RESEARCH CENTRE

Bordeaux - Sud-Ouest

IN PARTNERSHIP WITH:

Institut Polytechnique de Bordeaux

2020

ACTIVITY REPORT

Project-Team

CARDAMOM

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

IN COLLABORATION WITH: Institut de Mathématiques de Bordeaux (IMB)

DOMAIN

Applied Mathematics, Computation and Simulation

THEME

Numerical schemes and simulations

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Project-Team CARDAMOM

Creation of the Team: 2015 January 01, updated into Project-Team: 2016 June 01

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2 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 1^{st}, 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. Moreover, the full scale behaviour is 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 operational models used in parametric analysis and design cycles, by increasing both accuracy and confidence in the results. This is achieved by combining improved physical and numerical modelling, and assessment of output uncertainties. This requires a research program mixing of PDE analysis, high order discretizations, Uncertainty Quantification (UQ), and to some extend optimization and inverse modelling. These skiss need to be also combined with some specific engineering know how to tackle specific applications. Part of this scientific themes and of these activities have been part of the work of the BACCUS and MC teams. CARDAMOM harmonizes and gives new directions to this know how.

2.1 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 [82, 24]. An apllication with many similarities is the ablation of thermal protective layers during space re-entry. An important example of a front where the physical behaviour is radically impacted, although no actual material interface exists, is the transition between propagating and breaking free surface waves. Across breaking fronts the flow develops strong vorticity dynamics and dissipative effects, which are less predominant during propagation [30]. Depending on where breaking occurs, a full transition between non-hystrostatic and hydristatic behavior may laos occur. Similar examples exist in energy and material engineering, and they 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 [62, 24] or for wave energy conversion [45]), or parametric studies of complex environments (e.g. harbour dynamics [52], or estuarine hydrodynamics [22]), or hazard assessment and prevention [47]. In all cases, computationally affordable, fast, 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 [86]. 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 uncertainty in the data used in practice to define the problem geometry, the boundary conditions, the initial conditions, 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. The models are then calibrated with manipulated experimental data (filtering, averaging, etc ..), affected in turn by their own uncertainty. These model uncertainties are *epistemic*, as they relate to a deficiency due to a lack of knowledge [35, 74]. 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 [38]). 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.

2.2 Our approach

A standard way a certification study may be performed can be described as two embedded loops. The inner loop is the physical model itself, which is composed of 3 main elements: PDE system, mesh (generation and/or adaptation), and discretization of the PDE (numerical scheme). The outer loop is the certification involving: parameter (data) representation and sampling, physical model, and output post-processing. There are several possible interactions which can be exploited to improve the accuracy and efficiency of the process. In the context of high order methods [56] it is known that realistic industrial applications can only be envisioned in conjunction with $h-/p-/r-$ 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, as well as model adaptation itself in the context of a multi-fidelity approach etc.

As things stand today, we will not be able to take advantage of the potential of advanced 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 all the aspects involved in the construction and exploration of the model itself: approximation in space and time, mesh generation and adaptation, uncertainty quantification, PDE modelling. This is what we want to do in `CARDAMOM`. The team composition provides the unique combination of skills allowing to explore such interaction 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 information made available from parametric/sensitivity/uncertainty studies or optimization to construct a more efficient adaptation strategy in physical and/or parameter, 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 and in particular wave energy conversion ;
- Material engineering (self healing composite materials) ;
- Coastal and civil engineering (coastal protection, hazard assessment, hydraulics etc.).

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

3 Research program

3.1 Variational discrete asymptotic modelling

In many of the applications we consider, intermediate fidelity models are or can be derived using an asymptotic expansion for the relevant scale resolving PDEs, and eventually considering some averaged form of the resulting continuous equations. The resulting systems of PDEs are often very complex and their characterization, e.g. in terms of stability, is 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 [59, 61] 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 [18] 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 [23] by developing more robust nonlinear variants allowing to embed rapidly moving objects. For this the use of non-linear mesh PDEs (cf e.g. [72, 78, 31]), combined with Bezier type approximations for the mesh displacements to accommodate high order curved meshes [18], 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 [60, 63, 64] 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. [41, 84, 83] 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. [21, 49, 85, 39] 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 [23]. 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 [23]. 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. [58]). The use of penalization will also provide a natural setting to compute immediate approximations of the forces on the immersed body [62, 65]. 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 [50], or on some iterative Defect Correction method (see e.g. [33]) ;

- 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 [46] 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 [32], allowing to have a more flexible approach similar to the so-called P^nP^m method [44, 76]. 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 [48] ;

- 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 [29], as well as spatial partitioning techniques [55]. 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 [20]. 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 [20], 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 [20] 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 [36] ;

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.

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 [25] 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 [19, 65]. In these methods we compensate for the error at solid walls introduced by the penalization by using anisotropic mesh adaptation [42, 57, 58]. 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 [27]. 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 [28, 24] 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 [69], 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 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

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

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 [37]). 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:

- 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) ;
- 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 ;
- 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 [86], 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 [45], we will develope 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 [45], 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 OCEANEra-net 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).

4.3 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 [73].

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 [38, 43, 71]. We have demonstrated the potential of this model in showing the importance of taking into account the multi-dimensional topology of a fibre bundle (distribution of fibres) in the rupture mechanism.

This means that the 0-dimensional model used in most of the studies (see e.g. [34]) 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.

4.4 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 [54, 75, 68, 40], to hybrid methods coupling dispersive PDEs with hyperbolic ones, and trying to mimic wave breaking with travelling bores [80, 81, 79, 51, 46]. 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 [26].

5 Highlights of the year

- In December 2020 Elena Gaburro, previously post-doc at the University of Trento, has joined CARDAMOM with an Inria Starting Faculty Position.
- A new realease of the software ParMmg has been published in 2020 [70]. The source code, documentation and contributions are hosted at `https://github.com/MmgTools`.
- The year 2020 was marked by the covid crisis and its impact on society and its overall activity. The world of research was also greatly affected: Faculty members have seen their teaching load

increase significantly; PhD students and post-docs have often had to deal with a worsening of their working conditions, as well as with reduced interactions with their supervisors and colleagues; most scientific collaborations have been greatly affected, with many international activities cancelled or postponed to dates still to be defined.

6 New software and platforms

6.1 New software

6.1.1 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 2020, the following points were addressed in AeroSol:

- Update, documentation, and update of wiki for the test case

- Development of Continuous Galerkin based models for Advection, Diffusion and AdvectionDiffusion.

- Implementation of eddy viscosity models (k-epsilon, Spalart-Almarras) turbulence models.

- Keeping on the interfacing with PARMMG for parallel mesh adaptation.

- Development of a HLL flux for finite volume and DG discretizations

- Development of a filtering method for low Mach number flows

- Development of symmetric boundary conditions for Advection and Diffusion problems.

URL: https://team.inria.fr/cardamom/aerosol/

Authors: Vincent Perrier, Damien Genet, Maxime Mogé, Simon Delmas, Benjamin Lux, Dragan Amenga Mbengoue, Mario Ricchiuto

Contact: Vincent Perrier

Participants: Benjamin Lux, Damien Genet, Mario Ricchiuto, Vincent Perrier, Héloïse Beaugendre, Subodh Madhav Joshi, Christopher Poette, Marco Lorini, Jonathan Jung, Enrique Gutierrez Alvarez

Partner: BRGM

6.1.2 Mmg

Name: 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 allows to control the boundaries approximation: The "ideal" geometry is reconstructed 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:

- mmg2d: generation of a triangular mesh , adaptation and optimization of a triangular mesh.

- mmgs: adaptation and optimization of a surface triangulation representing a piecewise linear approximation of an underlying surface geometry.

- mmg3d: adaptation and optimization of a tetrahedral mesh and isovalue discretization.

The platform software performs local mesh modifications. The mesh is modified iteratively until it meets user-defined prerequisites.

Release Contributions: This release includes:

- the possibility to preserve input references when discretizing an isovalue with mmg3d (multi-material mode),

- the possibility to discretize an isovalue and to adapt over a metric in one mmg call (modification of existing APIs),

- the new -rmc option that allows to remove small parasitic components within an isovalue in isovalue discretization mode (bubbles removal),

- the preservation of input quadrangles in Mmg2d (modification of existing APIs),

- the possiblity to impose local parameters in Mmg2d,

- the preservation of points given as required even if not connected to the mesh,

- the new -nsd option that allows to save only one domain of a multi-domain mesh,

- the renaming of the -msh option into the -3dMedit one (modification of existing APIs),

- new I/Os (VTK file formats .vtk, .vtp, .vtu) and new outputs (Triangle and Tetgen file formats .node, .ele, .face, .edge, .neigh),

- the new -nreg option to enable normal regularization,

- the migration to Modern CMake,

- new preprocessors macros to help user to detect Mmg version.

