

RESEARCH CENTRE

Inria Paris Centre

IN PARTNERSHIP WITH:

Ecole des Ponts ParisTech

2023

ACTIVITY REPORT

Project-Team

SERENA

Simulation for the Environment: Reliable and Efficient Numerical Algorithms

IN COLLABORATION WITH: Centre d'Enseignement et de Recherche en
Mathématiques et Calcul Scientifique (CERMICS)

DOMAIN

Digital Health, Biology and Earth

THEME

**Earth, Environmental and Energy
Sciences**

Inria

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Project-Team SERENA

Creation of the Project-Team: 2017 April 01

Keywords

Computer sciences and digital sciences

- A2.1.3. – Object-oriented programming
- A2.1.4. – Functional programming
- A2.4.3. – Proofs
- A6.1.1. – Continuous Modeling (PDE, ODE)
- A6.1.4. – Multiscale modeling
- A6.1.5. – Multiphysics modeling
- A6.2.1. – Numerical analysis of PDE and ODE
- A6.2.5. – Numerical Linear Algebra
- A6.2.8. – Computational geometry and meshes
- A6.3.1. – Inverse problems
- A6.3.4. – Model reduction
- A6.3.5. – Uncertainty Quantification

Other research topics and application domains

- B3.1. – Sustainable development
- B3.3.1. – Earth and subsoil
- B3.4.2. – Industrial risks and waste
- B3.4.3. – Pollution
- B4.1. – Fossil energy production (oil, gas)
- B4.2.1. – Fission
- B5.5. – Materials

1 Team members, visitors, external collaborators

Research Scientists

- Martin Vohralík [Team leader, INRIA, Senior Researcher, HDR]
- François Clement [INRIA, Researcher]
- Zhaonan Dong [INRIA, Researcher]
- Gregor Gantner [INRIA, ISFP, until Oct 2023]
- Jean-Charles Gilbert [INRIA, Emeritus, from Oct 2023]
- Jean-Luc Guermond [Texas A&M University, Chair, Inria International Chair, HDR]
- Michel Kern [INRIA, Researcher]
- Geraldine Pichot [INRIA, Researcher]

Faculty Members

- Alexandre Ern [ENPC, Professor, HDR]
- Pierre Rousselin [UNIV PARIS XIII, Professor Delegation, from Sep 2023]

Post-Doctoral Fellows

- Akram Beni Hamad [INRIA, Post-Doctoral Fellow]
- Andre Harnist [INRIA, Post-Doctoral Fellow, until Aug 2023]

PhD Students

- Nicolas Hugot [CEA, from Nov 2023]
- Abbas Kabalan [Safran Tech]
- Clément Maradei [INRIA, from Oct 2023]
- Romain Mottier [ENPC, CEA]
- Houda Mouhcine [Inria Saclay]
- Stefano Piccardo [UPC Barcelona, until Dec 2023]
- Ari Rappaport [INRIA]
- Morgane Steins [CEA, until Dec 2023]
- Zuodong Wang [INRIA]
- Daniel Zegarra Vasquez [INRIA]

Technical Staff

- Sebastien Furic [INRIA, Engineer, until Oct 2023]
- Simon Legrand [Inria, Engineer]
- Raphaël Zanella [Inria, Engineer]

Interns and Apprentices

- Nicolas Hugot [ENSTA, Intern, from Apr 2023 until Oct 2023]
- Clement Maradei [INRIA, Intern, from Feb 2023 until Sep 2023]
- Alessandra Marelli [INRIA, Intern, from Apr 2023 until Sep 2023]

Administrative Assistant

- Derya Gok [INRIA]

Visiting Scientists

- Stefano Bonetti [ECOLE POLYT. MILAN, from May 2023 until Jul 2023]
- Roland Maier [UNIV JENA, from Feb 2023 until Feb 2023]
- Dirk Praetorius [TU WIEN, from Jun 2023 until Jun 2023]
- Fabio Vicini [ECOLE POLYT. TURIN, until Feb 2023]
- Pietro Zanotti [University of Pavia, from Apr 2023 until Feb 2023]
- Lina Zhao [City University of Hong Kong, from Jun 2023 until Jun 2023]

