RESEARCH CENTRE

Inria Centre at the University of Bordeaux

IN PARTNERSHIP WITH: Institut Polytechnique de Bordeaux

2023 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

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- 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

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- 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 extend optimization and inverse modelling. These skiss need to be also combined with some specific engineering know how to tackle specific applications. Part of this scientific themes and of these activities have been part of the work of the BACCHUS 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 [99, 41]. 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 [48, 72]. 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 [49]. For wave energies, as well as for aquifers, the transition between free surface and congested flows (below a solid surface) is another example [63]. 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 [101]. 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 mimimize the computational effort. To this end, the dynamics of some of the fronts can be modelled by appropriate asymptotic/homogeneised 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 ..) [57, 91]. 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 [58]). So the challenge is to construct computationally affordable models robust under variability of input paramters 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 [75] 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 sudied, 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 contraints 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 processs in realistic environments, and on the other of data possibly available for the proces 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:

- Aeronautics and aerospace engineering (de-anti icing systems, space re-entry, complex materials);
- Coastal engineering (coastal protection, hazard assessment etc.);
- · Energy engineering with a focus on wave energy conversion
- Large scale models on manifolds with a focus on geophysics and recent models from applications in astrophysics and relativity.

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 homogeneization 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 [93, 100].

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 of C-property [44, 90]) 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 [38, 83]. On Cartesian meshes several techniques exist to control the consistency order based on extrapolation/interpolation, or adaptive methods (cf e.g.[94, 80, 39, 55, 65, 59] and references therein). For discontinuities, we can learn from fitting techniques [45], and from some past work by Prof. Glimm and co-workers [54].

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 [95, 76]. 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 [67, 66] that will be further investigated.

3.3 Applications in physics and engineering

As already mentioned, our focus is on four main classes of problems:

- Aeronautics and aerospace engineering (de-anti icing systems, space re-entry, complex materials)
- · Coastal engineering (coastal protection, hazard assessment etc.)
- · Energy engineering with a focus on wave energy conversion
- Large scale models on manifolds with a focus on geophysics and recent models from applications in astrophysics and relativity.

There are several common aspects. One is the use of asymptotic vertically averaged approximations to produce efficient application-Taylored PDE models. Another common point is the construction of possibly high order constraint/property preserving numerical approximations. This entails the characterization of the underlying PDE models with a set of embedded properties, which go from classical conservation, to exact solutions (steady or moving), to the preservation of differential operators, to the thermodynamic adissibility (non-negativity, preservation of physical bounds). For all applications, the investigation of the parameter dependence of the results will take several forms from sensitivity analyses, to classical parametric studies to understand physical processes, to approximation in parameter space in the framework of hybrid PDE-meta-/reduced-order models.

4 Application domains

4.1 De-anti icing systems

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

In [42] 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 [38, 83]. In these methods we compensate for the error at solid walls introduced by the penalization by using anisotropic mesh adaptation [61, 77, 78]. 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 [43]. 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 [47, 41] 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 [86], 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 [101], 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 [63] [46] 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 [71, 70], and will be pursued in the comping 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. Out numerical developments will be performed withing 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 [89].

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

In collaboration wit the LCTS laboratory (a joint CNRS-CEA-SAFRAN-Bordeaux University lab devoted to the study of thermo-structural materials in Bordeaux), we are developing a multi-scale model in which a structural mechanics solver is coupled with a closure model for the crack physico chemistry. This model is obtained as a multi-dimensional asymptotic crack averaged approximation fo the transport equations (Fick's laws) with chemical reactions sources, plus a potential model for the flow of oxide [58, 62, 87]. 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.

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

This means that the 0-dimensional model used in most of the studies (see e.g. [56]) will underestimate appreciably the lifetime of the material. Based on these recent advances, we will further pursue the development of multi-scale multi-dimensional asymptotic closure models for the parametric design of self healing CMCs. Our objectives are to provide: (i) new, non-linear multi-dimensional mathematical model of CMCs, in which the physico-chemistry of the self-healing process is more strongly coupled to the two-phase (liquid gas) hydro-dynamics of the healing oxide ; (ii) a model to represent and couple crack networks ; (iii) a robust and efficient coupling with the structural mechanics code ; (iv) validate this platform with experimental data obtained at the LCTS laboratory. The final objective is to set up a multi-scale platform for the robust prediction of lifetime of SH-CMCs, which will be a helpful tool for the tailoring of the next generation of these materials.

4.4 Coastal and civil engineering

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

We will focus our effort in the understanding of the interactions between asymptotic 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 of by means of multilayer models. In the first case, there is an issue with the constraints on the numerical approximation. Investigations of approriated 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 [74, 92, 85, 60], to hybrid methods coupling dispersive PDEs with hyperbolic ones, and trying to mimic wave breaking with travelling bores [98, 97, 96, 73, 64]. In both cases, numerical dissipation plays an important role and the activation or not of the breaking closure, as well as on the establishement of stationary travelling profiles, or on the appearance of solitary waves. These aspects are related to the notion of numnerical 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 adressed 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 is 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 applciations in astrophysics which also involve similar issues. The idea is to consider both coordinate changes related to mesh movement, and in ALE formulations, as well as genuinely space-time manifolds as in hyperbolic reformulations of relativity [68], and combinations of both when for example considered mesh movement and adaptation in curvilinear coordinates [40]. 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 [40] and [69].

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

5.1 Carreer enhancements

• Héloïse Beaugendre has been promoted to a professor's position.

5.2 Awards won in 2023

• Elena Gaburro has been granted the Peter Lax Award, bestowed by the HYP conference as best young researcher (10 years from the PHD) in the community of hyperbolic PDEs research.

5.3 Grants obtained in 2023

- ERC StG 2023 ALcHyMia (PI Elena Gaburro). Funding: 1.500.000 euros. Starting in April 2024. Title: "Advanced Structure Preserving Lagrangian schemes for novel first order Hyperbolic Models: towards General Relativistic Astrophysics"
- ANR JCJC 2023 ImprEVu (PI Elena Gaburro). Funding: around 240.000 euros. (Declined due to incompatibility with the ERC).
- EU Horizon- MSCA-2022-DN: Resilient Solutions for Coastal, Urban, Estuarine and Riverine Environments. Starting in February 2024. contact: M. Kazolea.
- IMPT projets. N. Barral and M. Parisot have been awarded funds by IMPT for their respective projects on sea ice simulation on adaptive meshes, and simulation of aquifers.
- Partnership with AIRBUS: a new collaboration with AIRBUS has started around curved mesh adaptation and high order boundary conditions. The colaboration is sealed by joint participation to a DGAC project, plus the funding of a CIFRE PhD.

5.4 International events held in 2023

- NumHyp23, Bordeaux, July 2023. International conference with around 70 participants from Europe, USA and China. Co-organizers: Martin Parisot and Mario Ricchiuto.
- Bwaves23, Bordeaux May 30th/June 1st 2023. The workshop has hosted about 60 participants among which the leading personalities in coastal engineering and free surface hydrodynamics.
- HONOM 2024: the team is in charge of the organization of the next edition of HONOM which will be hald in Crete, Greece in September 2024. Among the organizers we have: Elena Gaburro (chair of the organizing committee), Maria Kazolea (co-chair) and Mario Ricchiuto.

6 New software, platforms, open data

6.1 New software

6.1.1 SLOWS

Name: Shallow-water fLOWS

Keywords: Simulation, Free surface flows, Unstructured meshes

- Scientific Description: Three different approaches are available, based on conditionally depth-positivity preserving implicit schemes, or on conditionally depth-positivity preserving genuinely explicit discretizations, or on an unconditionally depth-positivity preserving space-time approach. Newton and frozen Newton loops are used to solve the implicit nonlinear equations. The linear algebraic systems arising in the discretization can be solved either with the MUMPS library or with the MKL Intel library. Implicit and explicit (extrapolated) multistep higher order time integration methods are available, and a mesh adaptation technique based on simple mesh deformation are also included. This year a new higher order reconstruction for the FV scheme has been added.
- **Functional Description:** SLOWS is a C-platform allowing the simulation of free surface shallow water flows with friction. It can be used to simulate near shore hydrodynamics, wave transformations processes, etc.
- URL: https://team.inria.fr/cardamom/slows-shallow-water-flows/

Contact: Mario Ricchiuto

Participants: Maria Kazolea, Mario Ricchiuto

6.1.2 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.