It provides new API functions :

- MMG[2D|S]_Get_numberOfNonBdyEdges and MMG[2D|S]_Get_nonBdyEdge to get non boundary edges (for example for DG methods),

- MMG3D_Get_numberOfNonBdyTriangles and MMG3D_Get_nonBdyTriangle to get non boundary triangles (for example for DG methods),

- MMG2D_[S|G]et_quadrangle to provide quadrangle to mmg2d,

- MMG[2D|S|3D]_GetByIds_vertex to get a vertex from its index,

- MMG[2D|S]_Get_triangleQuality to get the quality of a triangular element,

- MMG3D_Get_tetrahedronQuality to get the quality of a tetrahedron,

- MMG[2D|S|3D]_Compute_eigenv function to compute eigenvalues and eigenvectors of an input metric tensor.

It also modifies some existing API functions :

- MMG[2D|S|3D]_mmg[2d|s|3d]ls functions now takes a third argument, the input metric (may be null),

- MMG2d_[S|G]et_meshSize functions takes a new argument before the number of edges, the number of quadrangles (may be 0 or null).

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).

URL: http://www.mmgtools.org

Authors: Algiane Froehly, Cécile Dobrzynski, Charles Dapogny, Pascal Frey

Contact: Algiane Froehly

Participants: Algiane Froehly, Charles Dapogny, Pascal Frey, Luca Cirrottola

Partners: Université de Bordeaux, CNRS, IPB, UPMC

6.1.3 MMG3D

Name: 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.

URL: http://www.mmgtools.org

Authors: Algiane Froehly, Cécile Dobrzynski, Charles Dapogny, Pascal Frey

Contact: Algiane Froehly

Participants: Algiane Froehly, Charles Dapogny, Pascal Frey, Luca Cirrottola

Partners: Université de Bordeaux, CNRS, IPB, UPMC

6.1.4 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.

Authors: Gregory Perrot, Guillaume Couegnat, Virginie Drean, Gérard Vignoles, Mario Ricchiuto, Gregory Perrot, Gregory Perrot

Contacts: Mario Ricchiuto, Guillaume Couegnat, Gérard Vignoles

Participants: Gérard Vignoles, Gregory Perrot, Guillaume Couegnat, Mario Ricchiuto, Giulia Bellezza

Partner: LCTS (UMR 5801)

6.1.5 SLOWS

Name: 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 can be solved either with the MUMPS library or with the MKL Intel library. Implicit and explicit (extrapolated) multistep higher order time integration methods are available, and a mesh adaptation technique based on simple mesh deformation are also included. This year a new higher order reconstruction for the FV scheme has been added.

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.

URL: https://team.inria.fr/cardamom/slows-shallow-water-flows/

Authors: Mario Ricchiuto, Maria Kazolea

Contacts: Maria Kazolea, Mario Ricchiuto

Participants: Maria Kazolea, Mario Ricchiuto

6.1.6 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.

Authors: Argiris Delis, Ioannis Nikolos, Maria Kazolea

Contacts: Maria Kazolea, Mario Ricchiuto

Participants: Argiris Delis, Ioannis Nikolos, Maria Kazolea

Partner: Technical University of Crete

6.1.7 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.

Contacts: Mario Ricchiuto, Algiane Froehly

Participants: Leo Nouveau, Luca Arpaia, Mario Ricchiuto, Luca Cirrottola

6.1.8 ParMmg

Keywords: 3D, Mesh adaptation, Anisotropic, Isotropic, Isovalue discretization, Distributed Applications, MPI communication

Functional Description: The ParMmg software build parallel (MPI based) mesh adaptation capabilities on top of the sequential open-source remesher Mmg, iteratively called over sub-meshes of the initial mesh.

ParMmg is available:

- through command line ,

- in library mode using the dedicated API.

Release Contributions: The version 1.3 of ParMmg provide 3D volume mesh adaptation with constrained surface.

This release introduces:

- improved scalability on more the 100 processes,

- a fix for an erroneous count of memory usage,

- the interpolation on the adapted mesh of user-defined solution fields (on mesh vertices),

- the possibility to speed-up interpolation through the configuration variable USE_POINTMAP,

- the ripristination of output mesh load balancing,

- additional API functions to ease the reconstruction of parallel communicators in node-based solvers.

URL: https://mmgtools.org

Contacts: Algiane Froehly, Luca Cirrottola

Participants: Algiane Froehly, Luca Cirrottola

Partners: FUI Icarus, ExaQUte

6.1.9 GeoFun

Keywords: Geophysical flows, Unified models, Finite volume methods

Scientific Description: GeoFun focuses on applications where different models in different regions in space are needed, with interfaces between these regions that depend on the solution. To deal with this complex boundary problem, the code aims at exploiting unified models available everywhere in the computational domain, and at using asymptotic preserving numerical schemes to recover specific regime flows without an a priori detection of the interfaces.

Functional Description: The GeoFun library is developed as a module on top of the kernel provided by AeroSol. Its objective is to simulate geophysical flows, free surface and underground, at large time and space scales. For this reason, unified vertically integrated (shallow water type) models are considered.

News of the Year: In 2020, the development of GeoFun focused on:

- Setup of the GitLab repository.

- Setup of Continuous Integration (both compilation and unitary tests).

- Setup of the compilation process with the inclusion of AeroSol and its dependencies.

- Verification of compilation process on different architectures with different compilers.

- Development of an interface with AeroSol to keep the library development fully independent.

- Development of specific numerical integrators.

- Development of specific time schemes.

- Implementation and verification of Dupuit-Forchheimer model.

- Implementation and verification of heat equation model to test purely diffusive models.

- Beginning of implementation of shallow water model.

- Reports, documentation and wiki redaction.

Authors: Martin Parisot, Marco Lorini

Contacts: Martin Parisot, Marco Lorini

Participants: Martin Parisot, Marco Lorini

6.1.10 UHAINA

Keywords: Simulation, Ocean waves, Unstructured meshes, Finite element modelling

Scientific Description: Operational platform for near shore coastal application based on the following main elements:

- Fully-nonlinear wave propagation.

- Wave breaking handled by some mechanism allowing to mimic the energy dissipation in breakers.

- A high order finite element discretization combined with mesh and polynomial order adaptation for optimal efficiency.

- An efficient parallel object oriented implementation based on a hierarchical view of all the data management aspects cared for by middle-ware libraries developed at Inria within the finite element platform Aerosol.

- A modular wrapping allowing for application tailored processing of all input/output data (including mesh generation, and high order visualization).

Functional Description: Waves simulation

Authors: Vincent Perrier, Mario Ricchiuto, Philippe Bonneton, Fabien Marche, David Lannes, Simon Delmas, Andrea Filippini, Sébastien de Brye

Contacts: Mario Ricchiuto, Vincent Perrier

Participants: Mario Ricchiuto, Philippe Bonneton, David Lannes, Fabien Marche

Partners: EPOC, IMAG, IMB

7 New results

7.1 High order well balanced discretizations

- Participants: Rémi Abgrall, Elena Gaburro, Sixtine Michel, Mario Ricchiuto, and Davide Torlo
- Corresponding member: Mario Ricchiuto

We have further generalized our work on the approximation of the shallow water equations in a more general setting. For large scale applications involving moving adaptive meshes, we have shown that the combination of the notion of well-balanced and of discrete geometric conservation is required to provide an appropriate notion of consistency. This has been put to practice in the context of second order residual distribution schemes. Applications to standard bechmarks in spherical coordinates as well as to realistic tsunami simulations on adaptive meshes are shown in [3]. In collaboration with the BRGM, we are currently improving this work by replacing the latituge longitude representation of the sphere used in the last reference with a hybrid 3D/2D-covariant form of the equations allowing to retain (on fixed meshes) both mass conservation and well balancing. Preliminary results with a discontinuous Galerkin approximation have been presented at the Eccomas WCCM2020 conference in Paris.

For the shallow water equations, we are also developping improved implicit-explicit time stepping procedures in the context of continuous finite element/residual distribution approximations. Preliminary results have been obtained using both a standard formulation with IMEX multi-step and Runge Kutta methods, and with a discrete kineic approach combined with an IMEX-Defect Correction method. Results have been presented at the Eccomas WCCM2020 conference in Paris.

A more general study of the issue of well-balancing and its relation with the concept of global fluxes as well as with methods allowing to embed solenoidal involutions are under investigation in collaboration with U. of Zurich (PhD of Lorenzo Micalizzi co-advised by R. Abgrall and M. Ricchiuto).

7.2 Modelling of free surface flows

- Participants: Mathieu Colin, Maria Kazolea, Martin Parisot, Mario Ricchiuto
- Corresponding member: Maria Kazolea

For non hydrostatic wave propagation, we are working on several axes.

For the solution of the Green-Naghdi model we exploit an algorithm consisting in projecting the solution of the shallow water model on a set of admissible ones, subject to a solenoidal constraint. Thanks to this observation, we have been able to derive a family of boundary conditions that preserve this projection property and hence leads to a robust numerical scheme. In addition to be used as classical boundary conditions, we show how our strategy can also be used to define transmission conditions in a coupling or the automatic adaptation between shallow water and Green-Naghdi models. Additional ongoing work is related to understanding the approximation constraints related to the projection step. On one hand, when coupling this step with a hyperbolic solver, e.g. based on a finite volume approximation, one has to properly define some of the coefficients involved in the projection, which depend on the preliminary solution provided by the hyperbolic solver, and hence on the approximation underlying this step. We have found that this aspect has tremendous impact on the overall accuracy. On the other hand, the projection itself introduces approximation constraits similar to those arising in incompressiible flows, and also bearing many similarities with problems arising when solving the Maxwell equations. Several avenues are under investigation to side-step the strict necessity of working with $H(\text{div})$ compatible discretizations.

