Activity Report 2018

Project-Team MEMPHIS

Modeling Enablers for Multi-PHysics and InteractionS
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Project-Team MEMPHIS

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

Keywords:

**Computer Science and Digital Science:**
- A6. - Modeling, simulation and control
- A6.1.1. - Continuous Modeling (PDE, ODE)
- A6.1.5. - Multiphysics modeling
- A6.2.1. - Numerical analysis of PDE and ODE
- A6.3.1. - Inverse problems
- A6.3.2. - Data assimilation
- A6.3.4. - Model reduction
- A6.5.2. - Fluid mechanics
- A9.2. - Machine learning

**Other Research Topics and Application Domains:**
- B1.1.7. - Bioinformatics
- B2.2.1. - Cardiovascular and respiratory diseases
- B4.3.2. - Hydro-energy
- B4.3.3. - Wind energy
- B5.2.1. - Road vehicles
- B5.2.3. - Aviation
- B5.2.4. - Aerospace
- B5.5. - Materials
- B8.4. - Security and personal assistance
- B8.4.1. - Crisis management

1. Team, Visitors, External Collaborators

**Research Scientists**
- Michel Bergmann [Inria, Researcher, HDR]
- Tommaso Taddei [Inria, Researcher, from Oct 2018]

**Faculty Members**
- Angelo Iollo [Team leader, Univ de Bordeaux, Professor, HDR]
- Afaf Bouharguane [Univ de Bordeaux, Associate Professor]
- Charles-Henri Bruneau [Univ de Bordeaux, Professor]

**PhD Students**
- Emanuela Abbate [Univ degli Studi dell’Insubria / Univ de Bordeaux]
- Luis Henrique Benetti Ramos [ONERA]
- Mathias Braun [IRSTEA]
- Michele Giuliano Carlino [Inria, from Oct 2018]
- Antoine Fondaneche [Univ de Bordeaux, from Sep 2018]
- Baptiste Lambert [Univ de Bordeaux]
- Claire Taymans [VALEOL, until Sep 2018]
- Stefano Pezzano [Inria, from Apr 2018 until Sep 2018]
2. Overall Objectives

2.1. Multi-physics numerical modeling

We aim at a step change in multi-physics numerical modeling by developing two fundamental enablers:

- **reduced-order models**;
- **hierarchical Cartesian schemes**.

Reduced-order models (ROMs) are simplified mathematical models derived from the full set of PDEs governing the physics of the phenomenon of interest. ROMs can be obtained exploiting first principles or be data-driven. With ROMs one trades accuracy for speed and scalability, and counteracts the curse of dimensionality of traditional high-fidelity solvers by significantly reducing the computational complexity. ROMs represent an ideal building block for systems with real-time requirements, like interactive decision support systems that offer the possibility to rapidly explore various alternatives.

Hierarchical Cartesian schemes allow the multi-scale solution of PDEs on non body-fitted meshes with a drastic reduction of the computational setup overhead. These methods are easily parallelizable and they can efficiently be mapped to high-performance computer architectures. They avoid dealing with grid generation, a prohibitive task when the boundaries are moving and the topology is complex and unsteady.

3. Research Program

3.1. Reduced-order models

Massive parallelization and rethinking of numerical schemes will allow the use of mathematical models for a broader class of physical problems. For industrial applications, there is an increasing need for rapid and reliable numerical simulators to tackle design and control tasks. To provide a concrete example, in the design process of an aircraft, the flight conditions and manoeuvres, which provide the largest aircraft loads, are not known a priori. Therefore, the aerodynamic and inertial forces are calculated for a large number of conditions to give an estimate of the maximum loads, and hence stresses, that the structure of the detailed aircraft design might experience in service. As a result, the number of simulations required for a realistic design problem could easily be in the order of tens of millions. Even with simplistic models of the aircraft behavior this is an unfeasible number of separate simulations. However, engineering experience is used to identify the most likely critical load conditions, meaning that approximately hundreds of thousands simulations are required for conventional aircraft configurations. Furthermore, these analyses have to be repeated every time that there is an update in the aircraft structure.
Compared to existing approaches for ROMs [32], our interest will be focused on two axes. On the one hand, we start from the consideration that small, highly nonlinear scales are typically concentrated in limited spatial regions of the full simulation domain. So for example, in the flow past a wing, the highly non-linear phenomena take place in the proximity of the walls at the scale of a millimeter, for computational domains that are of the order of hundreds of meters. Based on these considerations, we propose in [15] a multi-scale model where the large scales are described by far-field models based on ROMs and the small scales are simulated by high-fidelity models. The whole point for this approach is to optimally decouple the far field from the near field.