Contact: Martin Parisot

Participants: Martin Parisot, Marco Lorini

6.1.3 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).
 - Spherical coordinates based on a local projection on a real 3D spherical map (as of 2021)
 - Compilation with GUIX available (as of 2022)

- Homogenization and standardization of code outputs and hazard quatification (as of 2022)

- Correction of the management of dry/wet fronts in the presence of structures represented by a single high point (as of 2022)

- Use of FES for the calculation of the tide directly in UHAINA through an API. New compilation option for activation (as of 2022)

- Boundary conditions accounting tides from FES and corrected with the effect of the inverse barometer, for the simulation of the tidal propagation and the surge on domains at the regional scale (as of 2022)

- Hydraulic connections (e.g. sewers) in the simulation of urban flooding (as of 2022)

- Mass source term, for the injection of the volume of water overtopping structures not accounted in the elevation model during flooding episodes by sea surges (as of 2022)

Functional Description: Waves simulation

Contact: Mario Ricchiuto

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

Partners: EPOC, IMAG, IMB

6.1.4 AleVoronoi

- Name: Direct Arbitrary Lagrangian Eulerian Finite Volume and Discontinous Galerkin schemes on VORONOI moving meshes with topology changes
- Keywords: Finite volume methods, Discontinuous Galerkin, High order methods, Centroidal Voronoi tessellation, ALE, Fortran, OpenMP
- Scientific Description: We would like to remark that the implementation of AleVoronoi started in April 2018 as a collaboration between E. Gaburro, M. Dumbser (University of Trento, Italy) and W. Boscheri (University of Trento, then University of Ferrara, and now CNRS France). E. Gaburro was the main contributor in particular for what concerns the novelties, however, many parts of the code have been taken from existing codes of the other coauthors. Starting from July 2019, S. Chiocchetti (University of Trento, University of Stuttgart and now University of Cologne) joined the project, becoming a fundamental contributor to it. The work has continued during the years and have been moved to a git account in 2021. The main developers from 2021 up to now have been E. Gaburro and S. Chiocchetti. However, small contributions were introduced also by W. Boscheri and M. Ricchiuto. In addition, M. Dumbser has always participated int the scientific discussion concerning the development line of AleVoronoi.
- **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.

Publications: hal-03850200, hal-03865596, hal-03850195, hal-02411272

Authors: Elena Gaburro, Simone Chiocchetti, Michael Dumbser, Walter Boscheri, Mario Ricchiuto

Contact: Elena Gaburro

6.1.5 HOTHYPE

Name: High Order shock Tracking for HYPerbolic Equations

- **Keywords:** Finite volume methods, Discontinuous Galerkin, Partial differential equation, Delaunay triangulation
- Scientific Description: We would like to remark that this code born in December 2020, but it was quickly created because many of its part were taken from AleVoronoi and simplified/adapted to the purpose of this code. The code was created and mainly developed by E. Gaburro. However, all the original contributors of AleVoronoi should be acknowledged for their contributions to HOTHYPE: S. Chiocchetti, W. Boscheri, M. Dumbser. During the years, the code was mainly maintained and developed by E Gaburro. Another important contributor has been S. Chiocchetti. Minor parts of this code have been implemented by M. Ciallella under the supervision of M. Ricchiuto.
- **Functional Description:** High order ADER-type Finite Volume and Discontinuous Galerkin schemes on 2D triangular meshes for the solution of hyperbolic partial differential equations.

Publications: hal-03850196, hal-04341999, hal-03865587

Authors: Elena Gaburro, Simone Chiocchetti, Michael Dumbser, Mario Ricchiuto, Mirco Ciallella

Contact: Elena Gaburro

6.1.6 AeroSol

- **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:** The main highlight of 2022 concerning the AeroSol library was the hiring of Luca Cirrottola as an INRIA permanent engineer.

In 2022, the development of the library was focused on the following points

* Development environment - Work on the packaging with Guix. - Work on continuous integration by using Plafrim as gitlab runner, with dependencies handled by Guix (and Modules for legacy). - Fix of an old memory leak on PaMPA and integration in the packaging. - Beginning of work for merging the branch master, the branch used for Uhaina/Lagoon project, and the branch including turbulence models and axi models. - the development of a new library DM2 has started. It aims at replacing PaMPA.

* General numerical feature of the library - Postprocessing on wall and lines, including computation of Cp and Cf - New finite elements for quads and hexa, based on Gauss-Lobatto or Gauss-Lagrange elements were added.

* Work on SBM methods - Shifted boundary method for Neumann and Dirichlet boundary conditions, - development of high order derivative in some of the finite element classes

* Low Mach number flows: - Low Mach number filtering was extended on quads. Implementation of dicrete semi-norms div and grad, extension of some fixes to full Euler with arbitrary EOS.

* RANS turbulent flow computations: - Inlet/Outlet boundary conditions for Euler/Navier-Stokes systems allowing to get a stationary solution - HLLC numerical flux, exact jacobian with frozen wave speeds and extension to the RANS equations coupled to transport equations (turbulence models) -

test case: laminar and turbulent flat plate, development and documentation of axisymmetric test case, - Fix of Spalart-Almaras model, negative fix handle - Beginning of implementation of coupled elliptic problem with Neumann and Dirichlet boundary conditions on one variable.

* Flux-reconstruction - Implementation of Flux-Reconstruction methods on Cartesian meshes

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

Contact: Vincent Perrier

Participants: Mario Ricchiuto, Vincent Perrier, Heloise Beaugendre, Christopher Poette, Marco Lorini, Jonathan Jung, Anthony Bosco, Luca Cirrottola, Romaric Simo Tamou, Ibtissem Lannabi

6.1.7 DM2

Name: Distributed Mesh and Data Manager

Keywords: HPC, Data parallelism, High order finite elements, Unstructured meshes, Hybrid meshes

Functional Description: DM2 is a C++ library for managing mesh and data on mesh in a MPI parallel environment. It is conceived to provide parallel mesh and data management in high order finite element solvers for continuum mechanics.

The user should provide a mesh file which is read by the library. Then DM2 is able to:

- Read the mesh, and read the data provided in the mesh file, possibly in parallel

- Redistribute the mesh in order to distribute the data on a given set of processors. This redistribution is made through a graph partitioner such as PARMETIS or PT-SCOTCH.

- Allocate the memory in parallel if a number of unknown by entity type is provided by the user.

- Centralize the data.

- Compute the halo required for a numerical method. The halo is adapted for each of the possible discretization.

- Renumber mesh elements for making a difference between mesh elements that need or need not communication.
- Aggregate a mesh based on a metric for developing a multigrid method.
- **Release Contributions:** This version introduces overlap regions ("halos") among distributed mesh partitions. These halos are specialized for discontinuous or continuous schemes, but generic with respect to the (geometric) degree of the mesh cells. These halos allow to synchronize numerical data defined on a set of entities of the distributed mesh. Numerical data is again generic with respect to the degree of their polynomial approximation, the number and combinations of scalar/vector fields, and the size of the vector spaces.
- **News of the Year:** Contributions of this year are integrated in version v0.1. This version introduces overlap regions ("halos") among distributed mesh partitions. These halos are specialized for discontinuous or continuous schemes, but generic with respect to the (geometric) degree of the mesh cells. These halos allow to synchronize numerical data defined on a set of entities of the distributed mesh. Numerical data is again generic with respect to the degree of their polynomial approximation, the number and combinations of scalar/vector fields, and the size of the vector spaces. The continuous integration framework testes each commit on several 2D/3D hybrid meshes on which parallel mesh distribution and halos construction is performed, for each geometric and polynomial degree up to 4. Main classes are also covered by a set of unit tests.

Contact: Vincent Perrier

Participants: Vincent Perrier, Luca Cirrottola

7 New results

7.1 Structure preserving numerical methods for evolutionary PDEs

Participants: Rémi Abgrall, Elena Gaburro, Mario Ricchiuto, Vincent Pilorget.

• Corresponding member: Mario Ricchiuto

7.1.1 Stabilized continuous finite elements for hyperbolic PDEs

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 [81] 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 temps of CPU time for a given error. This year we have propose a multidimensional extension of this fully discrete analysis. The challenges in two-dimensions are related to the Fourier analysis. Here, we perform it on two types of periodic triangular meshes varying the angle of the advection, and we combine all the results for a general stability analysis. Due to the large number of modes involved, in the fully fiscrete case we have combined the basic Fourier stability criterion with the one obtained from Dahlquist's equation for the spatial discretization alone. Furthermore, we introduce additional a high order viscosity to stabilize the discontinuities, in order to show how to use these methods for tests of practical interest. A simple model for this non-linear term has been included in the spectral analysis as well. All the theoretical results are thoroughly validated numerically both on linear and non-linear problems, and error-CPU time curves are provided. Our final conclusions suggest that Cubature elements combined with SSPRK and OSS stabilization is the most promising combination. Work discussed in [14] (accepted on J.Sci.Comp.).

