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2021
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 Project-Team: 2016 June 01

Keywords

Computer sciences and digital sciences

- A6.1.1. – Continuous Modeling (PDE, ODE)
- A6.1.4. – Multiscale modeling
- A6.1.5. – Multiphysics modeling
- A6.2. – Scientific computing, Numerical Analysis & Optimization
- A6.2.1. – Numerical analysis of PDE and ODE
- A6.2.8. – Computational geometry and meshes
- A6.3. – Computation-data interaction
- A6.3.4. – Model reduction
- A6.3.5. – Uncertainty Quantification
- A6.5.2. – Fluid mechanics

Other research topics and application domains

- B3.3.2. – Water: sea & ocean, lake & river
- B3.3.3. – Nearshore
- B3.4.1. – Natural risks
- B4.3.2. – Hydro-energy
- B5.2.1. – Road vehicles
- B5.2.3. – Aviation
- B5.2.4. – Aerospace
- B5.5. – Materials

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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 1st, 2015 ([website](#)).

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 extent optimization and inverse modelling. These skills 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 CARDAMOM is to provide improved analysis and design tools for engineering applications involving fluid flows with moving fronts. In our applications *a front is either an actual material interface, a boundary of the domain, or a well identified 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 [92, 37]. Another application, relevant for space reentry, is the study of transitional regimes in high altitude gas dynamics in which extremely thin layers appear in the flow which cannot be analysed with classical continuous models (Navier-Stokes equations) used by engineers [44, 64]. A classical example relevant in coastal engineering is free surface flows. The free surface itself is a material interface, but we can identify also other fronts as e.g. the flooding line (wet/dry transition) or the transition between propagating and breaking waves, across which relevance of dissipation and vorticity changes dramatically [45]. For wave energies, as well as for aquifers, the transition between free surface and congested flows (below a solid surface) is another example [56]. Other similar examples exist in geophysics, astrophysics, aeronatic and aerospace engineering, civil engineering, energy engineering, material engineering, etc.

In all cases, computationally affordable, fast, and accurate numerical modelling is essential to allow reliable predictions in early stages of the design/analysis [94]. Such computational models are also needed for simulations over very long times, especially if changes in many variable input parameters need to be investigated.

To achieve this goal one needs to have a physically relevant Partial Differential Equation (PDE) model, which can be treated numerically efficiently and accurately, which means possibly with some adaptive numerical technique allowing to minimize the computational effort. To this end, the dynamics of some of the fronts can be modelled by appropriate asymptotic/homogenised PDEs, while other interfaces are explicitly described. Even in the best of circumstances in all practical applications the reliability of the numerical predictions is limited by the intrinsic uncertainty on the operational conditions (e.g. boundary/initial conditions, geometry, etc.). To this *aleatory* uncertainty we must add the structural *epistemic* uncertainty related possibly to the use of approximate PDE models. Besides the limited validity of the derivation assumptions, these models are often calibrated/validated with experimental data which is itself subject to errors and post-processing procedures (filtering, averaging, etc ..) [50, 83]. This is even worse in complex flows for which measurements are difficult or impossible to plan or perform due to the inherent exceptional character of the phenomenon (e.g. tsunami events), or technical issues and danger (e.g. high temperature reentry flows, or combustion), or impracticality due to the time scales involved (e.g. study of some new materials' micro-/meso- structure [51]). So the challenge is to construct computationally affordable models robust under variability of input parameters due to uncertainties, certification/optimization, as well as 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 and objectives

We propose a research program mixing asymptotic PDE analysis, high order adaptive discretizations, and uncertainty quantification. In a standard approach a certification study can be described as a modelling exercise involving two black boxes. The first box is the computational model itself, composed of: PDE system, mesh generation/adaptation, and discretization of the PDE (numerical scheme). The second box is the main robust certification loop which contains separate boxes involving the evaluation of the physical model, the post-processing of the output, and the exploration of the spaces of physical and stochastic parameters (uncertainties). Many interactions exist in this process. Exploiting these interactions could allow to tap as much as possible into the potential of high order methods [68] such as e.g. h-, p-, r- adaptation in the physical model w.r.t. some parametric quantity/sensitivity non necessarily associated to the solution's smoothness.

Our objective is to provide some fundamental advances allowing to bring closer to the operational level modern high order numerical techniques and multi-fidelity certification and optimization algorithms, possibly using some clever paradigm different from the 2-black box approaches above, and involving tight interactions between all the parts of the play: PDE modelling, numerical discretization techniques, uncertainty quantification methods, mesh generation/adaptation methods, physical model validation/calibration, etc. The initial composition of the team provided a unique combination of skills covering all the necessary topics allowing to explore such an avenue. The questions that need to be

tackled can be organized in the following main axes/scientific questions:

1. Continuous modelling: how to obtain the PDE description most suited for a given application, and make sure that on one hand its structure embeds sufficiently the physics studied, and on the other the system is in a form suitable for efficient numerical discretization ?
2. Higher order adaptive discretization: what are the relations between PDE model accuracy (e.g. asymptotic error), PDE constraints (e.g. entropy inequalities, particular steady states, etc) and the scheme consistency ? how to account for additional constraints in the scheme ?
3. Parameter uncertainty and robust modelling: how to properly account when build models on one hand for the variability of physical states defining a process in realistic environments, and on the other of data possibly available for the process in consideration ? is it possible to couple the sampling in the space of parameters with the approximation in physical space ?

These themes are discussed in the following sections together with some challenges specific to the engineering applications considered:

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

3 Research program

3.1 Continuous and discrete asymptotic modelling

In many of the applications we consider intermediate fidelity models can be derived using an asymptotic expansion for the relevant scale resolving PDEs, possibly combined with some form of homogenization or averaging. The resulting systems of PDEs are often very complex. One of the main challenges is to characterize the underlying structure of such systems: possible conservation laws embedded; additional constraints related to consistency with particular physical states (exact solutions), or to stability (entropy/energy dissipation); etc. A question of paramount importance in practical applications is also the formulation of the boundary conditions. The understanding of these properties is necessary for any new model. Moreover, different forms of the PDE may be better suited to enforce some of these properties at the numerical level.

Another issue when working with asymptotic approximations is that of closure. Indeed, important physical phenomena may be unaccounted for either due to some initial modelling assumptions, or because they involve scales much smaller than those modelled. A typical example is wave breaking in some depth averaged models. Another, relevant for our work, is the appropriate prediction of heat fluxes in turbulent flows.

So our main activities on this axis can be classified according to three main questions:

- what is the structure of the PDE model (exact solutions, stability and algebraic or differential constraints embedded, boundary conditions) ?
- what is the form of the model better suited to reproduce numerically certain constraints ?
- how to embed and design closure laws for relevant phenomena not modelled by the main PDE ?

3.2 High order discretizations on moving adaptive meshes

The efficient and robust discretization of complex PDEs is a classical and widespread research subject. The notion of efficiency is in general related to the combination of high order of accuracy and of some adaptation strategy based on an appropriate model of the error [85, 93].