A second characterizing feature of our ROM approach is non-linear interpolation. We start from the consideration that dynamical models derived from the projection of the PDE model in the reduced space are neither stable to numerical integration nor robust to parameter variation when hard non-linear multi-scale phenomena are considered. However, thanks to Proper Orthogonal Decomposition (POD) [38], [44], [28] we can accurately approximate large solution databases using a low-dimensional base. Recent techniques to investigate the temporal evolution of the POD modes (Koopman modes [39], [26], Dynamic Mode Decomposition [42]) and allow a dynamic discrimination of the role played by each of them. This in turn can be exploited to interpolate between modes in parameter space, thanks to ideas relying on optimal transportation [46], [29] that we have started developing in the FP7 project FFAST and H2020 AEROGUST.

3.2. Hierarchical Cartesian schemes

We intend to conceive schemes that will simplify the numerical approximation of problems involving complex unsteady objects together with multi-scale physical phenomena. Rather than using extremely optimized but non-scalable algorithms, we adopt robust alternatives that bypass the difficulties linked to grid generation. Even if the mesh problem can be tackled today thanks to powerful mesh generators, it still represents a severe difficulty, in particular when highly complex unsteady geometries need to be dealt with. Industrial experience and common practice shows that mesh generation accounts for about 20% of overall analysis time, whereas creation of a simulation-specific geometry requires about 60%, and only 20% of overall time is actually devoted to analysis. The methods that we develop bypass the generation of tedious geometrical models by automatic implicit geometry representation and hierarchical Cartesian schemes.

The approach that we plan to develop combines accurate enforcement of unfitted boundary conditions with adaptive octree and overset grids. The core idea is to use an octree/overset mesh for the approximation of the solution fields, while the geometry is captured by level set functions [43], [37] and boundary conditions are imposed using appropriate interpolation methods [25], [45], [41]. This eliminates the need for boundary-conforming meshes that require time-consuming and error-prone mesh generation procedures, and opens the door for simulation of very complex geometries. In particular, it will be possible to easily import the industrial geometry and to build the associated level set function used for simulation.

Hierarchical octree grids offer several considerable advantages over classical adaptive mesh refinement for body-fitted meshes, in terms of data management, memory footprint and parallel HPC performance. Typically, when refining unstructured grids, like for example tetrahedral grids, it is necessary to store the whole data tree corresponding to successive subdivisions of the elements and eventually recompute the full connectivity graph. In the linear octree case that we develop, only the tree leaves are stored in a linear array, with a considerable memory advantage. The mapping between the tree leaves and the linear array as well as the connectivity graph is efficiently computed thanks to an appropriate space-filling curve. Concerning parallelization, linear octrees guarantee a natural load balancing thanks to the linear data structure, whereas classical unstructured meshes require sophisticated (and moreover time consuming) tools to achieve proper load distribution (SCOTCH, METIS etc.). Of course, using unfitted hierarchical meshes requires further development and analysis of methods to handle the refinement at level jumps in a consistent and conservative way, accuracy analysis for new finite-volume or finite-difference schemes, efficient reconstructions at the boundaries to recover appropriate accuracy and robustness. These subjects, that are currently virtually absent at Inria, are among the main scientific challenges of our team.
4. Application Domains

4.1. Energy conversion

We apply the methods developed in our team to the domain of wind engineering and sea-wave converters. In Figure 1, we show results of a numerical model for a sea-wave energy converter. We here rely on a monolithic model to describe the interaction between the rigid floater, air and water; material properties such as densities, viscosities and rigidity vary across the domain. The appropriate boundary conditions are imposed at interfaces that arbitrarily cross the grid using adapted schemes built thanks to geometrical information computed via level set functions [43]. The background method for fluid-structure interface is the volume penalization method [25] where the level set functions is used to improve the degree of accuracy of the method [3] and also to follow the object. The underlined mathematical model is unsteady, and three dimensional; numerical simulations based on a grid with $\mathcal{O}(10^8)$ degrees of freedom are executed in parallel using 512 CPUs.