7.1.2 High order well balanced discretizations

Global flux based schemes. We have developed schemes based on a fully discrete well balanced criterion which exploits the idea of a global flux formulation. In this framework, classically some primitive function of the source terms is defined and included in the hyperbolic flux. In our work however this idea is mostly used to infer an ad-hoc quadrature strategy of the soource which we refer to as "global flux quadrature". This quadrature approach allows to establish a one to one correspondence, for a given local set of data on a given stencil, between the discretization of a non-local integral operator, and the discretization of the local steady differential problem. This equivalence is a discrete well balanced notion which allows to construct balanced schemes without explicit knowledge of the steady state, and in particular without the need of solving a local Cauchy problem. We have used this idea in the setting of finite elements, both discontinuous in [32] and continuous n the framerowk of the PhD of Lorenzo Micalizzi at U. Zurich, co-advised by R. Abgrall and M. Ricchiuto. We have shown that the used of specific finite element spaces allows to provide a very precice characterization of the discrete solution. For example, the use of Gauss-Lobatto elements provides a natural connection to continuous collocation methods for integral equations. This allows to prove super-convergence estimates for the steady discrete solution. In the continuous finite element case, this new well balanced criterion requires the design of compatible stabilization operators. This aspect was presented at the HONOM2022 conference. A paper on the latest developments is in preparation.

In the context of preserving stationary states, e.g. lake at rest and moving equilibria, a new formulation of the shallow water system, called Flux Globalization has been introduced by Cheng et al. (2019). This approach consists in including the integral of the source term in the global flux and reconstructing the new global flux rather than the conservative variables. The resulting scheme is able to preserve a large family of smooth and discontinuous steady state moving equilibria. In this work, we focus on an arbitrary high order WENO Finite Volume (FV) generalization of the global flux approach. The most delicate aspect

of the algorithm is the appropriate definition of the source flux (integral of the source term) and the quadrature strategy used to match it with the WENO reconstruction of the hyperbolic flux. When this construction is correctly done, one can show that the resulting WENO FV scheme admits exact discrete steady states characterized by constant global fluxes. We also show that, by an appropriate quadrature strategy for the source, we can embed exactly some particular steady states, e.g. the lake at rest for the shallow water equations. It can be shown that an exact approximation of global fluxes leads to a scheme with better convergence properties and improved solutions. The novel method has been tested and validated on classical cases: subcritical, supercritical and transcritical flows. The work published in Journal of Scientific Computing [8].

This year we presented a novel approach for solving the shallow water equations using a discontinuous Galerkin spectral element method. The method we propose has three main features. First, it enjoys a discrete wellbalanced property, in a spirit similar to the one of e.g. [52]. As in the reference, our scheme does not require any a-priori knowledge of the steady equilibrium, moreover it does not involve the explicit solution of any local auxiliary problem to approximate such equilibrium. The scheme is also arbitrarily high order, and verifies a continuous in time cell entropy equality. The latter becomes an inequality as soon as additional dissipation is added to the method. The method is constructed starting from a global flux approach in which an additional flux term is constructed as the primitive of the source. We show that, in the context of nodal spectral finite elements, this can be translated into a simple modification of the integral of the source term. We prove that, when using Gauss-Lobatto nodal finite elements this modified integration is equivalent at steady state to a high order Gauss collocation method applied to an ODE for the flux. This method is superconvergent at the collocation points, thus providing a discrete well-balanced property very similar in spirit to the one proposed in [52], albeit not needing the explicit computation of a local approximation of the steady state. To control the entropy production, we introduce artificial viscosity corrections at the cell level and incorporate them into the scheme. We provide theoretical and numerical characterizations of the accuracy and equilibrium preservation of these corrections. Through extensive numerical benchmarking, we validate our theoretical predictions, with considerable improvements in accuracy for steady states, as well as enhanced robustness for more complex scenarios. The work has been published in Journal of Computational Physics [13].

Shallow water equations on manifolds. The work on well balanced schemes for shallow water type models had major enhancements. We proposed a novel hyperbolic re-formulation of the shallow water model written in covariant coordinates, i.e. metric independent, and for this system we derived a cheap well balanced method able to maintain at machine precision water at rest equilibria for general metrics and complex-shaped domains. The obtained numerical results, both in 1D and 2D are reported in [6].

Astrophysics. Following the work in [68], we have continued our research on the implementation of robust and accurate numerical schemes for the simulation of hyperbolic models of general relativity. We investigated in particular the general relativistic magnetohydrodynamics (GRMHD) equations and the Einstein field equations with different first order reformulations as the Z4 and CCZ4 models. We also considered the Buchman [50] and the novel TEGR [88] tedrad formulations. The implementation work is done in a 3D Cartesian code. 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 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. A manuscript at this purpose has been submittes in July 2023: [30]. The obtained results have been presented during ICIAM 2023 (TOKYO, Japan) by E. Gaburro and in several other conferences by the coauthours of the paper.

Embedding WB in ALE schemes. A major work during the year has been also devoted to embedd well balanced techniques inside the AleVoronoi code of Elena Gaburro. Indeed, we are working on a novel family of high order accurate numerical schemes for the solution of hyperbolic PDEs which combines several geometrical and physical structure preserving properties. In particular, in the context of this work, and in particular in the framework of a complex moving mesh code, we have made, for the first time in literature, the full ADER DG scheme with *a posteriori* sub-cell FV limiter *well balanced*. Further details are given in the section below which describes the enhancements of our direct ALE algorithm and a paper is in preparation.

7.1.3 Schemes embedding additional discrete conservation constraints

Entropy conservative ADER-DG. We have developed a fully discrete entropy preserving ADER-Discontinuous Galerkin (ADER-DG) method. To obtain this result, we have equipped the space part of the method with entropy correction terms that balance the entropy production in space, inspired by the work of Abgrall. Whereas for the time-discretization we have applied the relaxation approach introduced by Ketcheson that allows to modify the timestep to preserve the entropy preserving ADER-DG scheme has been constructed. We have also verified our theoretical results with various numerical simulations, reporting our results in [9] which already has 10 citations in scopus.

A posteriori sub-cell conservative correction of nonconservative schemes. We proposed a novel quasi-conservative high order discontinuous Galerkin (DG) method able to capture contact discontinuities avoiding any spurious numerical artifacts, thanks to the PDE evolution in *primitive variables*, while at the same time being strongly conservative on shocks, thanks to a conservative *a posteriori* subcell finite volume (FV) limiter. In particular, we have verified the improved reliability of our scheme on the *multi-fluid Euler system* on examples like the interaction of a shock with a helium bubble. The obtained results have been presented at SIAM 2023 (Amsterdam) and at the CFC conference in Cannes (France); a manuscript is in preparation.

7.2 Modelling of free surface flows

Participants: Maria Kazolea, Martin Parisot, Mario Ricchiuto.

· Corresponding member: Maria Kazolea

Coupling dispersive and non-dispersive models. To study the coupling of Boussinesq-type equations with Saint-Venant equations a domain-decomposition approach was explored for linear/nonlinear and overlapping/nonoverlapping conditions. In the linear case only the overlapping condition would generate different results. When applied to the nonlinear equations though, it was observed that a different pattern of oscillations would appear at the interfaces, and that sometimes the numerical stability could be improved [37]. The numerical stability of the linearized discretization was also examined. From the linear nonoverlapping case the optimal convergence operators, in the iterative domain decomposition method used, were given by the theory of absorbing operators. This allowed a reformulation of the problem that allows to describe the artifacts introduced by the coupling strategy as reflections emanating from the interface. An accurate description of these was obtained, allowing to accurately asses the quality of the observed results. This is an ongoing work.

Dispersive waves with/without porous media. This year, our work for a conservative form of the extended Boussinesq equations for waves in porous media were publiced in the Ocean engineering journal [19]. This model can be used in both porous and non-porous media since it does not requires any boundary condition at the interface between the porous and non-porous media. A hybrid Finite Volume/Finite Difference (FV/FD) scheme has been coded in order to solve the conservative form of the extended Boussinesq equations for waves in porous media. For the hyperbolic part of the governing equations, the FV formulation is applied with Riemann solver of Roe approximation. Whereas, the dispersive and porosity terms are discretized by using the FD. The model is validated with experimental data for solitary waves interacting with porous structures and a porous dam break in a one-dimensional flow. The limitation of this scheme is that is not well-balanced when topography is present. Currently we are working on a well balanced numerical scheme for the model with out the dispersive terms and with the precence of topography. The scheme is based on the global flux approach. Furthermore we are working on the implementation of a well balanched numerical scheme for a shallow water the two layer model with the presence of porocity and topography.

At the same time we went back to fundamental question of whether full nonilearity in weakly dispersive Boussinesq type models is a necessity [12]. We reconsider the tests first used in the literature to address this issue, as well as a number of more demanding issues. We also consider different families of weakly nonlinear BT models, with different shoaling characteristics, especially when nonlinear waves are involved. Our study allows us to point out that for many cases, it is quite hard to conclude whether full nonlinearity is really necessary. There are a few discriminant cases, which are unfortunately not those mostly used in the literature proposing new models or new numerical methods.