This strategy is of course also part of our work. However, we are convinced that a more effective path to obtain effective discretizations consists in exploiting the knowledge of the PDE structure, embedding as much as possible the PDE structure in the discrete equations. This is related to the notion of enhanced consistency that goes in the direction of what is today often referred to as *constraint or property preserving* discretizations. For the type of PDE systems of our interest, the properties which are of paramount importance to be controlled are for example: the balance between flux divergence and forcing terms (so called well balanced or C-property [40, 82]) and the preservation of some specific steady states; the correct reproduction of the dispersion relation of the system, especially but not only for dispersive wave propagation; the preservation of some algebraic constraints, typically the non-negativity of some thermodynamic quantities; the respect of a discrete entropy/energy equality or inequality (for stability); the strong consistency with some asymptotic limit of the PDE (AP property); etc.

A fundamental issue is the efficient and accurate treatment of boundary and interface conditions. The idea is to have some approach which tolerates the use of non-conformal meshes, which is genuinely high order, and compatible with adaptation, and of course conformal meshing of the boundary/discontinuity. Techniques allowing the control of the geometrical error due to non-conformity is required. For discontinuities, this also requires an ad-hoc treatment of the jump condition. For wall boundaries, initial work using penalization has been done in CARDAMOM in the past [34, 74]. On Cartesian meshes several techniques exist to control the consistency order based on extrapolation/interpolation, or adaptive methods (cf e.g. [87, 73, 35, 48, 58, 52] and references therein). For discontinuities, we can learn from fitting techniques [41], and from some past work by Prof. Glimm and co-workers [46].

For efficiency, mesh adaptation plays a major role. Mesh size adaptation based on both deformation, r-adaptation, or remeshing h-adaptation, can be designed based on some error model representative. For unsteady flows, the capability to use moving meshes becomes necessary, and geometrical conservation (GCL) needs to be added to the list of constraints to be accounted for [88, 70]. In particular, one technique that provides meshes with optimal quality moving together with the unsteady flows, reduction of errors due to convective terms, GCL respected up to machine precision, and high order of accuracy, is offered by the Direct Arbitrary-Lagrangian-Eulerian (ALE) methods on moving Voronoi meshes with topology changes [60, 59] that will be further investigated.

3.3 Applications in physics and engineering

Some of the developments of the last years involve the application of the methods/models developed in applied studies. For example research in UQ is more focused on a black-box approach, however with an industrial perspective. In this sense, methods should be able to work with very expensive computer codes (physical samples), and with a very large number of uncertainties (order of hundreds), and still be able to evaluate single runs and provide as efficiently as possible reliable estimations in for sensitivity analysis, building of metamodels, optimization of design parameters, etc. A second example is the usage of free surface flow models in order to study realistic physical phenomena for tidal bores and tsunami waves. In this spirit, we can roughly divide our work in three main sub-axis. 1. Geophysics, 2. Aerospace science/icing, 3. Industrial problems related to materials for space re-entry objects.

4 Application domains

4.1 De-anti icing systems

Impact of large ice debris on downstream aerodynamic surfaces and ingestion by aft mounted engines must be considered during the aircraft certification process. It is typically the result of ice accumulation on unprotected surfaces, ice accretions downstream of ice protected areas, or ice growth on surfaces due to delayed activation of ice protection systems (IPS) or IPS failure. This raises the need for accurate ice trajectory simulation tools to support pre-design, design and certification phases while improving cost efficiency. Present ice trajectory simulation tools have limited capabilities due to the lack of appropriate experimental aerodynamic force and moment data for ice fragments and the large number of variables that can affect the trajectories of ice particles in the aircraft flow field like the shape, size, mass, initial velocity, shedding location, etc... There are generally two types of model used to track shed ice pieces. The first type of model makes the assumption that ice pieces do not significantly affect the flow. The

second type of model intends to take into account ice pieces interacting with the flow. We are concerned with the second type of models, involving fully coupled time-accurate aerodynamic and flight mechanics simulations, and thus requiring the use of high efficiency adaptive tools, and possibly tools allowing to easily track moving objects in the flow. We will in particular pursue and enhance our initial work based on adaptive immersed boundary capturing of moving ice debris, whose movements are computed using basic mechanical laws.

In [38] 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 [34, 74]. In these methods we compensate for the error at solid walls introduced by the penalization by using anisotropic mesh adaptation [54, 71, 72]. 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 [39]. 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 [43, 37] we will develop appropriate asymptotic PDE approximations to describe the water runoff on the wing surface, also accounting for phase change, thus allowing to describe the ice formation and possibly rupture and detachment. 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 [78], 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 Modeling of wave energy converters

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 [94], 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.

Our previous work [56][42] has shown the potential of depth-averaged models for simulating wave energy devices. The approach followed so far relies on an explicit coupling of the different domains involving the flow under the structure and the free surface region. This approach has the advantage to need efficient solvers of well-known system of equations (compressible and incompressible flow). However, the transmission condition between this two regimes is now always well understood, depending on the underlying PDE models. Moreover, several sources of numerical instabilities exist because of

the different nature of the regions involved (compressible/incompressible). A different approach is proposed in [63, 62], and will be pursued in the coming years. The idea is to solve a unique model in the whole computational domain, with the effect of the structure being accounted for by means of an appropriate pressure variable playing the role of a Lagrange multiplier. Our numerical developments will be performed with the parallel platform GeoFun, based on the Aerosol library. In order to simulate the dynamic of the floating structures, we will consider the coupling with the open source code tChrono¹, an external code specialized in the resolution of the rigid body dynamics. The coupling is still under development. In parallel, we will add closure for other complex physical effects as e.g. the modeling of air pocket trapped under the structures. Several industrial processes (SeaTurns, Hace...) are based on chamber compressing air inside by the movement of the water surface. This strategy has the advantage of taking the turbines for energy production out of the water. The strategy is based on a polytropic modeling of the gas dynamics taking into account merging and splitting of the pockets, without a major impact on the efficiency of the simulation (robustness and numerical cost). This works benefits of the associated team LARME with RISE (C. Eskilson).

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. 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 [81].

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

In collaboration with the LCTS laboratory (a joint CNRS-CEA-SAFRAN-Bordeaux University lab devoted to the study of thermo-structural materials in Bordeaux), we are developing a multi-scale model in which a structural mechanics solver is coupled with a closure model for the crack physico chemistry. This model is obtained as a multi-dimensional asymptotic crack averaged approximation for the transport equations (Fick's laws) with chemical reactions sources, plus a potential model for the flow of oxide [51, 55, 80]. 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. [49]) 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

¹Project Chrono: An Open Source Multi-physics Simulation Engine

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 approximation and numerical approximation. This is extremely important in several ways. An example is the capability of a numerical model to handle highly dispersive wave propagation. This is usually done by high accuracy asymptotic PDE expansions or by means of multilayer models. In the first case, there is an issue with the constraints on the numerical approximation. Investigations of appropriated error models for adaptivity in the horizontal may permit to alleviate some of these constraints, allowing a reasonable use of lower order discretizations. Concerning multi-layer models, we plan can use results concerning the relations between vertical asymptotic expansions and truncation/approximation error to improve the models by some adaptive approach.