![Figure 1. numerical modeling of a sea-wave converter by a monolithic model and Cartesian meshes.](image)

In the context of the Aerogust (Aeroelastic gust modelling) European project, together with Valorem, we investigated the behavior of wind turbine blades under gust loading. The aim of the project was to optimize the design of wind turbine blades to maximize the power extracted. A meteorological mast (Figure 2(a)) has been installed in March 2017 in Brittany to measure wind on-site: data provided by the mast have been exploited to initialize the mathematical model. Due to the large cost of the full-order mathematical model, we relied on a simplified model [35] to optimize the global twist. Then, we validated the optimal configuration using the full-order Cartesian model based on the NaScar solver. Figure 2(b) shows the flow around the optimized wind turbine rotor.

4.2. Impacts

Mathematical and numerical modelling of physical systems undergoing impacts is challenging due to the presence of large deformations and displacements of the solid part, and due to the strongly non-linear behaviour of the fluid part. At the same time, proper experiments of impact phenomena are particularly dangerous and require expensive facilities, which make them largely impractical. For this reason, there is a growing interest in the development of predictive models for impact phenomena.

In MEMPHIS, we rely on a fully Eulerian approach based on conservation laws, where the different materials are characterized by their specific constitutive laws, to address these tasks. This approach was introduced in [34] and subsequently pursued and extended in [40], [33], [27], [30] In Figure 3, we show the results of the numerical simulation of the impact of a copper projectile immersed in air over a copper shield. Results are obtained using a fully parallel monolithic Cartesian method, based on a $4000^2$ fixed Cartesian grid. Simulations
are performed on a cluster of 512 processors, and benefits from the isomorphism between grid partitioning and processor topology.

Figure 3. Impact and rebound of a copper projectile on a copper plate. Interface and schlieren at 50\(\mu\)s, 199\(\mu\)s, 398\(\mu\)s and 710\(\mu\)s.

4.3. Vascular flows

A new research direction pursued by the team is the mathematical modelling of vascular blood flows in arteries. Together with the start-up Nurea (http://nurea-soft.com/) and the surgeon Eric Ducasse, we aim at developing reliable and automatic procedures for aneurysm segmentation and for the prediction of aneurysm rupture risk. Our approach exploits two sources of information: (i) numerical simulations of blood flows in complex geometries, based on an octree discretization, and (ii) computed tomography angiography (CTA) data. Figure 4 shows the force distribution on the walls of the abdominal aorta in presence of an aneurysm; results are obtained using a parallelized hierarchical Cartesian scheme based on octrees.

5. Highlights of the Year
5.1. Highlights of the Year

5.1.1. Turbulent flow simulations using Octrees

We have initially developed and tested a 3D first-order Octree code for unsteady incompressible Navier-Stokes equations for full windmill simulations with an LES model and wall laws. We have validated this code on Occigen for complex flows at increasing Reynolds numbers. This step implied identifying stable and feasible schemes compatible with the parallel linear Octree structure. The validation has been conducted with respect to the results of a fully Cartesian code (NaSCAR) that we run on Turing (with significantly more degrees of freedom) and with respect to experimental results.

Subsequently, we have developed a second-order Octree scheme that has been validated on Occigen for a sphere at a moderate Reynolds number ($Re = 500$), see Table 1. Then, for a cylinder at ($Re = 140000$) (Figures 5(a) and 5(b)), close to real applications, we have preliminary validation results for the second-order scheme with respect to experimental drag coefficient (Table 2). Additional resources will be asked on Occigen to complete the study.

Table 1. Flow past a sphere at $Re = 500$. Results in the literature are spread between $C_D = 0.48$ and $C_D = 0.52$.