Hyperbolic-elliptic spliting. Our work on the use of the splitting between hyperbolic and elliptic steps published in journal of Ocean modelling [11]. In this paper we use a high order FV method to solve the hyperbolic step, and a standard P1 finite element method for 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 finale 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(div) spaces. However, it has been shown that perturbed problems involving similar operators with a small Laplace perturbation are well behaved in H1 provided that some numerical dissipation is embedded in the overall discretization. In our case, the use of upwind numerical fluxes in the hyperbolic step suffices to this end, allowing to not only obtain convergent results, but also provide the expected convergence rates.

Last but not least we focused on the numerical modelling of water waves by means of depth averaged models. We considered in particular PDE systems which consist in a nonlinear hyperbolic model plus a linear dispersive perturbation involving an elliptic operator. We proposed two strategies to construct reduced order models for these problems, with the main focus being the control of the overhead related to the inversion of the elliptic operators, as well as the robustness with respect to variations of the flow parameters. In a first approach, only a linear reduction strategies is applied only to the elliptic component, while the computations of the nonlinear fluxes are still performed explicitly. This hybrid approach, referred to as pdROM, is compared to a hyper-reduction strategy based on the empirical interpolation method to reduce also the nonlinear fluxes. We evaluated the two approaches on a variety of benchmarks involving a generalized variant of the BBM-KdV model with a variable bottom, and a one-dimensional enhanced weakly dispersive shallow water system. The results show the potential of both approaches in terms of cost reduction, with a clear advantage for the pdROM in terms of robustness, and for the EIMROM in terms of cost reduction. This work has been published in Mathematics and Computers in Simulation [18].

7.3 Modelling of icing and de-icing of aircrafts

Participants: Héloïse Beaugendre.

· Corresponding member: Héloïse Beaugendre

In-flight icing is a major source of incidents and accidents. The effects of atmospheric icing can be anticipated by Computational Fluid Dynamics (CFD). Experimental and numerical fluid dynamics studies highlight a change of flow structure in the presence of surface roughness. The changes involve both wall heat transfer and skin friction, and are mainly restricted to the inner region of the boundary layer. Aircraft in-flight icing is a typical application where rough surfaces play an important role in the airflow structure and the subsequent ice growth. The objective of this work [10] is to investigate how surface roughness is tackled in RANS with wall resolved boundary layers for aeronautics applications, with a focus on ice-induced roughness. The literature review shows that semi-empirical correlations were calibrated on experimental data to model flow changes in the presence of roughness. The correlations for RANS do not explicitly resolve the individual roughness. They principally involve turbulence model modifications to account for changes in the velocity and temperature profiles in the near-wall region. The equivalent sand grain roughness (ESGR) approach emerges as a popular metric to characterize roughness and is employed as a length scale for the RANS model. For in-flight icing, correlations were developed, accounting for both surface geometry and atmospheric conditions. Despite these research efforts, uncertainties are present in some specific conditions, where space and time roughness variations make the simulations difficult to calibrate. Research that addresses this gap could help improve ice accretion predictions.

CFD is a primary tool used to assess the in-flight effects of atmospheric icing on aircraft. In-flight ice accretion codes use CFD computed quantities, such as shear stress and heat transfer, to predict ice shape formation over rough surfaces. The equivalent sandgrain roughness approach is the model commonly used in icing codes for the prediction of skin friction and heat fluxes over iced surfaces. Additional turbulent Prandtl number corrections can be added to the Reynolds Averaged Navier-Stokes (RANS) equations turbulence model to refine the heat transfer. Still, uncertainties persist in identifying the roughness parameters to input into the thermal correction, leaving the characterization of rough surfaces incomplete in terms of research. Uncertainty quantification (UQ) could help quantify the impact of surface roughness parameters on the reliability of ice accretion prediction. This chapter [27] develops a methodology for the estimation of roughness input parameters based on the observation of experimental ice accretion. Metamodeling involving Polynomial Chaos Expansion (PCE) and calibration with a Bayesian inversion are employed. The methodology is applied to a NACA0012 airfoil, yielding a glaze ice cross-sectional area and maximum thickness with less than a 6% error from experiments. The approach opens perspectives for the estimation of appropriate case-dependent roughness parameters for RANS-based ice shape predictions.

7.4 High order embedded and immersed boundary methods

Participants: Héloïse Beaugendre, Tiffanie Carlier, Benjamin Constant, Elena Gaburro, Florent Nauleau, 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.

Shifted boundary method, extensions and developments. We have proposed several applications and extensions of the original ideas behind the shifted boundary method of [79]. This method is based on the simple idea that when applying the boundary conditions on a modified boundary we can modify the imposed conditions to account for this offset by means of a Taylor series expantion truncated to the desired accuracy. First of all, we extended the enriched formulation proposed in [84] to the approxiamtion of parabolic problems with moving interfaces, modeling phase change. In the PhD of T. Carlier [5, 21, 22] we present an extension of the shifted boundary method to simulate partial differential equations with moving internal interfaces. The objective is to apply the method to phase change problems modelled by the Stefan equation which is a parabolic heat equation with a discontinuity separating two phases, moving at a speed given by the normal flux jump. To obtain an accurate prediction of the temperature field on both sides of the discontinuity, and of the position of the discontinuity itself, we propose a variant of the shifted boundary method adapted to problems with moving fronts. This method is based on an enriched mixed form proposed by some of the present authors, which preserves a uniform second order accuracy in space and time. Stabilization terms are added on the whole domain to ensure convergence. Our approach [5] correctly predicts the position of the front when simulating the melting of a semi-infinite ice block. Note that the enrichment procedure is mandatory to obtain the willing second order accuracy, which justify the proposed mixed formulation.

Actually, we perform a stability analysis of the dimensionless Stefan model with a 2D motion of the phase front. Results on the numerical scheme will show the ability of the Shifted Boundary Method to handle perturbations at the interface and will show the character stable of the model. This ongoing work has been presented at CFC 2023 [21] and ENUMATH 2023 [22] and a paper is in preparation.

We have worked on extending the use of the same idea to higher orders. In this case the evaluation of the entire Taylor expansion in each boundary quadrature point is quite expensive. On the other hand, when using local data to evaluate the Taylor series this procedure can be readily shown to be simply a local change in polynomial basis. This has allowed to re-write the method via a simple but effective high order polynomial correction based on the polynomial representation already available in the cell. This approach has been thoroughly tested for hyperbolic problems in 2D and 3D in [7]. Its in depth study for elliptic problems is ongoing in collaboration with DTU compute and Duke University.

At the same time, we have tried to reformulate the problem based on 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 approaximation whose trace on the surrogate boundary is precisely the condition used in the shifted boundary method. This allows to design several boundary conditions within any desired order of accuracy. This work is perfomed in collaboration with L. Nouveau (INSA Rennes), and C. Poignard (Inria, MONC).

Immersed boundaries for turbulent flows. 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. New adaptive methods are investigated for the near-field reconstruction of aerodynamic forces in an immersed boundary context. The proposed developments take place during the pre- and postprocessing stages of the simulation workflow, and aim at increasing the accuracy of the approach for steady-state simulations of high Reynolds number turbulent flows around airfoil geometries in high-lift configurations. To this end, the location of the forcing points is further optimized prior to simulation, with an adaptive and local modeling height that accounts for the evolution of the turbulent boundary layer thickness, especially at the leading edge. In addition to that, the direct extrapolation of the pressure solution at the wall is replaced by first- and second-order reconstructions using the normal pressure gradients interpolated at a new set of image points, located further away from the modeled area. This second approach takes place after the simulation and prevents the degradation of the wall pressure in the presence of strong curvatures or thin boundary layers. The latest developments have been validated through the simulation of subsonic turbulent flows around the NACA0012 profile and 2D multi-element airfoil (2DMEA), facing flow incidences of ten and sixteen degrees respectively. Smooth and accurate skin pressure and friction coeficients are observed, in excellent agreement with body fitted wall-resolved solutions. Better drag and lift coefficients calculated by direct near-field integrations are also obtained, as well as accurate predictions of the near-wall ow physics throughout the turbulent boundary layer. The paper relating this work has been submitted.

This work continues with the thesis of Michele Romanelli. In [16], Michele presents a data-based methodology to build Reynolds-Averaged Navier–Stokes (RANS) wall models for aerodynamic simulations at low Mach numbers. Like classical approaches, the model is based on nondimensional local quantities derived from the wall friction velocity, the wall viscosity, and the wall density. A fully-connected neural network approximates the relation. We consider reference data (obtained with RANS simulations based on fine meshes up to the wall) of attached turbulent flows at various Reynolds numbers over different geometries of bumps, covering a range of wall pressure gradients. After training the neural networks on a subset of the reference data, the paper assesses their ability to accurately recover data for unseen conditions on meshes that have been trimmed from the wall up to an interface height where the learned wall law is applied. The network's interpolation and extrapolation capabilities, the neural network model shows good robustness and accuracy. The global error on the skin friction coefficient is a few percent and behaves consistently over all the considered test cases.