Another important aspect which is not understood well enough at the moment is the role of dissipation in the evolution of the free surface dynamics, and of course in wave breaking regions. There are several examples of breaking closure, going from algebraic and PDE-based eddy viscosity methods [67, 84, 77, 53], to hybrid methods coupling dispersive PDEs with hyperbolic ones, and trying to mimic wave breaking with travelling bores [90, 91, 89, 65, 57]. In both cases, numerical dissipation plays an important role and the activation or not of the breaking closure, as well as on the establishment of stationary travelling profiles, or on the appearance of solitary waves. These aspects are related to the notion of numerical dissipation, and to its impact on the resulting numerical solutions. These elements must be clarified to allow full control of adaptive techniques for the models used in this type of applications.

A fundamental issue that needs to be addressed is the proper discrete formulation of the boundary conditions for dispersive wave approximations. These conditions play of course a critical role in applications and remain an open problem for most Boussinesq models.

4.5 Geophysics and astrophysics

This work is related to large scale simulations requiring the solution of PDEs on manifolds. Examples are tsunami simulations, as those performed in the past in the **TANDEM** project, as well as some applications considered in the ANR LAGOON for climate change. The MSCA project SuPerMan proposes applications in astrophysics which also involve similar issues. The idea is to consider both coordinate changes related to mesh movement, as in ALE formulations, as well as genuinely space-time manifolds as in hyperbolic reformulations of relativity [10], and combinations of both when for example considered mesh movement and adaptation in curvilinear coordinates [36]. Challenges are related to the appropriate PDE formulation, and the respect of continuous constraints at the discrete level.

The objective here is to devise the most appropriate manifold representation, and formulate the PDE system in the appropriate way allowing to embed as many continuous constraints as possible (well balancing, energy conservation, positivity preservation, etc). Embedding the ALE mapping will be necessary to envisage adaptive strategies, improving on [36] and [61].

Geophysical applications are of interest for BRGM, while the more exploratory application to general relativity of the MSCA project SuPerMan will push the numerical discretizations to their limit, due to the great complexity of the model, and allow new collaborations in the domain of astrophysics, as e.g. with Max Planck institute.

5 Highlights of the year

- Elena Gaburro obtained the Marie Curie Individual Fellowship (MSCA-IF) *SuPerMan* (Structure Preserving schemes for Conservation Laws on Space Time Manifolds), funded by the Horizon 2020 programme.
- We co-organized the fourth edition of the B'Waves workshop on wave breaking has been organized as a virtual event. As in previous editions, leading scientists in the field of wave dynamics have

contributed to the talks, which have been hosted by Springer Nature with more than 200 registered participants. More information on the [main page of Springer Nature](#) and on the [dedicated page at Inria](#).

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 2021, the development of the library was focused on the following points

- * Development environment - Plugin : Uhaina, GeoFun, allow for plugins to register numerical schemes. - Time dependent data variables. - CI on Plafrim, intel compiler, Clang compiler
- * General numerical feature of the library - Implementation of the Taylor finite element basis. - Implementation of the Gauss-Lobatto finite element basis for quads and lines - Implementation of higher order derivatives into finite element basis. - Crouzeix-Raviart, Rannacher-Turek nonconforming methods for the Laplace equation. - Dual consistent integration of source term involving gradients
- * Work on SBM methods
- * Low Mach number flows: - Implementation of the Euler and Waves models with porosity - initialization of a vector with a potential function. - Implementation of the Bouchut-Chalons-Guisset numerical flux. - Low Mach number filtering.
- * CG implementations: - Implementation of cubature elements with mass lumping - Development of the Continuous Interior Penalty method - parallel validation of CG

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

Contact: Vincent Perrier

Participants: Benjamin Lux, Damien Genet, Mario Ricchiuto, Vincent Perrier, H lo se Beaugendre, Subodh Madhav Joshi, Christopher Poette, Marco Lorini, Jonathan Jung, Enrique Gutierrez Alvarez, Anthony Bosco

Partner: BRGM

6.1.2 Mmg

Name: Mmg Platform

Keywords: Mesh adaptation, Anisotropic, Mesh generation, Mesh, Isovalue discretization

Scientific Description: The Mmg platform 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 patches. 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 platform 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 possibility 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.mmgttools.org>

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 of 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. It is dedicated to the modification of 3D volume meshes. It performs the adaptation and the optimization of a tetrahedral mesh and allows to discretize an isovalue.

Mmg3d performs local mesh modifications. The mesh is iteratively modified until the user prescribes satisfaction.

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

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.

Contact: Mario Ricchiuto

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 is 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 transformation processes, etc.

URL: <https://team.inria.fr/cardamom/sloWS-shallow-water-flows/>

Contact: Mario Ricchiuto

Participants: Maria Kazolea, Mario Ricchiuto

6.1.6 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 addition 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.

Contact: Algiane Froehly

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

6.1.7 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>

Contact: Algiane Froehly

Participants: Algiane Froehly, Luca Cirrottola

Partners: FUI Icarus, ExaQute

6.1.8 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.

Contact: Martin Parisot

Participants: Martin Parisot, Marco Lorini

6.1.9 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

Contact: Mario Ricchiuto

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

Partners: EPOC, IMAG, IMB

6.1.10 AleVoronoi

Name: Direct Arbitrary Lagrangian Eulerian Finite Volume and Discontinuous Galerkin schemes on VORONOI moving meshes with topology changes

Keywords: Finite volume methods, Discontinuous Galerkin, High order methods, Centroidal Voronoi tessellation, ALE, Fortran, OpenMP

Functional Description: Explicit, arbitrary high order accurate, one step (ADER), Finite Volume and Discontinuous Galerkin schemes on 2D moving Voronoi meshes for the solution of general first-order hyperbolic PDEs. Main peculiarity: the Voronoi mesh is moved according to the fluid flow using a direct Arbitrary-Lagrangian-Eulerian (ALE) method achieving high quality of the moving mesh for long simulation times. The high quality of the mesh is maintained thanks to a) mesh optimization techniques and b) the additional freedom of allowing topology changes. The high quality of the results is obtained thanks to the high order ADER schemes. The main novelty is the capability of using high-order schemes on moving Voronoi meshes with topology changes.

The code is written in Fortran + OpenMP.

Contact: Elena Gaburro

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

Geophysics. We have further generalized our work on the approximation of the shallow water equations in a more general setting. For large scale applications an improved representation of the sphere based on a local parametrization has been proposed and combined with an efficient discontinuous Galerkin (DG) approximation. The discretization exploits a hybrid 3D/2D-covariant form of the equations allowing to decouple the equations for the velocity, while retaining mass conservation. A correction to ensure the well-balanced character of the scheme, and in particular the preservation of both the lake at rest and of the inverted manometer states [36].