The layerwise vertical discretization is an efficient strategy to take into account the vertical profile of the horizontal velocity in free surface flows. However, the strategy has failed to represent the discontinuity of the bathymetry or the free surface. We are working on an adaptive layered strategy that is able to take this discontinuity into account and reduce the number of layers to a minumum. The main objective of this model is the possibility to create a shear in the flow in particular for the simulation of hydraulic jump. The strategy is based on a variable density model which, as far as we know, is not taken into account anywhere else.

This year we also continued our work on wave breaking for Boussinesq type modeling and more precisely for the GN equations. Using the numerial model already discribed in [46] we attempted at providing some more understanding of the sensitivity of some closure approaches to the numerical set-up. More precisely and based on [53] we focus on two closure strategies for modelling wave breaking. The first one is the hybrid method consisting of suppressing the dispersive terms on a breaking region and the second one is an eddy viscosity approach based on the solution of a turbulent kinetic energy model. The two closures use the same conditions for the triggering of the breaking mechanisms. Both the triggering conditions and the breaking models themselves use case dependent, ad hoc, parameters which are affecting the numerical solution while changing. The scope of this work is to make use of sensitivity indexes computed by means of Analysis of Variance (ANOVA) to provide the sensitivity of wave breaking simulation to the variation of parameters such as the mesh size and the breaking parameters involved in each breaking model. The work has been accepted for presentation in WCCM-ECCOMAS Congress 2020, which due to covid-19 is held online on january 2021.

An other set of equations that can model free surface flows is the Isobe-Kakinuma model. The Isobe-Kakinuma model is a system of Euler-Lagrange equations for a Lagrangian approximating Luke's Lagrangian for water waves. We have initially worked on some theoretical properties of the model, and in particular on the existence of a family of small amplitude solitary wave solutions in the long wave regime [6]. Numerical analysis for large amplitude solitary wave solutions have also been performed and suggests the existence of a solitary wave of extreme form with a sharp crest. We are now focusing both on the numerical discretisation of this model, and on the study of its ability to represent correctly some physical parameters as phase dipersion and wave shoaling. The goal is to exploit possible advandages and/or limitations compared to other well known and widely used mathematical models such as the Green-Nagdi equations. This is an ongoing work.

7.3 Modelling of icing and de-icing of aircrafts

- Participants: Héloïse Beaugendre, Tiffany Carlier, Mathieu Colin and Francois Morency
- Corresponding member: Héloïse Beaugendre

In-flight icing is a major source of incidents and accidents. Accurate prediction of performance degradation linked to iced surfaces is a major concern for manufacturers to reduce risks. In the PhD of Gitsuzo De Brito Siqueira Tagawa, co-advised by François Morency and Heloise Beaugendre, we worked on improving the prediction of performance degradation linked to icing using hybrid RANS / LES methods. These DES methods are indeed capable of simulating massively separated flows while remaining affordable from a computational time point of view when applied to industrial geometries. The originality of this work consists in taking into account the surface roughness linked to the ice in the RANS part of the model. Previous works only consider smooth surfaces. This work therefore opens up new perspectives in the study of performance degradation linked to icing. Many questions arised which will require further research in this area.

Tiffany Carlier began her PhD in October 2020 and works on improved modelling of models water phase change using an enriched shifted boundary method previsouly developed in the team [66] in the context of de-icing systems.

7.4 High order embedded and immersed boundary methods

- Participants: Héloïse Beaugendre, Tiffanie Carlier, Mirco Ciallella, Benjamin Constant, Elena Gaburro, Florent Nauleau and Mario Ricchiuto
- Corresponding member: Héloïse Beaugendre

We have continued exploring new ideas allowing to improve the accuracy of immersed and embedded boundary methods, both on a fundamental level and in applications. For elliptic and parabilic problems, we are on one hand exploting and extending our previous work in the context of moving interfaces due to phase change in the PhD of T. Carlier. This work is based on a shifted boundary approach, consisting in applying the boundary conditions on a modified boundary. On this surrogate boundary (e.g. set faces closest to the physical boundary) we appropriately modify the imposed conditions to account for this offset by means of a backward Taylor series expantion truncated to the desired accuracy [66]. At the same time, we have tried to reformulate this approach by means of a continuous view of the scheme. Using the anisotropy of the thin region between the under-resolved and physical boundaries we have been able to derive a sub-grid asymptotic approximation whose trace on the surrogate boundary is precisely the condition used in the shifted boundary method. The availability of a continuous solution and the PDE setting used, however, allows both to set up a high order volume penalized approach, going beyond the limitations of the first order penalization method used e.g. in [67], and also to foresee a more consistent treatment of other PDEs. Preliminary results have been presented at the workshop on immersed methods of the Inria challenges: projet Surf. This work is perfomed in collaboration with L. Nouveau (INSA Rennes), and C. Poignard (Inria, MONC).

For hyperbolic problems we are following several directions to exploit and generalize the ideas of [77]. On one hand we are trying to recast the method in the setting of fully discontinuous approximations in space. This should allow further flexibility, and simplify somewhat the modification of the shifted boundary condition. Within the ANEMONE associated team we are also investigating the issue of the accuracy of the approximation of the distance. Finally, a very interesting extension is the use of this setting to embed shock waves. This has allowed to design a shock tracking method allowing to retain full second order of accuracy in presence of strong shock waves, combining a shock fitting approach with ideas similar to those undepinning the shifted boundary method [5]. Ongoing work on this topic, in collaboration with U. Roma La Sapienza (Prof. R. Paciorri) and U. della Basilicata (Prof. A. Bonfiglioli) is related to improving the accuracy, and handle interactions of several discontinuities. Preliminary results have been presented at the WCCM-ECCOMAS Congress 2020.

Realistic applications to external aerodynamics are being pursued in collaboration with ONERA and CEA-Cesta. Within the PhD of Benjamin Constant (ONERA) we have proposed an improved Immersed Boundary Method based on volume penalization for turbulent flow simulations on Cartesian grids. The proposed approach enables to remove spurious oscillations on the wall on skin pressure and friction coefficients. Results are compared to a body-fitted simulations using the same wall function, showing that the stair-step immersed boundary provides a smooth solution compared to the body-fitted one. The IBM has been modified to adapt the location of forced and forcing points involved in the immersed boundary reconstruction to the Reynolds number. This method has been validated either for subsonic and transonic flow regimes, through the simulation of the subsonic turbulent flow around a NACA0012 profile and the transonic flow around a RAE2822 profile and the three-dimensional ONERA M6 wing. This work has recently been accepted to be published in JCP. This work will be further pursued in the PhD of Florent Nauleau started in October 2020 in collaboration with the CEA cesta. In this project we aim at using immersed boundaries for large eddy simulations of hypersonic reentry vehicles.

7.5 Composites Materials

- Participants: Roberta Baggio, Giulia Bellezza, Mathieu Colin, Guillaume Couégnat, and Mario Ricchiuto
- Corresponding member: Mario Ricchiuto

This work involved the multiscale modelling of a class of complex ceramic composite materials known has self-healing ceramic matrix composites (SH-CMCs). The particular structure of the matrix of these composites is such that, upon craking in a corosive environment, a protective oxide is produced within the crack, protecting the carbon fibers, and providing extremely long lifetimes before failure. This makes these composites very interesting for applications e.g. in the aeronautic industry. Within the ANR Viscap, we are working on embedding the small scale physico-chemical dynamics into large scale mechanical simulations of the material's lifetime.

We have proposed improved analytical models for the progressive oxydation of the carbon fibers, and coupled them with a crack averaged model for the evolution of the reactive species. This model has been coupled with a simplified flow approximation for the protective oxide and coupled to the mechanical solver allowing to perform parametric studies of a single tow of fibers with transversal cracks. We are now completing a study showing the great advantage of including the multi-dimensional sub-crack model, as well as a first full investigation and sensitivity analysis of the lifetime dependence on the environnemental as well as structural parameters.

Modeling of the oxyde flow: lubrication and shallow water models, entropy conditions and numerical pproximation in 1D and 2D.

Our aim is also to include more phenomenon such as oxide spreading for example. To this end, a new model has been obtained, in the context of *thin-film long wave approximation*. The resulting lubrication obtained includes the oxide spreading by the use of an original right-hand-side term. We have also recast the system in a Shallow-water type's system, depending on a small parameter ε. The limit ε goes to 0 enables to recover the lubrication model. This formulation has the advantage that, considering that the RHS term is equal to 0, the system is given by an hyperbolic part and a second order part which is skew-symmetric with respect of the L2 scalar product. Furtehrmore, the augmented system admits a conservation law for the total energy density, which is useful for numerical simulations. Finally, some numerical test are under progress to validate this new model.

7.6 Adaptation techniques

- Participants: Nicolas Barral, Héloïse Beaugendre, Luca Cirrottola, Algiane Froehly, Mario Ricchiuto.