<table>
<thead>
<tr>
<th>Mesh</th>
<th>$\Delta x_{\text{min}}$</th>
<th>number of cells</th>
<th>$C_D$ (1st-order scheme)</th>
<th>$C_D$ (2nd-order scheme)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.094</td>
<td>$0.72 \cdot 10^5$</td>
<td>N.A.</td>
<td>0.526</td>
</tr>
<tr>
<td>2</td>
<td>0.047</td>
<td>$4.9 \cdot 10^5$</td>
<td>0.595</td>
<td>0.522</td>
</tr>
<tr>
<td>3</td>
<td>0.023</td>
<td>$4.7 \cdot 10^6$</td>
<td>0.546</td>
<td>0.492</td>
</tr>
<tr>
<td>4</td>
<td>0.012</td>
<td>$37.6 \cdot 10^6$</td>
<td>0.555</td>
<td>0.496</td>
</tr>
</tbody>
</table>

Table 2. Flow past a sphere at $Re = 14000$.

<table>
<thead>
<tr>
<th>Case</th>
<th>$C_D$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Octree, 1st-order scheme</td>
<td>1.007</td>
</tr>
<tr>
<td>Octree, 2nd-order scheme</td>
<td>1.157</td>
</tr>
<tr>
<td>Cartesian</td>
<td>1.188</td>
</tr>
<tr>
<td>Experimental estimate [31]</td>
<td>1.237</td>
</tr>
</tbody>
</table>
Figure 5. flow past a cylinder at $Re = 140000$. Left: vorticity contour lines. Right: streamwise velocity section and grid for the second-order Octree scheme.

6. New Software and Platforms

6.1. COCOFLOW

**KEYWORDS:** 3D - Elasticity - MPI - Compressible multimaterial flows

**FUNCTIONAL DESCRIPTION:** The code is written in fortran 95 with a MPI parallelization. It solves equations of conservation modeling 3D compressible flows with elastic models as equation of state.

- Contact: Florian Bernard
- URL: [https://gforge.inria.fr/projects/cocoflow](https://gforge.inria.fr/projects/cocoflow)

6.2. KOPPA

*Kinetic Octree Parallel PolyAtomic*

**FUNCTIONAL DESCRIPTION:** KOPPA is a C++/MPI numerical code solving a large range of rarefied flows from external to internal flows in 1D, 2D or 3D. Different kind of geometries can be treated such as moving geometries coming from CAO files or analytical geometries. The models can be solved on Octree grids with dynamic refinement.

- Participant: Florian Bernard
- Contact: Florian Bernard
- URL: [https://git.math.cnrs.fr/gitweb/?p=plm/fbernard/KOPPA.git;a=summary](https://git.math.cnrs.fr/gitweb/?p=plm/fbernard/KOPPA.git;a=summary)

6.3. NaSCar

*Navier-Stokes Cartesian*

**KEYWORDS:** HPC - Numerical analyse - Fluid mechanics - Langage C - PETSc

**SCIENTIFIC DESCRIPTION:** NaSCar can be used to simulate both hydrodynamic bio-locomotion as fish like swimming and aerodynamic flows such wake generated by a wind turbine.

**FUNCTIONAL DESCRIPTION:** This code is devoted to solve 3D-flows in around moving and deformable bodies. The incompressible Navier-Stokes equations are solved on fixed grids, and the bodies are taken into account thanks to penalization and/or immersed boundary methods. The interface between the fluid and the bodies is tracked with a level set function or in a Lagrangian way. The numerical code is fully second order (time and space). The numerical method is based on projection schemes of Chorin-Temam’s type. The code is written in C language and use Petsc library for the resolution of large linear systems in parallel.
NaSCar can be used to simulate both hydrodynamic bio-locomotion as fish like swimming and aerodynamic flows such wake generated by a wind turbine.

- Participant: Michel Bergmann
- Contact: Michel Bergmann
- URL: https://gforge.inria.fr/projects/nascar/

6.4. NS-penal

*Navier-Stokes-penalization*

**KEYWORDS:** 3D - Incompressible flows - 2D

**FUNCTIONAL DESCRIPTION:** The software can be used as a black box with the help of a data file if the obstacle is already proposed. For new geometries the user has to define them. It can be used with several boundary conditions (Dirichlet, Neumann, periodic) and for a wide range of Reynolds numbers.