Astrophysics. In [10], we have presented a novel second order accurate well balanced (WB) finite volume (FV) scheme for the solution of the general relativistic magnetohydrodynamics (GRMHD) equations and the first order CCZ4 formulation (FO-CCZ4) of the Einstein field equations of general relativity, as well as the fully coupled FO-CCZ4 + GRMHD system. These systems of *first order hyperbolic* PDEs allow to study the dynamics of the *matter* and the dynamics of the *space-time* according to the theory of general relativity. The new well balanced finite volume scheme proposed in this work exploits the knowledge of an equilibrium solution of interest when integrating the conservative fluxes, the nonconservative products and the algebraic source terms, and also when performing the piecewise linear data reconstruction. This results in a rather simple modification of the underlying second order FV scheme, which, however, being able to cancel numerical errors committed w.r.t. the equilibrium component of the numerical solution, substantially improves the accuracy and long-time stability of the numerical scheme when simulating small perturbations of stationary equilibria. In particular, the need for well balanced techniques appears to be more and more crucial as the applications increase their complexity and a series of numerical tests of increasing difficulty shows how that the well balancing significantly improves the long-time stability of the finite volume scheme compared to a standard one, in particular for the study of neutron stars. This work has been presented at the NUMHYP 2021 conference in Trento (Italy) and at the Hirshegg Workshop in Austria.

Fundamental work on schemes. To reduce the costs associated with the DG finite element method in the previous approach we study the use of (both continuous and discontinuous) cubature elements allowing a considerable reduction of the number of operations, including a full diagonalization of the mass matrix. In [13] we have provided a first investigation of the fully discrete linear stability of continuous finite elements with different stabilization operators. The theoretical results are confirmed by numerical computations on linear and nonlinear problems, confirming the potential of the cubature approach in terms of CPU time for a given error. The multidimensional generalization of this study and its implementation on the sphere is being performed in the PhD of S. Michel. Some of these results have been presented at NUMHYP 2021 conference in Italy and at the ICOSAHOM conference (Vienna).

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 [21]. Further study is ongoing in the framework of the PhD of Lorenzo Micalizzi at U. Zurich, co-advised by R. Abgrall and M. Ricchiuto. This issue has been presented at the Oberwolfach workshop *Hyperbolic Balance Laws: modeling, analysis, and numerics* in February, and at the SIAM GS21 conference.

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.

This year we finalised our work related to understanding the approximation constraints related to the projection step on the solution of the Green-Naghdi (GN) model. The FV method is used to solve the hyperbolic part, while a standard P1 finite element method is used to solve the elliptic system associated to the dispersive correction. We study the impact of the reconstruction used in the hyperbolic phase; the representation of the FV data in the FE method used in the elliptic phase and their impact on the theoretical accuracy of the method; the well-posedness of the overall method. For the first element we proposed a systematic implementation of an iterative reconstruction providing on arbitrary meshes up to third order solutions, full second order first derivatives, as well as a consistent approximation of the second derivatives. These properties are exploited to improve the assembly of the elliptic solver, showing dramatic improvement of the final accuracy, if the FV representation is correctly accounted for. Concerning the elliptic step, the original problem is usually better suited for an approximation in $H(\text{div})$ spaces. However, it has been shown that perturbed problems involving similar operators with a small Laplace perturbation are well behaved in H^1 . We show, based on both heuristic and strong numerical evidence, that numerical dissipation plays a major role in stabilizing the coupled method, and not only providing convergent results, but also providing the expected convergence rates. The work [27] submitted for publication in Ocean modelling.

This year we also continued our work on wave breaking for Boussinesq type modeling and more precisely for the GN equations. Using the numerical model already described in [57] we attempted at providing some more understanding of the sensitivity of some closure approaches to the numerical set-up. More precisely and based on [66] 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 breaking parameters involved in each breaking model. The work presented in WCCM-ECCOMAS Congress 2020, which due to covid-19 held online on January 2021 [33]. The paper will soon be submitted for publication in Water Waves journal.

An other topic that we are working on is the coupling of dispersive shallow water models, by deriving asymptotic interface operators. As shown by Lannes [69] from the Zakharov-Craig-Sulem (ZCS) formulation it is possible to derive shallow-water models in near-shore wave regimes by obtaining approximate asymptotic solutions of a Laplace equation that describes the vertical variations of the flow, and then truncating two evolution equations on horizontal variables to the chosen truncation order. Here we use this fact to derive boundary conditions for coupling and/or domain-decomposition of dispersive and non-dispersive shallow-water equations. First, from the ZCS formulation we study different boundary operators to be used on the interface of a Schwarz- based domain decomposition method for the 2D (1D in horizontal) Laplace equation discretized with the finite element method. Then, by taking the limit to the shallow-water regime, we show how these operators can translate into boundary conditions for different shallow water models such as the GN and Non-Linear Shallow Water equations. Initially, we examine the performance of this approach with a numerical implementation of the linearized SGN system. The work has been accepted for presentation in WCCM-XV/APCOM-VIII conference, to be held

in Yokohama, Japan 31/07-5/08 2022. This work is a part of the PhD of Jose Galaz. Its a common PhD project with the Lemon Inria team.

This year we started to work on the use of a hybrid formulation combining the direct solution of a PDE with morel reduction for some closure term. This has been performed to try to alleviate the overheads related to the approximation of dispersive effects. The numerical evidence suggests that not only this is possible, but the resulting discrete model provides accurate predictions with computational savings of at least one order of magnitude, with increased robustness compared to fully reduced approximations [30]. This work opens the way to many developments the first of which will be related to the extension of the initial results to breaking waves, and to the multidimensional case.

The projection structure of the time-discrete Green-Naghdi equations allowed to answer to several open questions at the discrete level. In particular, we proposed in [28] a numerical treatment of the boundary conditions that ensure the whole scheme to be entropy-stable, following the strategy of the incompressible models. In addition, we are currently working on a well-balanced numerical scheme, i.e. a scheme able to preserved all the steady states even not at rest, still based on the projection structure.

7.3 Modelling of icing and de-icing of aircrafts

- Participants: Héloïse Beaugendre, Mathieu Colin
- 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 [14]. In the PhD of Gitsuzo De Brito Siqueira Tagawa, co-advised by François Morency (ETS Montreal) 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.

The effects of atmospheric icing can be anticipated by Computational Fluid Dynamics (CFD). Past studies show that the convective heat transfer influences the ice accretion and is itself a function of surface roughness. Uncertainty quantification (UQ) could help quantify the impact of surface roughness parameters on the reliability of ice accretion prediction. This paper [11] aims to quantify ice accretion uncertainties and identify the key surface roughness correction parameters contributing the most to the uncertainties in a Reynolds-Averaged Navier-Stokes (RANS) formulation. Non-Intrusive Polynomial Chaos Expansion (NIPCE) metamodels are developed to predict the convective heat transfer and icing characteristics of the RANS database.

This year, the capabilities of the open-source SU2 CFD software, have been extended to 3D aircraft icing using the Eulerian droplet model formulation to solve the droplet impingement [18]. We also coded a Shallow Water Icing Model (SWIM) assuming that the shear stress driven runback film has a linear velocity profile in its thickness direction, with a non-slip condition at the water-wall interface [15]. The SWIM model enables to perform ice accretion simulations.