- Corresponding member: Nicolas Barral

ParMmg, the parallel version of the volume remesher Mmg3d, aims at allowing mesh adaptation in high performance computing. Supervised by Algiane Froehly (SED-BSO, DGD-I, Consortium Mmg), its development in 2020 has been pursued in the Cardamom team thanks to the FUI Icarus project and the ExaQUte European project http://exaqute.eu/ funding the postdoc of Luca Cirrottola. This work will be further pursued within the European project Microcard http://www.microcard.eu/, where Algiane Froehly is leading a work package on improving the performance of ParMmg with hybrid parallelism for applications in cardiac electrophysiology.

The source code, documentation and contributions are hosted at https://github.com/MmgTools. A minor release has been published in 2020[70], including:

- improved scalability on more the 100 processes;
- the interpolation on the adapted mesh of user-defined solution fields (on mesh vertices);
- additional API functions to ease the reconstruction of parallel communicators in the node-based solvers of the European partners.

Several software couplings have been refined or started in 2020. Foremost with the European partner solver Kratos, which couples and packages ParMmg since its release 8.1 in November 2020 https://github.com/KratosMultiphysics/Kratos/releases/tag/v8.1. As an independent third-party initiative, FreeFem developers have started coupling and packaging ParMmg since the FreeFem release 4.5 in February 2020 https://github.com/FreeFem/FreeFem-sources/releases/tag/v4.5. Other initiatives are currently under study. Debug and testing of ParMmg has been performed on PlaFRIM for parallel computations up to 1024 MPI processes.

The work on goal-oriented mesh adaptation techniques for geophysical flows has continued, in the context of the PhD thesis of Joseph Wallwork at Imperial College London, co-supervised by Nicolas Barral and Matthew Piggott (ICL).

A novel goal-oriented error estimate has been proposed for the nonlinear shallow water equations solved using a mixed discontinuous/continuous Galerkin approach. This error estimator takes into account the discontinuities in the discrete solution. Results are presented for simulations of two model tidal farm configurations computed using the Thetis coastal ocean model. Convergence analysis indicates that meshes resulting from the goal-oriented adaptation strategies permit accurate quantity of Interest estimation using fewer computational resources than uniform refinement.

The adjoint-based error estimates developped so far have been applied to advection-dominated tracer transport modelling problems in two and three dimensions, using the finite element package Firedrake. Goal-oriented meshes for an idealised time-dependent desalination outfall scenario are presented: the goal is the salinity at the plant inlet, which could be negatively impacted by the transport of brine from the plant's outfall.

Additional work performed has allowed to extend our previous results on moving mesh adaptation to curvilinear coordinates, and to 3D domains with curved conformally meshed boundaries.

7.7 Modeling of flows in aquifers

- Participants: Manon Carreau, Marco Lorini, Martin Parisot
- Corresponding member: Martin Parisot

This project started this year with the objective to propose a numerical tool (software GeoFun) for the simulation of flows in aquifers based on unified models. Different types of flows can appear in an aquifer: free surface flows (hyperbolic equations) for lakes and rivers, and porous flows (elliptic equations) for ground water. The variation in time of the domain where each type of flow must be solved makes the simulation of flows in aquifers a scientific challenge. Our strategy consists of writing a model that can be solved in the whole domain, i.e. without domain decomposition.

For the beginning of the project we start by considering only the saturated areas. We propose and study a unified model between shallow water and Dupuit-Forchheimer models, which are both classical models in each areas. In parallel, we work on the structure of the code in order to integrate more easily the furthers ideas. In particular, specific numerical integrators and time schemes have been implemented. All the code development has been documented in reports.

8 Bilateral contracts and grants with industry

8.1 Bilateral Contracts

CEA-DAM/DIF

- Title: Développement d'un modele numérique de tsunami: de la propagation au déferlement dans des environnements côtiers réels.
- Type: contrat d'accompagnement for Aurore Cauquis' PhD.
- Duration: 36 months
- Starting date : 1st Nov 2019
- Coordinator: Mario Ricchiuto and Philippe Heinrich (CEA)
- Summary: The objective of this contract is to develop efficient temporal and spatial discretizations for dispersive waves on Cartesian grids. The schemes are to be implemented in the code of CEA and applied to tsunami simulations in realistic environnements.

CEA-CESTA

- Title: Immersed boundary method applied to large eddy simulations of hypersonic reentry vehicles
- Duration: 36 months
- Starting date : 19 October 2020
- Coordinator: Heloise Beaugendre and Celine Baranger (CEA).
- Summary: This thesis topic is part of the aerothermal dimensioning approach of a re-entry vehicle and its main stake is to take up the technological challenges of such an approach while improving numerical predictions compared to existing methods. The primary criterion of the calculation code used by a team of designers, in addition to the control of its margin of error, is its speed of execution. In the context of aerothermal performance, codes are often based on Navier-Stokes averaged (RANS) equations and body-fitted structured meshes. These two technologies make it possible to obtain a time-averaged representation of phenomena in a reasonable time while capturing the flow and thermal close to the vehicle wall. Nevertheless, using an averaged field for the design implies less control of the maximum stresses that could be applied to the vehicle. The generation of "body-fitted" meshes can also become extremely time-consuming if the objects have geometric particularities. A second criterion, in a dimensioning environment, is based on the quality of the post-processing tools. As far as re-entry vehicles are concerned, because of the high Mach and Reynolds numbers involved, traditional analysis methods are often pushed to the limits of their applicability or even rendered obsolete.

  This thesis aims to contibute to the concerns cited above. In a first step, the flow resolution will be improved by the use of a Large Scale Simulation technology. To this end, a Direct Numerical Simulation (DNS) code (finite volumes, Cartesian mesh, hybrid parallelism, high order WENO type) already available will be equipped with a SGSM adapted to the presence of walls and the characteristics of a hypersonic flow. Regarding the cost of meshing, the PhD student will work on the technique of immersed boundaries to adapt it to the re-entry flows and will integrate an algorithm capable of taking advantage of the benefits related to the High Performance Computing environment present at the CEA. Finally, in order to exploit the results of simulations carried out for the development and validation of models, the PhD student will bring a critical look at them using a recent technique, topological data analysis (TDA) using the TTK open-source platform.

BRGM

- Title: dévéloppement d'une plateforme opérationnelle pour la simulation des risques côtiers (UHAINA)
- Duration: 30 months
- Starting date : 1st Steptember 2019
- Coordinator: Mario Ricchiuto and Rodrigo Pedreros (BRGM).
- Summary: The objective of this contract is to develop and implement the necessary functionalities to allow the use of the UHAINA platform in an operational context. This involves both pre- and post-processing tools based on standard data formats, as well as extension of the models themselves (non-uniform friction, wind forcing, curvilineear coordinates, etc). Applications to storm surge and real tsunami events are sought.

9 Partnerships and cooperations

9.1 International initiatives

Inria international Chairs:
IIC ABGRALL Rémi
Title: Numerical approximation of complex PDEs & Interaction between modes, schemes, data and ROMs
International Partner (Institution - Laboratory - Researcher):
ETH Zurich (Switzerland) - Institut fur Mathematik & Computational Science - Rémi Abgrall
Duration: 2019 - 2023
Start year: 2019

9.1.1 Inria Associate Team (not involved in an IIL)

ANEMONE

Title: AdvaNced Embedded MethOds for flows with NonlinEar moving fronts

Duration: 2020 - 2022

Coordinator: Mario Ricchiuto

Partners: Civil and Environnemental Engineering Department, Duke Univertsity (North Carolina, USA)

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

Inria contact: Mario Ricchiuto

Summary: ANEMONE focuses on the numerical treatment of flows with moving fronts with complex and possibly nonlinear dynamics. There exist many examples of such fronts, related to different physics. Some of these represent in some sense boundaries of the fluid domain, as for example the waterline in floods and tsunami inundations, or the rigid walls of bodies freely moving in the flow. Other fronts involve abrupt changes in the physics. This is the case for example of shock waves occurring in compressible flows (and in some flows with similar nonlinear behaviour), or fronts coupling flows with different behaviours, as it occurs in some models for wave-body interactions. To handle in an accurate and flexible manner these features, ANEMONE will focus on the improvement and application of high order embedding techniques based on ideas similar to the shifted boundary method, initially developed by the groupe at Duke University. This approach, initially developed to set boundary conditions on complex boundaries, will be extended to deal with several different types of nonlinear moving interfaces, while studying simplified formulations allowing an easier implementation, as well as the interaction of the accuracy of the embedding procedure with mesh adaptation. The results of ANEMONE are expected to have an impact on the activities of the participants in domains such as from wave energy extraction, coastal risk assessment, as well as applications in aeronautics related to wing icing.

