- Master : Héloïse Beaugendre , Projet fin d'études, 4h, M2, ENSEIRB-MATMÉCA, FRANCE
- Master: Mario Ricchiuto, Multi-Physics, 36hETD in the last year of the ENSEIRB-MATMÉCA school
- Post-Graduate: Mario Ricchiuto, Modelling of free surface flows, 12hETD post-graduate level short-course at Duke University
- Master : Mathieu Colin : Integration, M1, 54h, ENSEIRB-MATMÉCA, FRANCE
- Master : Mathieu Colin : Fortran 90, M1, 44h, ENSEIRB-MATMÉCA, FRANCE
- Master : Mathieu Colin : PDE, M1, 30h, University of Bordeaux, FRANCE
- Master : Mathieu Colin : Analysis, L1, 47h, ENSEIRB-MATMÉCA, FRANCE
- Master : Mathieu Colin : projet professionnel and internship responsibility : 15 h, ENSEIRB-MATMÉCA, FRANCE
- Master : Mathieu Colin : Encadrement de projets TER, 20h, ENSEIRB-MATMÉCA, FRANCE
- Master : Mathieu Colin : responsable relation entreprise formation en alternance ENSEIRB-MATMECA (30h)
- Master : Mathieu Colin : suivi d'apprenti en entreprise (28h).

10.2.2. Supervision

Lin Xi, Asymptotic modelling of incompressible reactive flows in self-healing composites, defended in October 2018.

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

Cortesi Andrea, Predictive numerical simulation for rebuilding freestream conditions in atmospheric entry flows, defented in March 2018

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

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

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

Mickael Rivier, Optimization under uncertainties of complex systems, started in May 2017.

Elie Solai, Efficient virtual prototyping of the EVE expander using robust multi-fidelity optimization, started in October 2018

Sixtine Michel, Parallel Coastal flood simulations using adaptive high order schemes with re-meshing and mesh deformation, PhD started in November 2018

10.2.3. Juries

Mario Ricchiuto has contributed to the following theses defense:

- Stephane Glockner: HDR U. de Bordeaux, June 2018 (as reviewer)
- Xi Lin: PhD U. Bordeaux, October 2018 (as examiner)
- Evi Noviani: PhD U. de Poitiers, November 2018 (as president of the jury)
- Kevin Pons: PhD U. de Toulon, December 2018 (as reviewer)
- Paola Bacigaluppi: PhD Zurich University, December 2018 (as reviewer)

Mathieu Colin has contributed to the following theses defense :

- Xi Lin: PhD U. Bordeaux, October 2018 (as director)

10.3. Popularization

10.3.1. Interventions

- Héloïse Beaugendre has co-organized (with PlaFRIM and CATIE) the Bordeaux session of the HPC hackathon sponsored by GENCI. This coding competition is open to students and young reserachers and has taken place at the Inria BOS center in December (for more information see `https://www.inria.fr/centre/bordeaux/agenda/hackathon-du-hpc-genci`)
- Algiane Froehly (Mmg-Consortium) and Mario Ricchiuto have set up and animated the CARDAMOM stand during the event "Fête des 10 Ans", held on September 27th, and celebrating the 10 years of the Inria BSO center

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