7.4 High order embedded and immersed boundary methods

- Participants: Héloïse Beaugendre, Tiffanie Carlier, Mirco Ciallella, Benjamin Constant, Elena Gaburro, Marco Lorini, 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 parabolic problems,

we are on one hand exploring 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 expansion truncated to the desired accuracy [75]. 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 [76], 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 performed 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 [86]. 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. Initial results, presented at the ECCOMAS Coupled Problems conference, are very encouraging. The method developed so far allows to achieve full order of accuracy in curved domains using linear meshes. 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 [47]. 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 been published in [9]. 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. We also investigate new visualization tools based on topological data analysis [16].

7.5 Composites Materials

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

On this application we have proposed and in depth characterization of the variability of the lifetime of a mini-composite (essentially a single tow) wrt the physical and model parameters. Tow failure depends on the statistical fibres initial strength, slow crack growth kinetic, and load transfer following fibres breakage, which is captured thanks to an approximate mechanical model. This approach has been applied to a virtual material consisting of Hi-Nicalon fibres immersed in an SiC/B4C matrix coating. Effects of temperature, spatial variation of the statistical distribution of fibres strength and applied load were examined in terms of material behaviour and lifetime prediction. The results prove the fundamental impact of the diffusion/reaction processes (healing) on the fibre breakage scenarios, highlighting the need

to model these processes appropriately. Besides, we show that the materials' lifetime is highly sensitive to the distribution of weak fibres and of their relative positions in the yarn completed a improved models for the progressive oxydation of the carbon fibers, and also some improvements 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 environmental as well as structural parameters. Work presented at the 8th ECCOMAS thematic conference COMPOSITES.

More work has been done this year to extend the modelling of the flow of the liquid oxide. Two approaches are compared: a lubrication approximation as well as an augmented shallow water system. The latter depends on a small parameter ϵ . In the limit ϵ goes to 0 we recover the lubrication model. The shallow water formulation however has the advantage to have an interesting structure involving a hyperbolic system, plus an operator which is skew symmetric wrt the L2 norm. This augmented system admits a conservation law for the total energy density, which is useful for numerical simulations. Numerical test are under progress to validate this new model.

7.6 Adaptation techniques

- Participants: Nicolas Barral, Héloïse Beaugendre, Luca Cirrottola, Algiane Froehly (SED), Elena Gaburro, 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 2021 has been pursued in the Cardamom team thanks to the [ExaQUte](#) European project funding the fixed-term engineering contract of Luca Cirrottola. A minor release has been published in 2021[79], to introduce parallel surface analysis and adaptation. These new functionalities have been integrated in several software couplings in 2021 thanks to external partners. Foremost by the European partner solver Kratos in its release 9.0 in November 2021, and as independent third-party initiatives in FreeFem and PETSc. Tasked-based parallelism using Mmg tools has started to be investigated within the European project [Microcard](#), where Algiane Froehly is leading a work package on the parallel generation of cardiac meshes for applications in cardiac electrophysiology, with the funding of Francesco Brarda fixed-term engineering contract and the Mariem Makni postdoc contract. This will also contribute to new research and developments on the handling of complex non-manifold geometries (originated for example from the membranes of the cardiac cells), and to the improvement of the software memory management also exploring shared-memory parallelization strategies. The source code, documentation and contributions to these projects are hosted at [github](#).

The work on goal-oriented mesh adaptation techniques for geophysical flows has continued, in the context of the collaboration with Imperial College London. The adjoint error model designed in previous years was applied to new cases.

Metric-based mesh adaptation methods were applied to advection-dominated tracer transport modelling problems in two and three dimensions, using the finite element package Firedrake [31]. In particular, the mesh adaptation methods considered are built upon goal-oriented estimates for the error incurred in evaluating a diagnostic quantity of interest (QoI). In the motivating example of modelling to support desalination plant outfall design, such a QoI could be the salinity at the plant inlet, which could be negatively impacted by the transport of brine from the plant's outfall. Four approaches were considered, one of which yields isotropic meshes. The focus on advection-dominated problems means that flows are often anisotropic; thus, three anisotropic approaches were also considered. Meshes resulting from each of the four approaches yield solutions to the tracer transport problem which give better approximations to QoI values than uniform meshing, for a given mesh size. The methodology was validated using an existing 2D tracer transport test case with a known analytical solution. Goal-oriented meshes for an idealised time-dependent desalination outfall scenario were also presented.

The modelling of a tidal array farm is an inherently multi-scale endeavour. It requires the simultaneous resolution of tidal processes across tens or hundreds of kilometres of coastal ocean (including estuaries, or even entire seas), the hydrodynamics in the neighbourhood of the farm (hundreds of metres), the wakes of individual turbines (metres, or tens of metres) and device hydrodynamics (sub-metre). As such, the construction of an accurate, computationally efficient numerical model requires careful consideration of the underlying discretisation. We applied time-dependent mesh adaptation techniques based on the Riemannian metric framework to an idealised tidal array and assessed the quality of the resulting approximations [32]. Whilst classical hierarchical mesh adaptation methods modify mesh element/cell size in order to improve resolution locally, the metric-based approach also allows for control of element shape and orientation, which can be especially advantageous for advection-dominated problems. Metrics are normalised in such a way that the resulting discretisation is multi-scale in both space and time. Typically, metrics are constructed from recovered derivatives of solution fields, such as fluid vorticity. Alternatively, metrics may be derived from goal-oriented error estimates, enabling accurate estimation of a diagnostic quantity of interest (QoI). In the context of tidal farm modelling, one clear QoI is the power output. Building upon the idealised steady-state test case considered in previous years, which represents turbines using a drag parametrisation in a depth-averaged shallow water model, we demonstrated that goal-oriented mesh adaptation can be used to obtain an accurate approximation of tidal farm power output using relatively few overall degrees of freedom.

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. In Cedrine Barandon's internship, we started to modify the classical hessian-based metric adaptation framework for applications in curvilinear coordinates on the sphere. The work on r-adaptation in 3D curved domains has aimed at improving the robustness of the approach. The idea of this work is to use a two-step procedure involving: an initial deformation of the mesh solving a Poisson equation with natural (homogenous) boundary conditions; a projection of the boundary nodes on the appropriate local spline approximation of the curved boundary. The main contribution of the work done is to write the update for the displacements by means of a nonlinear iterative projection allowing a full control on the non-negativity of the element volumes [8].

We have also started the development of a new code, called `AléVoronoi`: Direct Arbitrary Lagrangian Eulerian high order finite volume and discontinuous Galerkin schemes on VORONOI moving meshes with topology changes. The code is written in Fortran with the OpenMP parallel paradigm. It is arbitrary high order accurate, exploiting the ADER paradigm both for the Finite Volume and Discontinuous Galerkin case and can be already used for studying the Burgers equation, Euler equations, MHD equations, and the GPR model. The general purpose of the scheme is to be applied to any kind of first order hyperbolic PDEs. The work of 2021 has been devoted to make the code efficient, robust and accurate. The objective is to investigate the potential of previous work done of topology changing Voronoi meshes for adaptive simulations in several applications.