9.1.2 Inria international partners

Informal international partners

- U. Roma La Sapienza (Prof. R. Paciorri) and U. della Basilicata (Prof. A. Bongiglioli) : development of high order shock tracking and shock fitting techniques. Co-supervision of the PhD of M. Ciallella.
- ETS Ecole de Technologie Supérieure de Montréal (Prof. François Morency) co-supervision of Gitsuzo de Brito Siqueira Tagawa and Kevin Ignatowicz.
- RISE/U. Aalborg (Dr. C. Eskilsson) and DTU Compute (Prof. A.P. Engsig-Karup): modelling of wave energy devices using fully non-linear potential equations and depth averaged approaches. Associated team with RISE starting in 2021 (PI: M. Parisot).
- Imperial College London (Prof. M. Piggot): adjoint-based error estimation and goal-oriented mesh adaptation for Shallow Water flows.
- U. Aachen (Pr S. Noelle and Dr T. Tscherpel): on boundary condition for the Green-Naghdi model see 7.2. Further work on the definition of weak solution for the Grenn-Naghdi model.

9.2 European initiatives

9.2.1 FP7 & H2020 Projects

ExaQUte

Title: EXAscale Quantification of Uncertainties for Technology and Science Simulation

Duration: 01/06/2018 - 31/05/2021

Coordinator: CIMNE

Partners:

- Barcelona Supercomputing Center - Centro Nacional de Supercomputation (BSC, Spain)
- Centre Internacional de metodes Numerics en ENginyeria (CIMNE, Spain)
- Ecole Polytechnique Federale de Lausanne (Switzerland)
- Institute National de Recherce en Informatique et Automatique (INRIA, France)
- Str. Ucture GMBH (Germany)
- Technische Universitaet Muenchen (TUM, Germany)
- Universitat Politecnica de Catalunya (UPC, Spain)
- VSB - Technical University of Ostrava (Czech Republic)

Inria contact: Algian Froehly

Summary: 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.

9.3 National initiatives

ANR VISCAP

Title: VIrtual Self-healing Composites for Aeronautic Propulsion

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. 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. 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. It is planed to perform 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. Other characterizations are also 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.

ANR GEOFUN

Title: GEOphysical Flows with UNified models

Type: ANR

Duration: 48 months

Starting date : 1st Jan 2020

Coordinator: Martin Parizot

Abstract: The objective of the GeoFun project is to improve the modeling and simulation of geophysical flows involving at least two different processes. The main application we have in mind is water catchment areas, where a shallow free surface flow stands above a underground flow on porous medium. Our vision of water transport is often naive, because we first think of rivers, lakes, and flooding, but actually, 80% of water in continental areas is underground. Sometimes, the porous substrate is covered with an impermeable rock stratum, which confines the flow as in pipelines, except at certain points where springs and resurgences appear. Our long term goal is to propose a global and unified model of an aquifer. By global, we mean a complete description, including free surface flow (rivers), exchanges with the groundwater in unsaturated area, flows in caves, that might be congested or not, and might contain air pockets. By unified, we mean that we do not aim to decompose the domain and use different models for each part of the aquifer. On the contrary, we plan to propose and study models able to pick the relevant physic by themselves in a multi-physics context. The numerical approximation will be a main concern all along the way. The final contribution of the GeoFun project is the development of a scientific computing library, simulating complex flows in water catchment areas thanks to the numerical strategies analyzed in this project. Since unified models are design to be applied in the whole computational domain with no domain decomposition, the robustness of the numerical strategy at all regime are essential. Our unified numerical schemes will degenerate towards existing schemes in those regions, in order to guarantee a similar feasibility and robustness. Moreover, since the final goal is to test the library on realistic aquifers, the efficiency of the methods is of crucial importance.

Inria Challenges: SURF

Title: SURF: a ground-breaking project in oceanographic simulation

Type: Inria Challenges

Duration: 48 months

Starting date : 1st Jan 2019

Coordinator: Mario Ricchiuto

Abstract: Understanding the dynamics of the oceans is a key scientific issue. It has many applications in coastal zone management, the regulation of maritime traffic and the prevention of ecological, meteorological and industrial risks. While scientific computing is now one of the most widely-used tools to explain or predict changes in the ocean, simulation tools are still reserved for specific purposes. The SURF project brings together several Inria teams that are pooling their expertise to develop a common platform for computing oceanic flows in littoral and coastal zones.

9.4 Regional initiatives

EVE/VIPER

Title: Prototypage Virtuel Efficace du Moteur EVE

Type: Co-funded from Région Nouvelle-Aquitaine and INRIA

Duration: 36 months

Starting date : 01/01/2017

Coordinator: Pietro Congedo (H. Beaugendre)

Abstract: This project is in collaboration with the company EXOES. The main objective of the thesis is the construction of a numerical platform, for permitting an afficient simulation of battery thermal management system for a racing car. To perform optimization under uncertainties a multi-fidelity platform will be used. The idea is to evaluate the system performances by using massively the low-fidelity models and by correcting theses estimations via only few calculations with the high-fidelity code. High fidelity simulations are done using TrioCFD code. A first study is carried out on the uncertainties linked to the internal resistance model of batteries.

ETRURIA

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

Type: Apple à Projets Recherche Région Nouvelle-Aquitaine

Coordinator: M. Ricchiuto

Other partners: BRGM, UMR EPOC (P. Bonneton)

Abstract: The objective of this project is to combine high order continuous finite elements, with embedded methods and mesh adaptation in the simulation of coastal and urban inundation. Realistic validation cases will be provided by BRGM. This project co-funds (50%) the PhD of S. Michel.

FUI ICARUS

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

Type: FUI

Duration: January 2017 - December 2020

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.

10 Dissemination

10.1 Promoting scientific activities

10.1.1 Scientific events: organisation

Member of the Scientific Committees

- Mathieu Colin is a member of the scientific comittee of the "Journée Jeunes EDPistes"
- Mario Ricchiuto is member of the CFD Scientific Committee of the world conference in computational mechanics (WCCM2020)

Member of the organizing committees

- Maria Kazolea co-organized the session NH-017 Interdisciplinary Tsunami Science II at the AGU fall meeting, virtual Conference, 1-17 December 2020.
- Maria Kazolea co-organized the mini-symposium MS402 Numerical methods and Applications in Coastal Environments, at ECCOMAS WCCM 2020 in Paris.
- Mario Ricchiuto co-organized the mini-symposium MS207 Advances on (shock) fitting methods, at ECCOMAS WCCM 2020 in Paris.

- Mario Ricchiuto co-organized the mini-symposium MS130 Recent advances in immersed boundary, fictitious domain and unfitted discretization methods, at ECCOMAS WCCM 2020 in Paris.
- Nicolas Barral co-organized the mini-symposium MS413 Unstructured mesh adaptation: from mesh generation to applications, at ECCOMAS WCCM 2020 in Paris.

10.1.2 Scientific events: selection

10.1.3 Journal

Member of the editorial boards

- Mathieu Colin is a member of the Editorial board of Application and Applied Mathematics : An International Journal
- Mario Ricchiuto is a member of the editorial boards of Computers & Fluids (Elsevier) and of Water Waves (Springer)

Reviewer - reviewing activities

- Mathieu Colin : Nonlinearity, DCDS, Water Waves, SIMA
- Martin Parisot : International Journal for Numerical Methods in Fluid, Engineering Computations, International Journal of Aerospace Engineering, Journal of Applied Fluid Mechanics, Applied Mathematics and Computation
- Nicolas Barral : Journal of Computational Physics, Computer and Fluids, Journal of Scientific Computing
- Maria Kazolea: Wave motion, Journal of Fluid Mechanics, Applied Oscean Research , Computer and Fluids

10.1.4 Invited talks

- M. Ricchiuto, Bore propagation in channels with sloping banks: numerical and theoretical study, Journée Tsunami CEA DAM-DIF, September 2020

10.1.5 Research administration

- Mario Ricchiuto is deputy scientific head of the Inria Bordeaux Sud-Ouest center

10.2 Teaching - Supervision - Juries

10.2.1 Teaching

- License: Martin Parisot, TP Mécanique, 21h, M1, ENSEIRB-MATMÉCA, France
- License: Nicolas Barral, TD d'Analyse Numérique, 24h, L3, ENSEIRB-MATMÉCA, France
- Master : Nicolas Barral, TD C++, 48h, M1, ENSEIRB-MATMÉCA, France
- Master : Nicolas Barral, Calcul Haute Performance (OpenMP-MPI), 40h, M1, ENSEIRB-MATMÉCA et Université de Bordeaux, France
- Master : Nicolas Barral, Techniques de maillage, 36h, M2, ENSEIRB-MATMÉCA et Université de Bordeaux, France
- Master : Nicolas Barral, Encadrement de projet de Calcul Haute Performance, 14h, M2, ENSEIRB-MATMÉCA, France
- Master : Nicolas Barral : projet professionnel et suivi de stages, 10 h, ENSEIRB-MATMÉCA, France

- License: Héloïse Beaugendre, Encadrement de projets sur la modélisation de la portance, 20h, L3, ENSEIRB-MATMÉCA, France
- Master : Héloïse Beaugendre, TD C++, 48h, M1, ENSEIRB-MATMÉCA, France
- Master : Héloïse Beaugendre, Calcul Haute Performance (OpenMP-MPI), 40h, M1, ENSEIRB-MATMÉCA et Université de Bordeaux, France
- Master : Héloïse Beaugendre, 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, 11h, M2, ENSEIRB-MATMÉCA, 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 : 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 (35h)
- Master : Mario Ricchiuto, Multiphysics Course, 24h cours magistrale, M2, ENSEIRB-MATMÉCA, France