Florent Nauleau doctoral work aims at adapting the immersed boundary conditions (IBC) technique to three-dimensional (3D) large eddy simulations (LES) of viscous hypersonic flows around complex vehicles. The work relies on a pre-existing in-house IBC code, HYPERION (HYPERsonic vehicle design using Immersed bOuNdaries). The boundary conditions are imposed using a high-order reconstruction

algorithm based on HYPERION least squares. The condition number of this algorithm is related to the number of neighbors. In 3D configurations, we find that the number of neighbors must be high to ensure proper conditioning of the least squares matrix. Therefore, we successfully introduce an algorithm designed for a hybrid MPI/OpenMP environment based on migratory tasks to solve communication problems. In CFC 2023 conference [25], we discuss the implementation of LES capabilities in HYPERION. LES requires high-order schemes to limit numerical diffusion. However, considering reentry problems, HYPERION solvers should also be able to handle strongly shocked flows and high Reynolds number. Therefore, an important step in this work is to study the feasibility of embedding wall models in the IBC framework and reconstruction algorithm to try and counteract the low accuracy of the near-wall phenomena caused by the lack of body-fitted mesh.

Another aspect of the work of Florent Nauleau concerns scientific visualisation. This application paper [82] presents a comprehensive experimental evaluation of the suitability of Topological Data Analysis (TDA) for the quantitative comparison of turbulent flows. Specifically, our study documents the usage of the persistence diagram of the maxima of flow enstrophy (an established vorticity indicator), for the topological representation of 180 ensemble members, generated by a coarse sampling of the parameter space of five numerical solvers. We document five main hypotheses reported by domain experts, describing their expectations regarding the variability of the flows generated by the distinct solver configurations. We contribute three evaluation protocols to assess the validation of the above hypotheses by two comparison measures: (i) a standard distance used in scientific imaging (the L2 norm) and (ii) an established topological distance between persistence diagrams (the L2 -Wasserstein metric). Extensive experiments on the input ensemble demonstrate the superiority of the topological distance (ii) to report as close to each other flows which are expected to be similar by domain experts, due to the configuration of their vortices. Overall, the insights reported by our study bring an experimental evidence of the suitability of TDA for representing and comparing turbulent flows, thereby providing to the fluid dynamics community confidence for its usage in future work. Also, our flow data and evaluation protocols provide to the TDA community an application-approved benchmark for the evaluation and design of further topological distances.

7.5 Adaptation techniques

Participants: Nicolas Barral, Héloïse Beaugendre, Sourabh Bhat, Luca Cirrottola, Pierre Clouzet, Mario Ricchiuto, Ishak Tifouti.

• Corresponding member: Nicolas Barral

Mesh adpatation for sea ice modelling. Brieuc Praud's internship was dedicated to exploring the integration of MMG in neXtSIM, a sea ice dynamics model written by geophysicists in Grenoble and Norway. The model uses a Lagrangian paradigm, which requires frequent remeshing to preserve the quality of the mesh. We have developped a prototype of replacement of old library BAMG by MMG, and explored a simple ad hoc approach for the parallelisation of the remeshing step.

Goal oriented mesh adaptation. The work on goal-oriented mesh adaptation techniques for geophysical flows has continued, in the context of the collaboration with Imperial College London.

To examine the accuracy and sensitivity of tidal array performance assessment by numerical techniques applying goal-oriented mesh adaptation. The goal-oriented framework is designed to give rise to adaptive meshes upon which a given diagnostic quantity of interest (QoI) can be accurately captured, whilst maintaining a low overall computational cost. We seek to improve the accuracy of the discontinuous Galerkin method applied to a depth-averaged shallow water model of a tidal energy farm, where turbines are represented using a drag parametrisation and the energy output is specified as the QoI. Two goal-oriented adaptation strategies are considered, which give rise to meshes with isotropic and anisotropic elements. We present both fixed mesh and goal-oriented adaptive mesh simulations for an established test case involving an idealised tidal turbine array positioned in a channel. With both the fixed meshes and the goal-oriented methodologies, we reproduce results from the literature which demonstrate how a staggered array configuration extracts more energy than an aligned array. We also make detailed qualitative and quantitative comparisons between the fixed mesh and adaptive outputs. The proposed goal-oriented mesh adaptation strategies are validated for the purposes of tidal energy resource assessment. Using only a tenth of the number of degrees of freedom as a high-resolution fixed mesh benchmark and lower overall runtime, they are shown to enable energy output differences smaller than 2

Coupling mesh adaptation with model reduction. We propose an automated nonlinear model reduction and mesh adaptation framework for rapid and reliable solution of parameterized advection-dominated problems, with emphasis on compressible flows. The key features of our approach are threefold: (i) a metric-based mesh adaptation technique to generate an accurate mesh for a range of parameters, (ii) a general (i.e., independent of the underlying equations) registration procedure for the computation of a mapping Φ that tracks moving features of the solution field, and (iii) an hyper-reduced least-square Petrov-Galerkin reduced-order model for the rapid and reliable estimation of the mapped solution. We discuss a general paradigm — which mimics the refinement loop considered in mesh adaptation — to simultaneously construct the high-fidelity and the reduced-order approximations, and we discuss actionable strategies to accelerate the offline phase. We present extensive numerical investigations for a quasi-1D nozzle problem and for a two-dimensional inviscid flow past a Gaussian bump to display the many features of the methodology and to assess the performance for problems with discontinuous solutions.

7.6 Direct Arbitrary-Lagrangian Eulerian methods on Voronoi meshes

Participants: Elena Gaburro, Mario Ricchiuto.

· Corresponding member: Elena Gaburro

We have continued with the development of the code called AleVoronoi: Direct Arbitrary Lagrangian Eulerian high order finite volume and discontinous Galerkin schemes on VORONOI moving meshes with topology changes. The code is written in Fortran with the OpenMP parallel paradigm. It implements an arbitrary high order accurate numerical scheme which exploits the ADER paradigm both for the Finite Volume and Discontinous Galerkin case and can be used for studying the Burgers equation, Euler equations, multi-material Euler equations, Shallow Water models written in various system of coordinates and in covariant form, MHD equations, and the GPR model. It belongs to the family of Arbitrary-Lagrangian-Eulerian methods, so it can be used in fixed Eulerian framework or with a moving Voronoi mesh regenerated at each time step. Its peculiarity is the capability of dealing with topology changes maintaining the high order of accuracy.

The work of 2023 has been devoted to the following major improvements. First, we have completed the implementation of our robust a posteriori subcell Finite Volume limiter and we have continued our exploration on novel sofisticated mesh adaptation techniques. We have also collected the salient examples of the effectiveness of our moving mesh scheme in [26].

Then, we have continued our work on a novel quasi-conservative strategy to deal with multi-material flow simulations that we have already described above and for which here we want just to underline that the method has been implemented in two-dimension on unstructured Voronoi meshes.

Finally, we have inserted in the code powerful well balanced techniques which allow to study with increased accuracy the evolution of small perturbations arising over moving equilibrium solutions. A manuscript which reports these novel results with benchmarks performed on the Euler equations and the MHD equations is in preparation. We remark, that this is the first time in literature that the full ADER DG scheme with *a posteriori* sub-cell FV limiter has been made *well balanced*. This has been obtained by assuring that any projection, reconstruction and integration procedures were always performed by summing up the exact value of the equilibria plus the high order accurate evolution of the fluctuations.

The main developer of AleVoronoi is Elena Gaburro. The described work has been realized in collaboration with Simone Chiocchetti (University of Trento, Italy) and Mario Ricchiuto. This work has been presented at Numhyp 2023 (Bordeaux), ICIAM 2023 (Tokyo, Japan), ENUMATH 2023 (Lisbon, Portugal) and in several seminars at the department level (as at i. Politecnico di Milano, Italy, ii. École Polytechnique Paris, France, iii. University of Stuttgart. Germany ...).

7.7 Modeling of flows in aquifers

Participants: Manon Carreau, 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. In [51], 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.

In [15], 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 conververters such are the solution of Seaturns of Hace. In parallel, we work on the structure of the code in order to integrate more easily the furthers ideas. In particular, specific numerical integrators and time schemes have been implemented.

7.8 Uncertainty quantifications

Participants: Héloïse Beaugendre.