7.7 Modeling of flows in aquifers

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

The objective of this project is 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. A numerical scheme has been proposed and analysed. It satisfies a discrete entropy dissipation which ensure a strong stability. We also propose a model and a numerical strategy to take into account the air pockets that can be trapped under a impermeable structure. This work can also

be used for the simulation of some marine energy converters such as the solution of Seaturms of Hacc. In parallel, we work on the structure of the code in order to integrate more easily the further 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: Development of a numerical model for tsunamis: from propagation to breaking in realistic coastal environments.
- 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 based on ad hoc Lax-Wendroff finite difference methods combined with WENO approximations. The schemes are to be implemented in the code of CEA and applied to tsunami simulations in realistic coastal environments.

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: The aim of this work is to provide improved tools for the aerothermal dimensioning of a re-entry vehicle. Operational codes are based on Navier-Stokes averaged (RANS) equations and body-fitted structured meshes. The project aims at developing an LES code based on an existing DNS one (finite volumes, Cartesian mesh, hybrid parallelism, high order WENO type) to be enhanced with an SGSM closure adapted to hypersonic flows. The work will include immersed boundaries on Cartesian grids and to adapt the technique to re-entry flows. 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.

UNAINA intercarnot

- Title: développement d'une plateforme opérationnelle pour la simulation des risques côtiers (UHAINA)
- Duration: 30 months
- Starting date : 1st September 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, curvilinear coordinates, etc). Applications to storm surge and real tsunami events are sought.

9 Partnerships and cooperations

9.1 International initiatives

9.1.1 Associate Teams in the framework of an Inria International Lab or in the framework of an Inria International Program

LARME

Title: Large-scale simulations of renewable marine energy

Duration: 2021 ->

Coordinator: Claes Eskilsson (claes.eskilsson@ri.se)

Partners:

- Rise
- Aalborg University

Inria contact: Martin Parisot

Summary: LARME aims improving numerical methods for the simulation of renewable marine energy at large time and space scale. The vertical integrated models as well as the potential flow models are compared though the many scientific locks of this application: Multi-dimensional simulation, Improvement of water dynamics, Improvement of structure dynamics, High-Performance Computing, Validation of the strategies.

9.1.2 Inria associate team not involved in an IIL or an international program

ANEMONE

Title: AdvANced Embedded MethOds for flows with NonlinEar moving fronts

Duration: The project was approved at the end of 2019 and has been greatly affected by the sanitary crisis with virtually no activities taking place.

Coordinator: Guglielmo Scovazzi (guglielmo.scovazzi@duke.edu)

Partners:

- Duke University

Inria contact: Mario Ricchiuto

Summary: ANEMONE aims improving high order (second or more) embedded and immersed boundary methods to describe moving interfaces as well as moving boundary conditions on unstructured grids.

9.2 International research visitors

9.2.1 Visits of international scientists

- Philipp Rudolf Offner from Johannes Gutenberg Universitat, Department of Mathematics visited Mario Ricchiuto in Oct 2021, for three weeks. They worked on energy preserving numerical methods for hyperbolic equations.
- Jose Galaz Moralez from Inria Lemon team in Montpellier, visited Maria Kazolea in July 2021 and in October 2021 for three weeks in total to work on coupling methods for dispersive equations.

Inria International Chair

IIC ABGRALL Rémi

Name of the chair: Scientific Computing

Institution of origin: ETH Zurich, Institut für Mathematik & Computational Science

Country: Switzerland

Dates: From Tue Jan 01 2019 to Sun Dec 31 2023

Title: Numerical approximation of complex PDEs & Interaction between modes, schemes, data and ROMs

Summary: In 2021, he visited Inria from 01/02/2021 to 31/07/2021

9.3 European initiatives

9.3.1 FP7 & H2020 projects

ExaQute (730)

Title: EXAscale Quantification of Uncertainties for Technology and Science Simulation

Duration: 1/06/2018-30/11/2021

Coordinator: CIMNE

Partners:

- BARCELONA SUPERCOMPUTING CENTER - CENTRO NACIONAL DE SUPERCOMPUTACION (Spain)
- CENTRE INTERNACIONAL DE METODES NUMERICIS EN ENGINYERIA (Spain)
- ECOLE POLYTECHNIQUE FEDERALE DE LAUSANNE (Switzerland)
- INSTITUT POLYTECHNIQUE DE BORDEAUX (France)
- STR.UCTURE GMBH (Germany)
- TECHNISCHE UNIVERSITAET MUENCHEN (Germany)
- UNIVERSITAT POLITECNICA DE CATALUNYA (Spain)
- VYSOKA SKOLA BANSKA - TECHNICKA UNIVERZITA OSTRAVA (Czech Republic)

Inria contact: Mario Ricchiuto

Summary: The ExaQute project aims at constructing a framework to enable Uncertainty Quantification and Optimization Under Uncertainties in complex engineering problems, using computational simulations on Exascale systems.

eFlowsHPC

Title: Enabling dynamic and Intelligent workflows in the future EuroHPC ecosystem

Duration: 1/01/2021-31/12/2023

Coordinator: Barcelona Supercomputer Center

Partners:

- BARCELONA SUPERCOMPUTING CENTER - CENTRO NACIONAL DE SUPERCOMPUTACION (Spain)
- CENTRE INTERNACIONAL DE METODES NUMERICIS EN ENGINYERIA (CIMNE) (Spain)
- JULICH (Germany)

- UNIVERSITAT POLITECNICA DE VALENCIA (Spain)
- BULL Atos technologies (France)
- DtokLab (Italy)
- Centro Euro-Mediterraneo sui Cambiamenti Climatici (Italy)
- Scuola Internazionale Superiore di Studi Avanzati (Italy)
- Poznan Supercomputing and Networking Center (Poland)
- Universidad de Malaga (Spain)
- Alfred Wegener institute (Denmark)
- Istituto Nazionale di Geofisica e Vulcanologia (Italy)
- ETH Zurich (Switzerland)
- SIEMENS
- NGI (Norway)

Inria contact: Mario Ricchiuto

Summary: eFlows4HPC aims to create a European workflow platform to enable the design of complex applications that integrate HPC, data analytics and artificial intelligence and widen the access of HPC to selected user communities.

MICROCARD

Title: Numerical modeling of cardiac electrophysiology at the cellular scale

Duration: 04/2021-09/2024

Coordinator: University of Bordeaux (France)

Partners:

- University of Bordeaux (France)
- Inria (France)
- University of Strasbourg (France)
- Karlsruhe Institute of Technology (Germany)
- Zuse Institute Berlin (Germany)
- Megware (Germany)
- Numericor (Austria)
- Simula (Norway)
- Università della Svizzera Italiana (Switzerland)
- Università di Pavia (Italy)
- Orobix (Italy)

Inria contact: Nicolas Barral

Summary: MICROCARD is a European research project to build software that can simulate cardiac electrophysiology using whole-heart models with sub-cellular resolution, on future exascale supercomputers.