- Partner: Université de Bordeaux
- Contact: Charles-Henri Bruneau

7. New Results

7.1. Hybrid FOM/ROM simulations for turbulent flows

We present below results concerning the application of the hybrid FOM/ROM method to a realistic problem in CFD. The purpose of the study is to investigate the behavior of the flow past a car for several front bumper configurations. We here resort to Free-Form Deformation (FFD) based on two parameters to determine a satisfactory parametrization of all possible configurations, and we consider a steady RANS solver at $Re = 4.87 \cdot 10^6$ with Spalart-Allmaras turbulence model to simulate the flow. Simulations are performed in collaboration with OPTIMAD (http://www.optimad.it/) exploiting the methodology proposed in [15].

Figure 6 (left) shows the domain decomposition; in the blue region we solve the Full-Order model, while in the outer region we rely on a POD-Galerkin Reduced Order model. The partitioning is obtained adaptively using the algorithm described in [15]. Figure 6 (right) shows the flow prediction error relative to dynamic pressure for the worst-case parameter: the proposed method leads to $2\%$ accurate results with a speed-up compared to the full-order model of 8.

*Figure 6. hybrid FOM/ROM approach; application to RANS modelling of the flow around a car.*
7.2. All-speed multi-material schemes

We are interested in the development of numerical models for phenomena involving fluid flows and elastic material deformations. We pursue a monolithic approach, which describes the behavior of each material (gas, liquid or solid) through a system of conservation laws and appropriate constitutive relationships. Our method is designed to handle both high-Mach and low-Mach regimes.

It is well-known that Godunov-type schemes are inadequate for low-Mach problems: first, they introduce an excessive amount of numerical artificial viscosity; second, they require the enforcement of a CFL stability condition which leads to unpractical time steps. For this reason, we resort to the relaxation method proposed in [36], to derive a novel discretization scheme which can be applied to problems characterized by a broad range of Mach numbers. As opposed to [36], we propose in [1] to treat the advective term implicitly.

Figure 7 shows results for a quasi 1D de Laval nozzle problem in water: the flow is low-Mach and almost incompressible. In the present simulation, we impose at the inlet the total pressure \( P_{\text{tot}} = 10 \text{Pa} \) and the absolute temperature \( T = 280 \text{K} \) and at the outlet the pressure \( p_{\text{out}} = 1 \text{Pa} \). Figure 7(center) shows results for the explicit scheme proposed in [36], while Figure 7(right) shows results of our implicit scheme; for the explicit schemes, we impose the acoustic CFL \( \nu_{\text{ac}} = 0.4 \), while for the implicit scheme, we consider \( \nu_{\text{ac}} = 100 \). We observe that our method outperforms the method in [36].

![Figure 7. all-speed relaxation scheme. Left: de Laval nozzle. Center: pressure distribution predicted by the explicit method in [36] (\( \nu_{\text{ac}} = 0.4 \)). Right: pressure distribution predicted by the implicit method proposed in [1] (\( \nu_{\text{ac}} = 100 \)).](image)

7.3. Thermal convection on a hemisphere

Hamid Kellay (LOMA) performs a physical experiment using a half soap bubble heated at the equator. This device allows to study thermal convection and the movement of large scale structures on the surface of the bubble. The results show strong similarities with atmospheric flows on the earth. In particular large vortical structures on the half bubble and tropical cyclones in the atmosphere have the same dynamics.

Using a stereographic transform we solve Navier-Stokes equations on the half bubble and get very good agreement with the experiment. In addition we find that the Nusselt and Reynolds numbers verify scaling laws quite close to the scaling law given in the literature for Rayleigh-Bénard convection: \( \text{Nu} \propto \text{Ra}^{0.34} \) and \( \text{Re} \propto \text{Ra}^{1/2} \). Finally a Bolgiovino regime is found with scaling as \( \text{Ra}^{-1/4} \).

Adding the rotation like on the earth we show that the rotation changes the nature of turbulent fluctuations and a new scaling regime is obtained for the temperature field.