This paper [17] is part of Elie Solai's PhD and proposes an innovative way to deal with the uncertainties related to internal resistance of Li-ion batteries using experimental data and numerical simulation. First, a CFD model is used to reproduce an experimental configuration representing the behavior of heated Li-ion battery cells under constant discharging current conditions. Secondly, an Uncertainty Quantification based methodology is proposed to represent the internal resistance and its inherent uncertainties. The impact of those uncertainties on the temperature evolution of Li-ion cells is quantified. A Bayesian inference of the internal resistance model parameters using experimental measurements is performed, reducing the prediction uncertainty by almost 95% for some temperatures of interest. Finally, an enhanced internal model is constructed by considering the state of charge and temperature dependency on internal resistance. The resulting temperature evolution computed with the two different resistance models is compared for the low state of charge situations.

8 Bilateral contracts and grants with industry

8.1 Bilateral Contracts

CEA-DAM/DIF

Participants: Mario Ricchiuto.

- Title: Development of a numerical model for tsunamis: from propagation to breking in realistic coastal environnements.
- 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, possibly combined with WENO approximations. The schemes are to be implemented in the code of CEA and applied to tsunami simulations in realistic coastal environmements.

CEA-CESTA

Participants: Héloïse Beaugendre.

- Title: Immersed boundary method applied to large eddy simulations of hypersonic reentry vehicles
- Type: contrat d'accompagnement for Florent Nauleau's PhD.
- Duration: 36 months
- Starting date : 19 October 2020
- Coordinator: Heloise Beaugendre Fabien Vivodtzev and Thibault Bridel-Bertomeu (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.

CEA-CESTA

Participants: Héloïse Beaugendre.

- Title: Development of models and numerical methods for the degradation of a pyrolysable material
- Type: contrat d'accompagnement for Alexis Cas's PhD.
- Duration: 36 months
- Starting date : 1st October 2023
- Coordinator: Heloise Beaugendre Celine Baranger and Simon Peluchon(CEA)

• Summary: During re-entry into the atmosphere, a spacecraft is subjected to considerable mechanical stress and heat flows. These heat flows, applied to the vehicle's wall, cause the heat shield to heat up significantly. The heat shield is made up of materials that chemically degrade under the effect of heat to limit the temperature rise inside the vehicle. These reactions are known as pyrolysis. Similarly, on the surface, these materials undergo physical degradation known as ablation. Understanding these two phenomena is essential for the design of heat shields. The design of such a shield requires precise numerical simulations of the airflow that is created around the vehicle throughout its trajectory. This airflow must be coupled with ablation and pyrolysis phenomena.

EDF

Participants: Bastien Jouy, Mario Ricchiuto.

- · Title: Numerical modelling of Favre waves and undular bores in channels with banks
- Duration: 36 months
- Starting date : 08 November 2021
- Coordinator: Mario Ricchiuto
- Summary: The collaboration with EDF (Eleectricité de France) focuses on the improvement of their in house code TELEMAC-Mascaret, initially for the advection of passive scalars (pollutant transport), and more recently for the simulation of hydrostatic and dispersive (undular) bore dynamics in networks of channels (application to abrupt closing/opening of valves). The past work on advection schemes has been done with J.M. Hervouet (retired) and R. Ata (riadh.ata@edf.fr currently at FLOW-3D) was an informal collaboration. The ongoing collaboration on bore dynamics is with D. Violeau (damien.violeau@edf.fr) is object of a CIFRE contract. This work aims at increasing the capabilities of EDF's code to simulate the undulating bores studied in [53].

9 Partnerships and cooperations

9.1 International initiatives

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

LARME

Title: Large-scale simulations of renewable marine energy

Duration: 2021 ->

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

Partners:

Rise/Aalborg University (Danemark)

Inria contact: Martin Parisot

Summary: During this collaboration, we propose to focus on the modeling and simulation of marine renewable energy converters based on wave or current energy. Among marine renewable energies, only offshore wind energy is truly exploited today. However, this sector only uses large marine surfaces, without exploiting the true potential of the sea. Indeed, water being 1000 times heavier than air, its energy potential is also much higher.

9.2 International research visitors

9.2.1 Visits of international scientists

Inria International Chair

This year R. Abgrall has visited the team for one moth during which joint work with M. Ricchiuto and L. Micalizzi (U. Zurich) on well balanced schemes, and staggered discretizations for balance laws has been performed.

9.3 European initiatives

9.3.1 H2020 projects

SuPerMan SuPerMan project on cordis.europa.eu

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

Duration: From June 1, 2021 to May 31, 2023

Partners:

• INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET AUTOMATIQUE (INRIA), France

Inria contact: Elena GABURRO

Coordinator: 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.

Indeed, nonlinear systems of hyperbolic PDEs are characterized by invariants, whose preservation at the discrete level is not trivial, but plays a fundamental role in improving the long term predictivity and reducing the computational effort of modern algorithms. Besides mass and linear momentum conservation, typical of any Finite Volume scheme, the preservation of stationary and moving equilibria, asymptotic limits and interfaces still represents an open challenge, especially in astrophysical applications, such as turbulent flows in gas clouds rotating around black holes.

In this project, our focus will thus be on General Relativistic Hydrodynamics (GRHD) for which such Well Balanced (WB) Structure Preserving (SP) schemes have never been studied before. In particular, we plan to devise smart methods, independent of the coordinate system. This will be achieved by directly including the metric, implicitly contained in the covariant derivative, as a conserved variable inside the GRHD model.

This approach will first be tested on the Euler equations of gasdynamics with Newtonian gravity, extending already existing WB-SP techniques to general coordinate systems. All novel features will be carefully proven theoretically. Next, the new schemes will be incorporated inside a massively parallel high order accurate Arbitrary-Lagrangian-Eulerian Finite Volume (FV) and Discontinuous Galerkin (DG) code, to be released as open source. The feasibility of the project is guaranteed by the strong network surrounding the ER, including experts on WB-SP techniques and mesh adaptation (INRIA France), FV-DG schemes and GRHD (UniTN Italy) and computational astrophysics (MPG Germany). This MSCA project will allow the applicant transition to become an independent researcher.

eFlows4HPC eFlows4HPC project on cordis.europa.eu

Title: Enabling dynamic and Intelligent workflows in the future EuroHPCecosystem

Duration: From January 1, 2021 to February 29, 2024

Partners:

- INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET AUTOMATIQUE (INRIA), France
- DTOK LAB SRL, Italy
- FORSCHUNGSZENTRUM JULICH GMBH (FZJ), Germany
- SCUOLA INTERNAZIONALE SUPERIORE DI STUDI AVANZATI DI TRIESTE (SISSA), Italy
- INSTYTUT CHEMII BIOORGANICZNEJ POLSKIEJ AKADEMII NAUK, Poland
- ALFRED-WEGENER-INSTITUT HELMHOLTZ-ZENTRUM FUR POLAR- UND MEERESFORSCHUNG (AWI), Germany
- EIDGENOESSISCHE TECHNISCHE HOCHSCHULE ZUERICH (ETH Zürich), Switzerland
- INSTITUT POLYTECHNIQUE DE BORDEAUX (Bordeaux INP), France
- STIFTELSEN NORGES GEOTEKNISKE INSTITUTT (NGI), Norway
- BULL SAS (BULL), France
- CENTRE INTERNACIONAL DE METODES NUMERICS EN ENGINYERIA (CIMNE-CERCA), Spain
- UNIVERSIDAD DE MALAGA (UMA), Spain
- UNIVERSITAT POLITECNICA DE VALENCIA (UPV), Spain
- ISTITUTO NAZIONALE DI GEOFISICA E VULCANOLOGIA, Italy
- FONDAZIONE CENTRO EURO-MEDITERRANEOSUI CAMBIAMENTI CLIMATICI (FONDAZIONE CMCC), Italy
- SIEMENS AKTIENGESELLSCHAFT, Germany
- BARCELONA SUPERCOMPUTING CENTER CENTRO NACIONAL DE SUPERCOMPUTACION (BSC CNS), Spain

Inria contact: Mario RICCHIUTO

Coordinator:

Summary: eFlows4HPC aims to deliver a workflow software stack and an additional set of services to enable the integration of HPC simulation and modelling with big data analytics and machine learning in scientific and industrial applications.

To demonstrate the workflow software stack, use cases from three thematic pillars have been selected. Pillar I focuses on the construction of DigitalTwins for the prototyping of complex manufactured objects integrating state-of-the-art adaptive solvers with machine learning and datamining, contributing to the Industry 4.0 vision. Pillar II develops innovative adaptive workflows for climate and for the study of Tropical Cyclones (TC) in the context of the CMIP6 experiment, including in-situ analytics. Pillar III explores the modelling of natural catastrophes - in particular, earthquakes and their associated tsunamis- shortly after such an event is recorded. Leveraging two existing workflows, the Pillar will work of integrating them with the eFlows4HPC software stack and on producing policies for urgent access to supercomputers. The pillar results will be demonstrated in the target community CoEs to foster adoption and get feedback.

9.4 National initiatives

ANR GEOFUN

Participants: Manon Carreau, Martin Parisot.