SuPerMan-IF MCSA

Title: Structure Preserving schemes for Conservation Laws on Space Time Manifolds.

Duration: 1/06/2021-31/05/2023

Inria contact: Elena Gaburro

Summary: SuPerMan proposes the development and efficient implementation of new structure preserving schemes for conservation laws formulated in an elegant and universal form through covariant derivatives on spacetime manifolds.

9.4 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. 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 planned 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.

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.

ANR LAGOON

Title: Large scale global storm surge simulations

Type: ANR

Duration: 48 months

Starting date : 1st Oct 2021

Coordinator: Vincent Perrier (U.Pau et des Pays de l'Adour)

Abstract: The aim of the project is to develop an all-scale shallow water storm-surge model simulating different features of oceanic flows: from large scale linear waves in open ocean to small scale non-linear flows in coastal areas, and using high resolution by combining novel numerical approaches on unstructured grids and high performance computing.

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.

9.5 Regional initiatives

ETRURIA

Title: Evaluating coastal risks using high order finite element approaches

Duration: 60 months

Starting date : 19 Jan. 2018

Coordinator: Mario Ricchiuto

Partners: BRGM

Abstract: this project is devoted to the study of improved numerical approaches for coastal risk assessment, with applications to realistic cases relevant for the région Nouvelle Aquitaine. The final objective is to propose numerical methods which are optimal from the point of view of accuracy of results for a given number of elements and, more importantly, computational cost. The implementation will be done in the UHAINA platform co-developed with BRGM.

RENOVABLES

Title: Relaunch of renewable energies by providing high-level training for the Offshore sector within the Blue Economy Value Chain and establishing synergies within the Euroregion

Duration: 18 months

Starting date : 17 Dec. 2020

Coordinator: Martin Parisot

Partners: The RENEWABLES project is made up of nine main partners, three for each of the areas of the Euroregion, Esuskadi, Navarra and Nueva Aquitaine. On the part of the Basque Country, the University of the Basque Country, the Basque Center for Applied Mathematics and the ALERION company. On the part of Navarra, the Public University of Navarra, the National Center for Renewable Energies and the Automotive and Mechatronics Technological Center and on the part of Nueva Aquitaine the TRENT Chair, the Bordeaux Institute of Mathematics and INRIA.

Abstract: The RENEWABLES project seeks to foster strategic cooperation between the Euroregion's socio-economic stakeholders to drive the blue economy around the Bay of Biscay. This will be achieved by focusing on offshore renewable energies, whose promising development in the "blue economy" is a strategic focal point and also given its important value chain in the case of the Basque Country. The aim is to promote synergies, based on a high-level training cross-border network and whose existence is justified by its energy potential. Its goal will be to become a leading driver hub within the marine sector in the Euroregion, in the context of a climate neutral Europe.

EVE

Title: Robust prototyping of energy via exhaust (EVE) engines

Duration: 36 months

Starting date : 01 Jan. 2017

Coordinator: Pietro Congedo (H. Beaugendre)

Partners: EXOES

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 efficient simulation of battery thermal management system for electric vehicles. To perform optimization under uncertainties a multi-fidelity platform is used. The idea is to evaluate the system performances by using massively the low-fidelity models and by correcting these estimations via only few calculations with the high-fidelity code. High fidelity simulations are done using TrioCFD code. In Elie's PhD, we illustrate an experiment using a set up of immersion cooling battery pack with EXOES. The temperatures, voltage and electrical current evolution of the Li-ion batteries are monitored. A numerical model is implemented to simulate the heat transfer and electrical behavior of an immersion cooling Battery Thermal Management System. The uncertainties coming from multi-physics input parameters are considered. Bayesian calibration of the input parameters is performed using the experimental measurements directly [17].

10 Dissemination

10.1 Promoting scientific activities

10.1.1 Scientific events: organisation

General chair, scientific chair

- Mathieu Colin is a member of the scientific committee of the "Journée Jeunes EDPistes".
- Mario Ricchiuto is member of the scientific committee of the [EmrSim conference](#).

Member of the organizing committees

- Nicolas Barral co-organized the mini-symposium Unstructured mesh adaptation: from mesh generation to applications, MS413 at ECCOMAS-WCCM 2020 (held in January 2021).
- Maria Kazolea co-organized the Interdisciplinary Tsunami Science session in AGU fall meeting, New Orleans LA 13-17 December 2021.
- Mario Ricchiuto co-organized the mini-symposium Immersed Discretizations in Computational Mechanics: Mathematics, Algorithms, and Applications, MS609 at the 16th USCCM Conference, 2021.
- Mario Ricchiuto co-organized the mini-symposium Well-Balanced Numerical Discretizations of Geophysical Models, MS1 and MS9 at the SIAM-GS21 Conference.
- Elena Gaburro and Mario Ricchiuto co-organized the workshops *Journée Calcul & Simulation en Nouvelle-Aquitaine*, Arcachon, 6-7 December 2021.
- Martin Parisot co-organized the conference [EmrSim](#) on the optimization and simulation for renewable energies.
- Mario Ricchiuto co-organized the fourth edition of the [B'Waves](#) workshop on wave breaking, virtual event held in June 2021 and hosted by Springer Nature.

10.1.2 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 and Fluids (Elsevier), Journal of Computational Physics (Elsevier), and of Water Waves (Springer).

Reviewer - reviewing activities

- Nicolas Barral served as reviewer for the following international journals: *Journal of Computational Physics*, *Journal of Scientific Computing*, *Computer and Fluids*.
- Elena Gaburro served as reviewer for the following international journals: *Journal of Computational Physics* (6), *Journal of Scientific Computing* (4), *Computers and Fluids* (2), *International Journal for Numerical Methods in Fluids* (1), *SIAM Journal on Scientific Computing* (1).
- Maria Kazolea served as a reviewer for the following international journals: *Journal of Fluid Mechanics*, *Ocean engineering*, *Wave Motion*.
- Martin Parisot served as a reviewer for the following international journals: *AIMS Mathematics*, *Journal of Computational Physics*, *Applied Mathematics and Computation*.

10.1.3 Invited talks

- SMAI, Montpellier, France, June 2021 (Elena Gaburro)
- NumHyp2021, Trento, Italy, July 2021 (Elena Gaburro and Martin Parisot)
- NumAsp, Verona, Italy, December 2021 (Elena Gaburro)
- Oberwolfach workshop *Hyperbolic Balance Laws: modeling, analysis, and numerics*, February 2021 (Mario Ricchiuto)
- von Karman Institute 65th anniversary celebration and conference (Mario Ricchiuto)

10.1.4 Scientific expertise

- Mario Ricchiuto is member of the scientific committee of the [GDR MahGeoPhy](#)

10.1.5 Research administration

- Mathieu Colin is Director of the Mathematics department of the ENSEIRB-MATMECA/Bordeaux INP school
- Mario Ricchiuto is deputy scientific head of the Inria Bordeaux Sud-Ouest center.