10.2.2 Supervision

- PhD in progress : E. Solai, Multi-fidelity modeling of an immersive battery cooling system for electric vehicles, started in November 2018, co-supervised by H. Beaugendre and P.M. Congedo
- PhD in progress: B. Constant, High order immersed methods for turbulent flows, started in September 2019, supervised by H. Beaugendre
- PhD in progress : S. Michel, Shallow water simulations with immersed higher order residual methods on adaptive meshes, started in November 2018, supervised by M. Ricchiuto
- PhD in progress : G. Bellezza, Multi scale modelling for self-healing composite materials, started in February 2019, supervised by M. Ricchiuto and G. Vignoles (LCTS)
- PhD in progress : M. Ciallella, Bridging shock fitting and embedded methods to handle shock waves in hyperbolic systems, started in October 2019, supervised by M. Ricchiuto and R. Paciorri (U. Roma La Sapienza)
- PhD in progress : A. Cauquis, High order shock capturing methods for tsunami simulations, started in November 2019, supervised by M. Ricchiuto and P. Heinrich (CEA)

- PhD in progress : N. Boulos Al Makary, Numerical analysis and simulation of a shallow water model with two velocities, started in November 2018, co-supervised by N. Aguillon, M. Parisot and E. Audusse.
- PhD in progress : M. Carreau, Modeling, analysis and scientific computing for the simulation of geophysical flows with unified models, started in November 2020, co-supervised by M. Parisot and R. Masson.
- PhD in progess : T. Carlier, Modeling of an icing system using shifted boundary method, started in October 2020, co-supervised by H. Beaugendre and M. Colin.
- Post-Doc in progress: R. Baggio, Transversal/longitudinal single crack PDE and FEM model for self-healing ceramix-matrix composite materials, supervised by D. Bresch and M. Colin.
- Post-Doc in progress: D. Torlo, Hybrid PDE-ROM modeling for dispersive waves, supervised by M. Ricchiuto
- Post-Doc in progress: C. Poette, Development of an operational platform for near shore hydrodynamics, supervised by M. Ricchiuto and R. Pedreros
- Post-Doc: L. Cirrottola (until Oct 2020), Development of parallel adaptive re-meshing and adaptive moving mesh technqiues, supervised by A. Frohely and M. Ricchiuto
- Post-Doc: S. Madhav Joshi (until Apr 2020), Robust and high order modelling of dispersive wave propagation and wave breaking, supervised by M. Kazolea, D. Lannes and M. Ricchiuto.

10.3 Popularization

10.3.1 Education

- 01/12/2020: Elena Gaburro. Dissemination seminar on educational strategies. Title: A simple but efficient concept of blended teaching of mathematics for engineering students during the COVID-19 pandemic. Almath Verona seminar.

11 Scientific production

11.1 Major publications

[1] L. Arpaia and M. Ricchiuto. 'Well balanced residual distribution for the ALE spherical shallow water equations on moving adaptive meshes'. In: *Journal of Computational Physics* 405 (2020), p. 109173. DOI: 10.1016/j.jcp.2019.109173. URL: https://hal.inria.fr/hal-02422335.

[2] F. Morency and H. Beaugendre. 'Comparison of turbulent Prandtl number correction models for the Stanton evaluation over rough surfaces'. In: *International Journal of Computational Fluid Dynamics* 34.4 (Apr. 2020), pp. 278–298. DOI: 10.1080/10618562.2020.1753712. URL: https://hal.inria.fr/hal-02896481.

11.2 Publications of the year

International journals

[3] L. Arpaia and M. Ricchiuto. 'Well balanced residual distribution for the ALE spherical shallow water equations on moving adaptive meshes'. In: *Journal of Computational Physics* 405 (2020), p. 109173. DOI: 10.1016/j.jcp.2019.109173. URL: https://hal.inria.fr/hal-02422335.

[4] S. Busto, M. Dumbser and E. Gaburro. 'A simple but efficient concept of blended teaching of mathematics for engineering students during the COVID-19 pandemic'. In: *Education Sciences* (2nd Feb. 2021). DOI: 10.3390/educsci11020056. URL: https://hal.archives-ouvertes.fr/hal-03111979.

[5] M. Ciallella, M. Ricchiuto, R. Paciorri and A. Bonfiglioli. 'Extrapolated Shock Tracking: bridging shock-fitting and embedded boundary methods'. In: *Journal of Computational Physics* (Apr. 2020), p. 109440. DOI: 10.1016/j.jcp.2020.109440. URL: https://hal.archives-ouvertes.fr/hal-02536539.

[6] M. Colin and T. Higuchi. 'Solitary wave solutions to the Isobe-Kakinuma model for water waves'. In: *Studies in Applied Mathematics* (2020). URL: https://hal.archives-ouvertes.fr/hal-02364653.

[7] A. F. Cortesi, P. G. Constantine, T. Magin and P. M. Congedo. 'Forward and backward uncertainty quantification with active subspaces: application to hypersonic flows around a cylinder'. In: *Journal of Computational Physics* 407 (15th Apr. 2020), p. 109079. DOI: 10.1016/j.jcp.2019.109079. URL: https://hal.inria.fr/hal-03052824.

[8] M. Galbraith, P. Caplan, H. Carson, M. Park, A. Balan, W. K. Anderson, T. A. Michal, J. J. Krakos, D. Kamenetskiy, A. Loseille, F. Alauzet, L. Frazza and N. Barral. 'Verification of Unstructured Grid Adaptation Components'. In: *AIAA Journal* (June 2020), pp. 1–16. DOI: 10.2514/1.J058783. URL: https://hal.inria.fr/hal-02904421.

[9] M. Hubbard, M. Ricchiuto and D. Sarmany. 'Space-time residual distribution on moving meshes'. In: *Computers and Mathematics with Applications* (2020). DOI: 10.1016/j.camwa.2019.09.019. URL: https://hal.inria.fr/hal-02310394.

[10] M. Lorini, F. Bassi, A. Colombo, A. Ghidoni and G. Noventa. 'Discontinuous Galerkin solution of the RANS and $\mathrm{kL}-\mathrm{k}-\log(\omega)$ equations for natural and bypass transition'. In: *Computers and Fluids* 214 (Jan. 2021), p. 104767. DOI: 10.1016/j.compfluid.2020.104767. URL: https://hal.archives-ouvertes.fr/hal-03115177.

[11] F. Morency and H. Beaugendre. 'Comparison of turbulent Prandtl number correction models for the Stanton evaluation over rough surfaces'. In: *International Journal of Computational Fluid Dynamics* 34.4 (20th Apr. 2020), pp. 278–298. DOI: 10.1080/10618562.2020.1753712. URL: https://hal.inria.fr/hal-02896481.

[12] J. Wallwork, N. Barral, S. Kramer, D. Ham and M. Piggott. 'Goal-oriented error estimation and mesh adaptation for shallow water modelling'. In: *SN Applied Sciences* 2.6 (June 2020). DOI: 10.1007/s42452-020-2745-9. URL: https://hal.inria.fr/hal-02904413.

Scientific book chapters

[13] P. Poullet, P. Ramsamy and M. Ricchiuto. 'Residual based method for sediment transport'. In: *Recent Advances in Numerical methods for Hyperbolic PDE Systems. Selected talks of Numhyp 2019*. 2020. URL: https://hal.archives-ouvertes.fr/hal-03089375.

Reports & preprints

[14] E. Audusse, L. Boittin and M. Parisot. *On the Exner model and non-local approximations: modeling, analysis and numerical simulations*. 24th Nov. 2020. URL: https://hal.archives-ouvertes.fr/hal-03001671.

[15] A. Canteaut, M. A. Fernández, L. Maranget, S. Perin, M. Ricchiuto, M. Serrano and E. Thomé. *Évaluation des Logiciels*. Inria, 14th Jan. 2021. URL: https://hal.inria.fr/hal-03110723.

[16] A. Canteaut, M. A. Fernández, L. Maranget, S. Perin, M. Ricchiuto, M. Serrano and E. Thomé. *Software Evaluation*. Inria, 14th Jan. 2021. URL: https://hal.inria.fr/hal-03110728.

[17] J. A. Carrillo, M. Parisot and Z. Szymańska. *Mathematical Modelling of Collagen Fibers Rearrangement During Tendon Healing Process*. 8th Apr. 2020. URL: https://hal.inria.fr/hal-02537528.

11.3 Cited publications

[18] R. Abgrall, C. Dobrzynski and A. Froehly. ‘A method for computing curved meshes via the linear elasticity analogy, application to fluid dynamics problems’. In: *International Journal for Numerical Methods in Fluids* 76.4 (2014), pp. 246–266.

[19] R. Abgrall, H. Beaugendre and C. Dobrzynski. ‘An immersed boundary method using unstructured anisotropic mesh adaptation combined with level-sets and penalization techniques’. In: *Journal of Computational Physics* 257 (2014), pp. 83–101. URL: https://hal.inria.fr/hal-00940302.