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

Participants: Maria Kazolea, Martin Parisot, Mario Ricchiuto.

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

Participants: Maria Kazolea, Mario Ricchiuto.

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

Type: Inria Challenges

Duration: 48 months

Starting date: 1st Jan 2019

Coordinator: Arthur Vidard (AirSea)

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.

Inria Action Exploratoire: AM²OR

Participants: Nicolas Barral.

Title: AM²OR: Adaptive meshes for Model Order Reduction

Type: Inria Action Exploratoire

Duration: 48 months

Starting date: 1st October 2022

Coordinator: Nicolas Barral

Partner: Tommaso Taddei (Inria MEMPHIS)

Abstract: Mesh adaptation and Model Order Reduction both aim at reducing significantly the computational cost of numerical simulations by taking advantage of the solution's features. Reduced Order Modelling is a method that builds lighter surrogate models of a system's response over a range of parameters, which is particularly useful in the solution of design and optimization inverse problems. Reduced-order models rely on a high-fidelity (e.g., finite element) approximation that should be sufficiently accurate over the whole range of parameters considered: in presence of structures such as shocks and boundary layers, standard mesh refinement techniques would lead to high-fidelity models of intractable size. In this project, we propose a novel adaptive procedure to simultaneously construct a high-fidelity mesh (and associated discretisation) and a reduced-order model for a range of parameters, with particular emphasis on inverse problems in computational fluid dynamics.

10 Dissemination

10.1 Promoting scientific activities

10.1.1 Scientific events: organisation

General chair, scientific chair

• The team is activiley organizing the next edition of the HONOM (High-Order NOnlinear numerical Methods for evolutionary PDEs: theory and applications) conference to be held on 8-13 of Steptember 2024, KAM Conference Center Chania, Crete Island, Greece. Conference Chairs are E. Gaburro and M. Kazolea (co-chair).

Member of the organizing committees

- Martin Parisot: member of the organizing commitee of NumHyp23 'Numerical Methods for Hyperbolic Problems' 26-30 June 2023 Bordeaux (France). member of the organizing commitee of the
- Mario Ricchiuto: member of the organizing commitee of NumHyp23 and B'WAVES.
- Maria Kazolea and Martin Parisot were mebers of the organizing commitee of the MS3-03 Advanced numerical modeling for dispersive free surface water waves on the CFC2023, 26-28 April, Cannes, France.

10.1.2 Scientific events: selection

Member of scientific committees

- · Mario Ricchiuto is deputy head of science of the Inria center at University of Bordeaux
- Elena Gaburro is member of the scientific committees of the CEDYA international conference (June 2024, Spain) and the MultiMat 2024 international conference (August 2024, Colorado, USA).
- Mario Ricchiuto: member of the ICCFD series scientific committee (next edition Kobe, Japan in 2024), member of the IACM Computational Fluids Conference international scientific committee (Cannes, 2023), member of the scientific commitee of the GdR MathGeoPhy.

10.1.3 Journal

Member of the editorial boards

- Elena Gaburro: associate editor of Applied Mathematics and Computations, Elsevier journal;
- Martin Parisot: managing editor of J.Comput.Math. (Smai);
- Mario Ricchiuto : J.Comput.Physics (Elsevier), Computers and Fluids (Elsevier), Numerical Methods for Partial Differential Equations (Whiley), Water Waves (Springer).

Reviewer - reviewing activities

- Nicolas Barral: Journal of Computational Physics, Communications on Applied Mathematics and Computation
- Elena Gaburro : Applied Mathematics and Computations, Computer and Fluids, Journal of Computational Physics, Journal of Scientific Computing, International Journal for Numerical Methods in Fluids, Journal of Computational and Applied Mathematics, SIAM Journal on Scientific Computing
- Maria Kazolea: Journal of Computational Physics,
- Martin Parisot : Applied Mathematics and Computation, Computers and Fluids
- Mario Ricchiuto : J.Comput.Physics (Elsevier), J.Sci.Compput. (Springer), M2AN (ESAIM)
- Heloise Beaugendre : CMAME (Elsevier), MDPI

10.1.4 Invited talks

- Elena Gaburro: invited talk at a mini synposium at ICIAM 2023 (Tokyo, Japan);
- Maria Kazolea: invited talk at the NOAA seminar series (May 2023)
- Martin Parisot: invited talk at the Jean-Paul Vila's 66th birthday seminar (Mars 2023) and at 'Journées de Modélisation des Vagues à Phases Résolues' (Octobre 2023) and at the inria-Brazil seminar (Décember 2023).
- Mario Ricchiuto: plenary talks at the 11th SMAI Biennial (May 2023, Guadeloupe), Workshop on numerical approximation of hyperbolic PDEs in honor of Prof. Carlos Parés (November 2023, Malaga), Colloquium in memory of Serguei Godunov (November 2023, Marseille)

10.2 Teaching - Supervision - Juries

10.2.1 Teaching

- License: Nicolas Barral, Calcul Scientifique en Fortran 90, 22h, L3, ENSEIRB-MATMÉCA, France
- License : Nicolas Barral, TP Fortran 90, 44h, M1, ENSEIRB-MATMÉCA, France
- Master : Nicolas Barral, Calcul Haute Performance (OpenMP-MPI), 45h, M1, ENSEIRB-MATMÉCA et Université de Bordeaux, 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
- License: Martin Parisot, TP Fortran, 21h, M1, ENSEIRB-MATMÉCA, France
- Master : Mario Ricchiuto and Martin Parisot, Multiphysics Course, 26h cours magistrale, M2, ENSEIRB-MATMÉCA, France
- Master and PhD: Elena Gaburro, Advanced Numerical Methods for the solution of Hyperbolic Equations, 12h (University of Verona, Italy)

10.2.2 Supervision

- PhD in progress: J. Galaz Mora, Coupling of free surface coastal models, started in February 2021, co-supervised by M. Kazolea and A. Rousseau.
- 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 (defended in March 2023) : B. Constant, Amélioration d'une méthode de frontières immergées pour la simulation d'écoulements turbulents autour de géométries complexes, supervised by H. Beaugendre and S. Péron (ONERA).
- PhD (defended in December 2023) : T. Carlier, Modeling of an icing system using shifted boundary method, co-supervised by H. Beaugendre and M. Colin.
- PhD (defended in December 2023) : F. Nauleau, Immersed boundary method applied to large eddy simulations of hypersonic reentry vehicles, 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: B. Jouy, Simulation of Favre waves in channels with variable section, started in November 2021, co-supervised by M. Ricchiuto and D. Violeau (EDF).
- PhD in progress: V. Pilorget, High order DG modelling of global storm surges for very long term inundation simulations, started in January 2022, co-supervised by A.-G. Filippini (BRGM) and M. Ricchiuto.
- PhD in progress: A. Cas, Development of models and numerical methods for the degradation of a pyrolysable material, started in October 2023, co-supervised by C. Baranger and S. Peluchon (CEA) and H. Beaugendre.

10.2.3 Juries

- Mario Ricchiuto has contributed to the works of the PhD juries of A. Assonitis (U. Roma La Sapienza) in January 2023 (as reviewer), F.N. Mojarrad (U. Zurich) in March 2023 (as reviewer), T. Marchal (CERFACS) in April 2023 (as reviwer), L. Micalizzi (U. Zurich) in December 2023.
- Heloise Beaugendre has contributed to the works of the PhD juries of P. Benez (Coria/Insa Rouen) in July 2023 (as reviewer), M. Stuck (ONERA/CEA ISAE Sup AERO) in December 2023 (as reviewer), the HDR of Emmanuel Radenac (ONERA) in December 2023.

10.3 Popularization

10.3.1 Interventions

- Maria Kazolea participated in the European night of the researchers, 29 September 2023, Cap Sciences-Bordeaux
- Mario Ricchiuto participated to the 'Journées portes fermées' in December 2023 with a presentation on *The continnuum Modelling-HPC-Heterogeneous architectures*
- Martin Parisot participated to the 'Journée Emploi Maths et Interactions' in November 2023

11 Scientific production

11.1 Major publications

- T. Carlier, L. Nouveau, H. Beaugendre, M. Colin and M. Ricchiuto. 'An Enriched Shifted Boundary Method to Account For Moving Fronts'. In: *Journal of Computational Physics* 489 (2023). DOI: 10.1016/j.jcp.2023.112295. URL: https://inria.hal.science/hal-03661072.
- [2] M. Ciallella, D. Torlo and M. Ricchiuto. 'Arbitrary High Order WENO Finite Volume Scheme with Flux Globalization for Moving Equilibria Preservation'. In: *Journal of Scientific Computing* 96.2 (30th June 2023), p. 53. DOI: 10.1007/s10915-023-02280-9. URL: https://inria.hal.scie nce/hal-04372541.
- [3] M. Kazolea and M. Ricchiuto. 'Full nonlinearity in weakly dispersive Boussinesq models: luxury or necessity?' In: *Journal of Hydraulic Engineering* 150.1 (Jan. 2024). DOI: 10.1061/JHEND8.HYENG-13718. URL: https://inria.hal.science/hal-04334853.