8. Partnerships and Cooperations
8.1. Regional Initiatives

Leading team of the regional project "Investigation and Modeling of Suspensions with the LOMA and LOF labs in Bordeaux.

8.2. National Initiatives

We are part of the GDR AMORE on ROMs.

9. Dissemination

9.1. Promoting Scientific Activities

9.1.1. Scientific Events Organisation

The team organized a conference in honour of Charles-Henri Bruneau. Several scientific presentations have been given by his many collaborators and friends. This conference was organized over two half-days: the afternoon of September 13 and the morning of September 14. The presentations are in a 30-minute format.  

https://indico.math.cnrs.fr/event/3768/

The team organized a half-day workshop on numerical modelling of swimming on December 12th 2018. Participants: Patrick Babin (MRGM), Michel Bergmann, Afaf Bouharguane, Marie Couliou (ONERA), Hamid Kellay (LOMA), Angelo Iollo, Olivier Marquet (ONERA).

9.1.2. Reviewer - Reviewing Activities

9.1.3. Invited Talks

Angelo Iollo was invited as plenary speaker to SIMAI 2018, [https://ocs.simai.eu/index.php/SIMAIcongress/SIMA12018](https://ocs.simai.eu/index.php/SIMAIcongress/SIMA12018).

Angelo Iollo was invited to Gran Sasso Science Institute for the Intensive Week on Fluids and Waves [https://fluidsandwaves.wordpress.com/blog/](https://fluidsandwaves.wordpress.com/blog/).

9.1.4. Scientific Expertise

Angelo Iollo is an expert for the European Union for the program FET OPEN.

9.2. Teaching - Supervision - Juries

9.2.1. Teaching

Four members of the team are Professors or Assistant Professors at Bordeaux University and have teaching duties, which consist in courses and practical exercises in numerical analysis and scientific computing. Michel Bergmann (CR) also teaches around 64 hours per year (practical exercises in programming for scientific computing).

9.2.2. Supervision

PhD: Federico Tesser. *Parallel solver for the Poisson equation on a hierarchy of superimposed meshes, under a Python framework*, University of Bordeaux and Insubria University. 11/09/2018.

Advisors: Michel Bergmann, Angelo Iollo.


Advisors: Michel Bergmann, Angelo Iollo.


Advisors: Michel Bergmann, Lisl Weynans.


Advisors: Angelo Iollo, Gabriella Puppo.


Advisors: Michel Bergmann, Angelo Iollo.


Advisor: Michel Bergmann, Angelo Iollo.

PhD in progress: Mathias Braun. *Reduced-order modelling for increased resilience of water distribution networks*. 01/10/2015.

Advisors: Angelo Iollo, Iraj Mortazavi, Olivier Piller.

PhD in progress: *Numerical simulation and modeling of zebra fish swimming for the study of human diseases of genetic and toxicological origin*. 01/10/2015.

Advisors: Afaf Bouharguane, Patrick Babin.

9.2.3. Juries

Angelo Iollo has been reviewer of the PhD thesis of Nicola Pozzi *Numerical Modeling and Experimental Testing of a Pendulum Wave Energy Converter (PeWEC)*, Politecnico di Torino, DIMEAS, May 2018.

Tommaso Taddei has participated to the PhD thesis of Nicolas Cagniart *A few nonlinear approaches in model order reduction*, Sorbonne University, LJLL, November 2018.
9.3. Popularization

Afaf Bouharguane has presented her research at the event Unithé ou Café at Inria Bordeaux, November 2018. Michel Bergmann, "Modéliser et optimiser les énergies renouvelables". Stand for the 10-th year anniversary of Inria Bordeaux South West centre, October 13th 2018.

10. Bibliography

Major publications by the team in recent years


Publications of the year

Doctoral Dissertations and Habilitation Theses


Articles in International Peer-Reviewed Journals


International Conferences with Proceedings


Conferences without Proceedings


Research Reports


References in notes


[34] S. GODUNOV. Elements of continuum mechanics, Nauka Moscow, 1978

[35] X. JIN. Construction d’une chaîne d’outils numériques pour la conception aérodynamique de pales d’éoliennes, Université de Bordeaux, 2014