[20] R. Abgrall, P. M. Congedo and G. Geraci. ‘A One-Time Truncate and Encode Multiresolution Stochastic Framework’. In: *Journal of Computational Physics* 257 (Jan. 2014), pp. 19–56. URL: https://hal.inria.fr/hal-00851760.

[21] F. Alauzet and G. Olivier. ‘Extension of metric-based anisotropic mesh adaptation to time-dependent problems involving moving geometries’. In: *49th AIAA Aerospace Sciences Meeting and Exhibit, Orlando (FL)*. AIAA paper 2011-0896. 2011.

[22] L. Arpaia, A. Filippini, P. Bonneton and M. Ricchiuto. ‘Modelling analysis of tidal bore formation in convergent estuaries’. In: *36th International Association for Hydro-Environnement Engineering and Research (IAHR) World Conference*. submitted to *Ocean Modelling*. The Hague, Netherlands, June 2015. URL: https://hal.inria.fr/hal-01169254.

[23] L. Arpaia and M. Ricchiuto. ‘r-adaptation for shallow water flows: conservation, well balancedness, efficiency’. In: *Computers & Fluids* 160 (2017), pp. 175–203.

[24] H. Beaugendre and F. Morency. ‘Development of a Second Generation In-flight Icing Simulation Code’. In: *Journal of Fluids Engineering* 128 (2006).

[25] H. Beaugendre, F. Morency, F. Gallizio and S. Laurens. ‘Computation of Ice Shedding Trajectories Using Cartesian Grids, Penalization, and Level Sets’. In: *Modelling and Simulation in Engineering* 2011 (2011), pp. 1–15. URL: https://hal.inria.fr/hal-00653224.

[26] S. Bellec, M. Colin and M. Ricchiuto. ‘Discrete asymptotic equations for long wave propagation’. In: *SIAM J. Numer. Anal.* 54 (2016), pp. 3280–3299.

[27] L. Bennani, P. Villedieu, M. Salaun and P. Trontin. ‘Numerical simulation and modeling of ice shedding: Process initiation’. In: *Computers & Structures* 142 (2014), pp. 15–27.

[28] Y. Bourgault, H. Beaugendre and W. Habashi. ‘Development of a Shallow-Water icing model in FENSAP-ICE’. In: *Journal of Aircraft* 37 (2000).

[29] C. Bresten, S. Gottlieb, Z. Grant, D. Higgs, D. Ketcheson and A. Németh. ‘Strong Stability Preserving Multistep Runge-Kutta Methods’. In: *arXiv:1307.8058 [math.NA]* (2014).

[30] M. Brocchini. ‘A reasoned overview on Boussinesq-type models: the interplay between physics, mathematics and numerics’. In: *Proc. Royal Soc. A* 469 (2014).

[31] C. Budd, W. Huang and R. Russell. ‘Adaptivity with moving grids’. In: *Acta Numerica* 18 (May 2009), pp. 111–241.

[32] D. Caraeni and L. Fuchs. ‘Compact third-order multidimensional upwind discretization for steady and unsteady flow simulations’. In: *Computers and Fluids* 34.4-5 (2005), pp. 419–441.

[33] A. J. Christlieb, Y. Liu and Z. Xu. ‘High order operator splitting methods based on an integral deferred correction framework’. In: *Journal of Computational Physics* 294 (2015), pp. 224–242. DOI: http://dx.doi.org/10.1016/j.jcp.2015.03.032. URL: http://www.sciencedirect.com/science/article/pii/S0021999115001795.

[34] C. Cluzel, E. Baranger, P. Ladevèze and A. Mouret. ‘Mechanical behaviour and lifetime modelling of self-healing ceramic-matrix composites subjected to thermomechanical loading in air’. In: *Composites Part A: Applied Science and Manufacturing* 40.8 (2009), pp. 976–984.

[35] C. F. D. Committee. *Guide for the Verification and Validation of Computational Fluid Dynamics Simulations*. American Institute for Aeronautics and Astronautics, 1998.

[36] P. Congedo, J. Witteveen and G. Iaccarino. 'A simplex-based numerical framework for simple and efficient robust design optimization'. In: *Computational Optimization and Applications* 56 (2013), pp. 231–251.

[37] P. M. Congedo, P. Cinnella and C. E. Corre. 'Numerical investigation of dense-gas effects in turbomachinery'. In: *Computers and Fluids* 49.1 (2011), pp. 290–301. URL: https://hal.inria.fr/inria-00601545.

[38] G. Couégnat, G. L. Vignoles, V. Drean, C. Mulat, W. Ros, G. Perrot, T. Haurat, J. El-Yagoubi, M. Eric, M. Ricchiuto, C. Germain and M. Cataldi. 'Virtual material approach to self-healing CMCs'. In: *4th European Conference for Aerospace Sciences (EUCASS)*. Saint Petersurg, Russia, July 2011. URL: https://hal.archives-ouvertes.fr/hal-00624479.

[39] C. Dapogny, C. Dobrzynski and P. Frey. 'Three-dimensional adaptive domain remeshing, implicit domain meshing, and applications to free and moving boundary problems'. In: *Journal of Computational Physics* 262 (Apr. 2014), pp. 358–378. URL: https://hal.archives-ouvertes.fr/hal-01110395.

[40] Z. Demirbilek, A. Zundel and O. Nwogu. 'Boussinesq Modeling of Wave Propagation and Runup over Fringing Coral Reefs, Model Evaluation Report'. In: *Coastal and Hydraulics Laboratory Technical Note CHLTR0712*. Vicksburg, MS: U.S. Army Engineer Research and Development Center. 2007.

[41] V. A. Dobrev, T. V. Kolev and R. N. Rieben. 'High order curvilinear finite elements for elasticoplastic Lagrangian dynamics'. In: *Journal of Computational Physics* 257, Part B (2014). Physics-compatible numerical methods, pp. 1062–1080. DOI: http://dx.doi.org/10.1016/j.jcp.2013.01.015. URL: http://www.sciencedirect.com/science/article/pii/S0021999113000466.

[42] C. Dobrzynski, P. Frey, B. Mohammadi and O. Pironneau. 'Fast and accurate simulations of air-cooled structures'. In: *Computer Methods in Applied Mechanics and Engineering* 195 (2006), pp. 3168–3180. URL: https://hal.archives-ouvertes.fr/hal-00112976.

[43] V. Drean, G. Perrot, G. Couégnat, M. Ricchiuto and G. Vignoles. 'Image-Based 2D Numerical Modeling of Oxide Formation in Self-Healing CMCs'. In: *Developments in Strategic Materials and Computational Design III*. John Wiley & Sons, Inc., 2013, pp. 117–125. URL: http://dx.doi.org/10.1002/9781118217542.ch11.

[44] M. Dumbser. 'Arbitrary high order PNPM schemes on unstructured meshes for the compressible Navier-Stokes equations'. In: *Computers & Fluids* 39.1 (2010), pp. 60–76.

[45] C. Eskilsson, J. Palm, A. P. Engsig-Karup, U. Bosi and M. Ricchiuto. 'Wave Induced Motions of Point-Absorbers: a Hierarchical Investigation of Hydrodynamic Models'. In: *11th European Wave and Tidal Energy Conference (EWTEC)*. Nantes, France, Sept. 2015. URL: https://hal.archives-ouvertes.fr/hal-01168780.

[46] A. Filippini, M. Kazolea and M. Ricchiuto. 'A flexible genuinely nonlinear approach for nonlinear wave propagation, breaking and runup'. In: *Journal of Computational Physics* 310 (2016).

[47] H. Hébert, S. Abadie, M. Benoit, R. Créach, C. Duluc, A. Frère, A. Gailler, S. Garziglia, Y. Hayashi, A. Lemoine, A. Loevenbruck, O. Macary, A. Maspataud, R. Marcer, D. Morichon, R. Pedreros, V. Rebour, M. Ricchiuto, F. Schindelé, R. S. Jacinto, M. Terrier, S. Toucanne, P. Traversa and D. Violeau. 'TANDEM (Tsunamis in the Atlantic and the English ChaNnel: Definition of the Effects through numerical Modeling): a French initiative to draw lessons from the Tohoku-oki tsunami on French coastal nuclear facilities'. In: *EGU 2014 General Assembly*. Vienna, 2014.

[48] M. Hubbard. 'Non-oscillatory third order fluctuation splitting schemes for steady scalar conservation laws'. In: *Journal of Computational Physics* 222.2 (2007), pp. 740–768.

[49] D. Isola, A. Guardone and G. Quaranta. 'Arbitrary Lagrangian Eulerian formulation for two-dimensional flows using dynamic meshes with edge swapping'. In: *J. Comp. Phys.* 230 (2011), pp. 7706–7722.

[50] H. Jia and K. Li. 'A third accurate operator splitting method'. In: *Mathematical and Computer Modelling* 53.102 (2011), pp. 387–396. DOI: http://dx.doi.org/10.1016/j.mcm.2010.09.005. URL: http://www.sciencedirect.com/science/article/pii/S089571771000436X.

[51] M. Kazolea, A. Delis and C. Synolakis. 'Numerical treatment of wave-breaking on unstructured finite volume approximations for extended Boussinesq-type equations'. In: *Journal of Computational Physics* 271 (2014).