11.2 Publications of the year

International journals

- [4] N. Barral, T. Taddei and I. Tifouti. 'Registration-based model reduction of parameterized PDEs with spatio-parameter adaptivity'. In: *Journal of Computational Physics* 499 (Feb. 2024), p. 112727. DOI: 10.1016/j.jcp.2023.112727. URL: https://inria.hal.science/hal-04371531.
- [5] T. Carlier, L. Nouveau, H. Beaugendre, M. Colin and M. Ricchiuto. 'An Enriched Shifted Boundary Method to Account For Moving Fronts'. In: *Journal of Computational Physics* 489 (2023). DOI: 10.1016/j.jcp.2023.112295. URL: https://inria.hal.science/hal-03661072.
- [6] M. G. Carlino and E. Gaburro. 'Well balanced finite volume schemes for shallow water equations on manifolds'. In: *Applied Mathematics and Computation* 441 (Mar. 2023), p. 127676. DOI: 10.1016 /j.amc.2022.127676. URL: https://hal.science/hal-03850195.
- [7] M. Ciallella, E. Gaburro, M. Lorini and M. Ricchiuto. 'Shifted boundary polynomial corrections for compressible flows: high order on curved domains using linear meshes'. In: *Applied Mathematics and Computation* 441.15 (Mar. 2023), p. 127698. DOI: 10.1016/j.amc.2022.127698. URL: https://hal.science/hal-03865587.
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- [9] E. Gaburro, P. Öffner, M. Ricchiuto and D. Torlo. 'High order entropy preserving ADER-DG schemes'. In: Applied Mathematics and Computation 440 (Mar. 2023), p. 127644. DOI: 10.10 16/j.amc.2022.127644. URL: https://hal.science/hal-03850196.
- [10] K. Ignatowicz, F. Morency and H. Beaugendre. 'Surface Roughness in RANS Applied to Aircraft Ice Accretion Simulation: A Review'. In: *Fluids* 8.10 (15th Oct. 2023), p. 278. DOI: 10.3390/fluids81 00278. URL: https://inria.hal.science/hal-04359324.
- [11] M. Kazolea, A. G. Filippini and M. Ricchiuto. 'Low dispersion finite volume/element discretization of the enhanced Green-Naghdi equations for wave propagation, breaking and runup on unstructured meshes'. In: Ocean Modelling 182 (1st Apr. 2023), p. 102157. DOI: 10.1016/j.ocemod.202 2.102157. URL: https://inria.hal.science/hal-03402701.
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- [13] Y. Mantri, P. Öffner and M. Ricchiuto. 'Fully well-balanced entropy controlled discontinuous Galerkin spectral element method for shallow water flows: global flux quadrature and cell entropy correction'. In: *Journal of Computational Physics* 498 (Feb. 2024), p. 112673. DOI: 10.1016/j.jcp .2023.112673.URL: https://inria.hal.science/hal-04334768.

- [14] S. Michel, D. Torlo, M. Ricchiuto and R. Abgrall. 'Spectral analysis of high order continuous FEM for hyperbolic PDEs on triangular meshes: influence of approximation, stabilization, and time-stepping'. In: *Journal of Scientific Computing* 94.49 (21st Jan. 2023). DOI: 10.1007/s10915-022-02087-0. URL: https://inria.hal.science/hal-03940122.
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International peer-reviewed conferences

- [21] T. Carlier, B. T. Helenbrook, H. Beaugendre and M. Colin. 'Stability Analysis and Numerical Study of Stefan Problems for Embedded Computation of Moving Internal Boundaries'. In: CFC 2023 -22nd Computational Fluids Conference. Cannes, France, 25th Apr. 2023. URL: https://inria.h al.science/hal-04359856.
- T. Carlier, B. T. Helenbrook, H. Beaugendre, M. Colin and L. Nouveau. 'Numerical Analysis of Stefan Problems for Embedded Computation of Moving Internal Boundaries'. In: ENUMATH 2023
 The European Conference on Numerical Mathematics and Advanced Applications. Lisbonne, Portugal, 4th Sept. 2023. URL: https://inria.hal.science/hal-04359844.
- [23] C. Peugeot, E. Le Roux, V. Wendling, G. Panthou, P.-A. Raynal, A. Ba, I. Bouzou Moussa, J.-M. Cohard, J. Demarty, F. Gangneron, M. Grippa, B. Hector, T. Lebel, P. Hiernaux, L. Kergoat, E. Lawin, J. D. Galaz Mora, É. Mougin, C. Pierre, J.-L. Rajot and T. Project. 'A drought-triggered hydrological tipping point in the central Sahel: an attribution study using system dynamics modelling'. In: 2nd conference internationale TERENO-OZCAR. Bonn, Germany, 2023. URL: https://imt-mines-a les.hal.science/hal-04286359.

Conferences without proceedings

[24] K. Ignatowicz, F. Morency and H. Beaugendre. 'BAYESIAN CALIBRATION OF GLAZE ICE SUR-FACE ROUGHNESS FOR AIRCRAFT ICE ACCRETION SIMULATION'. In: Canadian Society for Mechanical Engineering International Congress 2023 - CSME Congress 2023. Sherbrooke, Canada, 28th May 2023. URL: https://inria.hal.science/hal-04359820. [25] F. Nauleau, H. Beaugendre, T. Bridel-Bertomeu and F. Vivodtzev. 'Immersed boundaries in hypersonic flows with considerations about high-order for LES simulations'. In: IACM 22nd Computational Fluids Conference - CFC 2023. Cannes, France, 25th Apr. 2023. URL: https://inria.hal .science/hal-04360180.

Scientific book chapters

- [26] E. Gaburro and S. Chiocchetti. 'High-order Arbitrary-Lagrangian-Eulerian schemes on crazy moving Voronoi meshes'. In: *Numerical aspects of hyperbolic balance laws and related problems*. 1st July 2023. DOI: 10.1007/978-3-031-29875-2_5. URL: https://hal.science/hal-03850 200.
- [27] K. Ignatowicz, H. Beaugendre and F. Morency. 'Numerical Simulation of In-Flight Iced Surface Roughness'. In: *Handbook of Numerical Simulation of In-Flight Icing*. Springer International Publishing, 4th May 2023, pp. 1–48. DOI: 10.1007/978-3-030-64725-4_29-1. URL: https://i nria.hal.science/hal-04358583.

Edition (books, proceedings, special issue of a journal)

[28] K. Ignatowicz, F. Morency and H. Beaugendre, eds. *Data-driven Roughness Estimation for Glaze Ice Accretion Simulation*. International Conference on Icing of Aircraft, Engines, and Structures. Vol. SAE Technical paper 2023-01-1449. 15th June 2023. DOI: 10.4271/2023-01-1449. URL: https://inria.hal.science/hal-04359770.

Reports & preprints

- [29] M. Ciallella, S. Clain, E. Gaburro and M. Ricchiuto. Very high order treatment of embedded curved boundaries in compressible flows: ADER discontinuous Galerkin with a space-time Reconstruction for Off-site data. 2023. DOI: 10.48550/arXiv.2312.07170. URL: https://inria.hal.scienc e/hal-04341999.
- [30] M. Dumbser, O. Zanotti, E. Gaburro and I. Peshkov. A well-balanced discontinuous Galerkin method for the first-order Z4 formulation of the Einstein-Euler system. 13th July 2023. URL: https: //hal.science/hal-04341812.
- [31] M. Kazolea and M. Ricchiuto. *Full nonlinearity in weakly dispersive Boussinesq models: luxury or necessity* ? 26th Mar. 2023. URL: https://inria.hal.science/hal-04046699.
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- [33] L. Micalizzi, M. Ricchiuto and R. Abgrall. Novel well-balanced continuous interior penalty stabilizations. 2023. DOI: 10.48550/arXiv.2307.09697. URL: https://inria.hal.science/hal-0 4342011.
- [34] J. Visbech, A. P. Engsig-Karup and M. Ricchiuto. A spectral element solution of the Poisson equation with shifted boundary polynomial corrections: influence of the surrogate to true boundary mapping and an asymptotically preserving Robin formulation. 2023. DOI: 10.48550/arXiv.2310.17621. URL: https://inria.hal.science/hal-04342005.
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[37] J. Galaz, M. Kazolea and A. Rousseau. 'Modeling wave breaking by coupling dispersive and hyperbolic water wave models'. In: MOMI 2023 - Le Monde des Mathématiques Industrielles 2023: Smart Environment. Sophia Antipolis, France, 2023. URL: https://inria.hal.science/hal-0 4189458.

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