10.2 Teaching - Supervision - Juries

10.2.1 Teaching

- License: Nicolas Barral, TD d'Analyse Numérique, 24h, L3, ENSEIRB-MATMÉCA, France
- License : Nicolas Barral, TP Fortran 90, 44h, M1, ENSEIRB-MATMÉCA, France
- Master : Nicolas Barral, TD C++, 48h, M1, ENSEIRB-MATMÉCA, France
- Master : Nicolas Barral, Calcul Haute Performance (OpenMP-MPI), 45h, 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, 14 h, ENSEIRB-MATMÉCA, France
- Master : Nicolas Barral : responsable des stages 2A, 20 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)
- License: Martin Parisot, TP Fortran, 21h, M1, ENSEIRB-MATMÉCA, France
- Master : Mario Ricchiuto, Multiphysics Course, 24h cours magistrale, M2, ENSEIRB-MATMÉCA, France
- Doctorat: Elena Gaburro, Advanced Numerical Methods for the solution of Hyperbolic Equations, 12h (EDMI-Université de Bordeaux)

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 (ONERA).
- 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).
- 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 progress : T. Carlier, Modeling of an icing system using shifted boundary method, started in October 2020, co-supervised by H. Beaugendre and M. Colin.
- PhD in progress : F. Nauleau, Immersed boundary method applied to large eddy simulations of hypersonic reentry vehicles, started in October 2020, co-supervised by H. Beaugendre and T. Bridel-Bertomeu and F. Vivodtzev (CEA).
- PhD in progress: M. Romanelli, Deep Wall Models for Aerodynamic Simulations, started in october 2021, co-supervised by H. Beaugendre and M. Bergmann (MEMPHIS).
- PhD in progress: J. Galaz Mora, Coupling of free surface coastal models, started in February 2021, co-supervised by M. Kazolea and A. Rousseau.
- Post-doc in progress: Mariem Makni (Université de Bordeaux, EU project MICROCARD).
- Post-doc in progress: Michele Giuliano Carlino (Inria).
- Post-doc: Post-Doc in progress: R. Baggio (until July 2021), Transversal/longitudinal single crack PDE and FEM model for self-healing ceramix-matrix composite materials, supervised by D. Bresch and M. Colin.
- Post-Doc: D. Torlo (until November 2021), Hybrid PDE-ROM modeling for dispersive waves, supervised by M. Ricchiuto.

10.2.3 Juries

- Yann Marchenay, Modélisation de la turbulence en présence de rugosité et de soufflage en régime hypersonique, PhD U. de Toulouse (ISAE), December 2021 (Heloise Beaugendre, reviewer) ;
- Benjamin Martin, Méthodes numériques et conditions limites pour la simulation aux grandes échelles du couplage entre plusieurs composantes d'une turbomachine, PhD U. de Toulouse (CERFACS), December 2021 (Mario Ricchiuto, reviewer) ;
- Ali Pourzangbar, Study of the influence of bottom boundary layer (BBL) and suspended sediment transport (SST) for the computation of the evolution of natural sand bars, PhD Università Politecnica della Marche, May 2021 (Mario Ricchiuto, reviewer).

10.3 Popularization

10.3.1 Articles and contents

- Elena Gaburro et al. proposed a simple but efficient concept of blended teaching of mathematics for engineering students during the COVID-19 pandemic, also published in [5].

11 Scientific production

11.1 Major publications

- [1] L. Arpaia, M. Ricchiuto, A. G. Filippini and R. Pedreros. ‘An efficient covariant frame for the spherical shallow water equations: Well balanced DG approximation and application to tsunami and storm surge’. In: *Ocean Modelling* (Nov. 2021), p. 101915. DOI: [10.1016/j.ocemod.2021.101915](https://doi.org/10.1016/j.ocemod.2021.101915). URL: <https://hal.inria.fr/hal-03421078>.
- [2] B. Constant, S. Péron, H. Beaugendre and C. Benoit. ‘An improved Immersed Boundary Method for turbulent flow simulations on Cartesian grids’. In: *Journal of Computational Physics* 435 (15th June 2021), p. 110240. DOI: [10.1016/j.jcp.2021.110240](https://doi.org/10.1016/j.jcp.2021.110240). URL: <https://hal.archives-ouvertes.fr/hal-03182402>.

11.2 Publications of the year

International journals

- [3] L. Arpaia, M. Ricchiuto, A. G. Filippini and R. Pedreros. ‘An efficient covariant frame for the spherical shallow water equations: Well balanced DG approximation and application to tsunami and storm surge’. In: *Ocean Modelling* (Nov. 2021), p. 101915. DOI: [10.1016/j.ocemod.2021.101915](https://doi.org/10.1016/j.ocemod.2021.101915). URL: <https://hal.inria.fr/hal-03421078>.
- [4] E. Audusse, L. Boittin and M. Parisot. ‘Asymptotic derivation and simulations of a non-local Exner model in large viscosity regime’. In: *ESAIM: Mathematical Modelling and Numerical Analysis* 55.4 (July 2021), pp. 1635–1668. DOI: [10.1051/m2an/2021031](https://doi.org/10.1051/m2an/2021031). URL: <https://hal.archives-ouvertes.fr/hal-03312836>.
- [5] 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](https://doi.org/10.3390/educsci11020056). URL: <https://hal.archives-ouvertes.fr/hal-03111979>.
- [6] L. Campoli, A. Assonitis, M. Ciallella, R. Paciorri, A. Bonfiglioli and M. Ricchiuto. ‘UnDiFi-2D: an Unstructured Discontinuity Fitting code for 2D grids’. In: *Computer Physics Communications* 271 (29th May 2021), p. 108202. DOI: [10.1016/j.cpc.2021.108202](https://doi.org/10.1016/j.cpc.2021.108202). URL: <https://hal.inria.fr/hal-03408117>.
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- [8] L. Cirrottola, M. Ricchiuto, A. Froehly, B. Re, A. Guardone and G. Quaranta. ‘Adaptive deformation of 3D unstructured meshes with curved body fitted boundaries with application to unsteady compressible flows’. In: *Journal of Computational Physics* 433 (May 2021), p. 110177. DOI: [10.1016/j.jcp.2021.110177](https://doi.org/10.1016/j.jcp.2021.110177). URL: <https://hal.inria.fr/hal-03194100>.
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- [15] K. Ignatowicz, F. Morency and H. Beaugendre. ‘Extention of SU2 CFD capabilities to 3D aircraft icing simulation’. In: CFDSC2021 - 29th Annual Conference of the Computational Fluid Dynamics Society of Canada. Virtual, Canada, 27th July 2021. URL: <https://hal.inria.fr/hal-03434919>.
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- [20] F. Desmons. ‘Numerical study of the breaking process for capillary-gravity waves’. Université de Bordeaux, 12th Feb. 2021. URL: <https://tel.archives-ouvertes.fr/tel-03204107>.

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- [23] L. Arpaia, M. Ricchiuto, A. G. Filippini and R. Pedreros. *An efficient 3d/2d-covariant formulation of the spherical shallow water equations: well balanced DG approximation and application to tsunami and storm surge*. 24th Apr. 2021. URL: <https://hal-brgm.archives-ouvertes.fr/hal-03207171>.
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