[52] M. Kazolea, N. Kalligeris, N. Maravelakis, C. E. Synolakis, A. Delis and P. J. Lynett. 'Numerical study of wave conditions for the old Venetian harbour of Chania in Crete, Greece'. In: *36th International Association for Hydro-Environnement Engineering and Research (IAHR) World Conference*. The Hague, Netherlands, June 2015.

[53] M. Kazolea and M. Ricchiuto. 'On wave breaking for Boussinesq-type models'. In: *Ocean Modelling* 123 (2018), pp. 16–39.

[54] A. Kennedy, J. T. Kirby and R. Dalrymple. 'Boussinesq modeling of wave transformation, breaking and runup. Part I: 1D'. In: *J. Waterw. PortCoast. Ocean Eng.* 126 (2000), pp. 39–47.

[55] D. Ketcheson, C. Macdonald and S. Ruuth. 'Spatially partitioned embedded Runge-Kutta mehods'. In: *SIAM J. Numer. Anal.* 51.5 (2013), pp. 2887–2910.

[56] N. Kroll, T. Leicht, C. Hirsch, F. Bassi, C. Johnston, K. Sorensen and K. Hillewaert. 'Results and Conclusions of the European Project IDIHOM on High-Order Methods for Industrial Aerodynamic Applications'. In: *53rd AIAA Aerospace Sciences Meeting*. 2015.

[57] A. Loseille and F. Alauzet. 'Continuous mesh framework, Part II: validations and applications'. In: *SIAM in Numerical Analysis* 49.1 (2011).

[58] A. Loseille, A. Dervieux, P. Frey and F. Alauzet. 'Achievement of global second-order mesh convergence for discontinuous flows with adapted unstructured meshes'. In: *18th AIAA Computational Fluid Dynamics Conference, Miami (FL)*. AIAA paper 2007-4186. 2007.

[59] T. Lundquist and J. Nordstrom. 'The SBP-SAT technique for initial value problems'. In: *Journal of Computational Physics* 270 (2014), pp. 86–104.

[60] A. Mazaheri and H. Nishikawa. 'Very efficient high-order hyperbolic schemes for time-dependent advection-diffusion problems: Third-, fourth-, and sixth-order'. In: *Computers and Fluids* 102 (2014), pp. 131–147.

[61] G. Mengaldo, D. de Grazia, D. Mozey, P. Vincent and S. Sherwin. 'Dealiasing techniques for high-order spectral element methods on regular and irregular grids'. In: *Journal of Computational Physics* 299 (2015), pp. 56–81.

[62] F. Morency, H. Beaugendre and F. Gallizio. 'Aerodynamic force evaluation for ice shedding phenomenon using vortex in cell scheme, penalisation and level set approaches'. In: *International Journal of Computational Fluid Dynamics* 26.9-10 (2012), pp. 435–450. URL: https://hal.inria.fr/hal-00768349.

[63] H. Nishikawa. 'First-, Second-, and Third-Order Finite-Volume Schemes for Diffusion'. In: *J.Comput.Phys.* 273 (2014), pp. 287–309. URL: http://www.hiroakinishikawa.com/My_papers/nishikawa_jcp2014v273pp287-309_preprint.pdf.

[64] H. Nishikawa. 'Beyond Interface Gradient: A General Principle for Constructing Diffusion Schemes'. In: *40th AIAA Fluid Dynamics Conference and Exhibit*. AIAA Paper 2010-5093. Chicago, 2010.

[65] L. Nouveau, H. Beaugendre, C. Dobrzynski, R. Abgrall and M. Ricchiuto. 'An explicit, adaptive, residual based splitting approach for the steardy and time dependent penalized Navier Stokes equations'. In: *Comput. Meth. Appl. Mech. Engrg.* 303 (2016), pp. 208–230.

[66] L. Nouveau, M. Ricchiuto and G. Scovazzi. 'High-Order Gradients with the Shifted Boundary Method: An Embedded Enriched Mixed Formulation for Elliptic PDEs'. In: *Journal of Computational Physics* (2019), p. 108898.

[67] L. Nouveau, H. Beaugendre, M. Ricchiuto, C. Dobrzynski and R. Abgrall. 'An adaptive ALE residual based penalization approach for laminar flows with moving bodies'. PhD thesis. INRIA Bordeaux, équipe CARDAMOM, 2016.

[68] O. Nwogu. 'Numerical prediction of breaking waves and currents with a Boussinesq model'. In: *Proceedings 25th International Conference on Coastal Engineering*. 1996.

[69] M. Papadakis, H. Yeong and I. Suares. 'Simulation of Ice Shedding from a Business Jet Aircraft'. In: *AIAA, Aerospace Sciences Meeting and Exhibit, 45 th, Reno, NV.* AIAA Paper 2007-506. 2007.

[70] *ParMmg version 1.3.0*. REPOSITORY: https://github.com/MmgTools/ParMmg.

[71] G. Perrot, G. Couégnat, M. Ricchiuto and G. Vignoles. '2D numerical modelling of the two-scale lifetime of self-healing CMCs'. In: *International Workshop on Testing and Modeling Ceramic and Carbon Matrix Composites.* Abstract review. ENS Cachan, France, June 2014.

[72] P.-O. Persson and J. Peraire. 'Curved mesh generation and mesh refinement using Lagrangian solid mechanics'. In: *Proc. of the 47th AIAA Aerospace Sciences Meeting and Exhibit.* LBNL-1426E. Ernest Orlando Lawrence Berkeley National Laboratory, Berkeley, CA (US). 2008.

[73] F. Rebillat. 'Advances in self-healing ceramic matrix composites'. In: *Advances in Ceramic Matrix Composites.* Ed. by I. Low. Woodhead, 2014, pp. 369–409.

[74] P. J. Roache. *Verification and validation in computational science and engineering.* Albuquerque, NM: Hermosa, 1998. URL: https://cds.cern.ch/record/580994.

[75] V. Roeber, K. Cheung and M. Kobayashi. 'Shock-capturing Boussinesq-type model for nearshore wave processes'. In: *Coastal Engineering* 57 (2010), pp. 407–423.

[76] L. Shi, Z. Wang, L. Zhang, W. Liu and S. Fu. 'A PnPm CPR Framework for Hyperbolic Conservation Laws'. In: *Journal of Scientific Computing* 61.2 (2014), pp. 281–307.

[77] T. Song, A. Main, G. Scovazzi and M. Ricchiuto. 'The shifted boundary method for hyperbolic systems: Embedded domain computations of linear waves and shallow water flows'. In: *Journal of Computational Physics* 369 (2018), pp. 45–79.

[78] P. Thoutireddy and M. Ortiz. 'A variational r-adaption and shape-optimization method for finite-deformation elasticity'. In: *International Journal for Numerical Methods in Engineering* 61.1 (2004), pp. 1–21. DOI: 10.1002/nme.1052. URL: http://dx.doi.org/10.1002/nme.1052.

[79] M. Tissier, P. Bonneton, F. Marche, F. Chazel and D. Lannes. 'A new approach to handle wave breaking in fully non-linear Boussinesq models'. In: *Coastal Engineering* 67 (2012), pp. 54–66. DOI: http://dx.doi.org/10.1016/j.coastaleng.2012.04.004. URL: http://www.sciencedirect.com/science/article/pii/S0378383912000749.

[80] M. Tonelli and M. Petti. 'Hybrid finite volume-finite difference scheme for 2DH improved Boussinesq equations'. In: *Coastal Engineering 56* (2009), pp. 609–620.

[81] M. Tonelli and M. Petti. 'Simulation of wave breaking over complex bathymetries by a Boussinesq model'. In: *Journal of Hydraulic Research* 49.4 (2011), pp. 473–486.

[82] P. Tran, P. Benquet, G. Baruzzi and W. Habashi. 'Design of Ice Protection Systems and Icing Certification Through Cost - Effective Use of CFD'. In: *AIAA Aerospace Sciences Meeting and Exhibit.* AIAA-CP 2002-0382. 2002.

[83] F. Vilar, P.-H. Maire and R. Abgrall. 'A discontinuous Galerkin discretization for solving the two-dimensional gas dynamics equations written under total Lagrangian formulation on general unstructured grids'. In: *Journal of Computational Physics* 276 (2014), pp. 188–234.

[84] J. Waltz, N. R. Morgan, T. R. Canfield, M. R. J. Charest and J. G. Wohlbier. 'A nodal Godunov method for Lagrangian shock hydrodynamics on unstructured tetrahedral grids'. In: *International Journal for Numerical Methods in Fluids* 76.3 (2014), pp. 129–146. DOI: 10.1002/fld.3928. URL: http://dx.doi.org/10.1002/fld.3928.

[85] L. Wang and P.-O. Persson. 'A high-order discontinuous Galerkin method with unstructured space-time meshes for two-dimensional compressible flows on domains with large deformations'. In: *Comput. & Fluids* 118 (2015), pp. 53–68.

[86] J. Weber. 'WEC Technology Readiness and Performance Matrix, finding the best research technology development trajectory'. In: *4th International Conference on Ocean Engineering - ICOE.* 2012.