External Collaborators

- Guy Chavent [retired from Inria]
- François Delebecque [retired from Inria]
- Andre Harnist [UTC, from Sep 2023]
- Jérôme Jaffré [retired from Inria, HDR]
- Caroline Japhet [UNIV PARIS XIII]
- Habib Jreige [SciWorks]
- Vincent Martin [UTC]
- Koondanibha Mitra [UNIV EINDHOVEN]
- Jean Roberts [retired from Inria, HDR]
- Pierre Weiss [retired from Inria]

2 Overall objectives

The project-team SERENA is concerned with **numerical methods** for **environmental problems**. The main topics are the conception and analysis of *models* based on *partial differential equations*, the study of their *precise and efficient numerical approximation*, and implementation issues with special concern for *reliability and correctness of programs*. We are in particular interested in *guaranteeing the quality* of the *overall simulation process*.

3 Research program

3.1 PDE level

Within our project, we start from the conception and analysis of *models* based on *partial differential equations* (PDEs). We namely address the question of *coupling* of different models, such as simultaneous fluid flow in a discrete network of two-dimensional *fractures* and in the surrounding three-dimensional porous medium, or interaction of a (compressible) flow with the surrounding elastic *deformable structure*. The key physical characteristics need to be captured, whereas existence, uniqueness, and continuous dependence on the data are minimal analytic requirements that we seek to satisfy. We are also interested in *localization*, *approximation*, and *model reduction*.

3.2 Advanced numerical discretization methods

We consequently design *numerical methods* for the devised model, while focusing on enabling general *polytopal meshes*, in particular in response to a high demand from our industrial partners (namely EDF, CEA, and IFP Energies Nouvelles). We in particular promote *structure-preserving* approaches that mimic at the discrete level the fundamental properties of the underlying PDEs, such as conservation principles and preservation of invariants. We perform numerical analysis in particular in singularly perturbed, unsteady, and nonlinear cases (reaction–diffusion and wave problems, eigenvalue problems, interface problems, variational inequalities, contact problems, degenerate parabolic equations), we apply these methods to challenging problems from fluid and solid mechanics involving large deformations, plasticity, and phase appearance and disappearance, and we develop a comprehensive software implementing them.

3.3 Iterative linearization, domain decomposition, and multigrid solvers

We next concentrate an intensive effort on the development and analysis of efficient solvers for the systems of nonlinear algebraic equations that result from the above discretizations. We work on *iterative linearization* schemes and analysis. We place a particular emphasis on parallelization achieved via the *domain decomposition* method, including the *space-time parallelization* for time-dependent problems. This allows the use of different time steps in different parts of the computational domain, particularly useful in our applications where evolution speed varies significantly from one part of the computational domain to another. We have also recently devised novel *geometric multigrid solvers* with the contraction factor independent of the approximation polynomial degree. The solver itself is *adaptively steered* at each execution step by an a posteriori error estimate giving a two-sided control of the algebraic error.

3.4 Reliability by a posteriori error control

The fourth part of our theoretical efforts goes towards assessing the precision of the results obtained at the end of the numerical simulation. Here a key ingredient is the development of rigorous *a posteriori estimates* that make it possible to estimate in a fully computable way the error between the unknown exact solution and its numerical approximation. Our estimates also allow to distinguish the different *components* of the overall *error*, namely the errors coming from modeling, the discretization scheme, the nonlinear (Picard, Newton) solver, and the linear algebraic (domain decomposition, multigrid) solver. A new concept here is that of *local stopping criteria*, where all the error components are balanced locally within each computational mesh element. This naturally connects all parts of the numerical simulation process and gives rise to novel *fully adaptive algorithms*. We derive a guaranteed error reduction factor at each adaptive loop iteration in model cases together with cost-optimality in the sense that, up to a generic constant, the *smallest possible computational effort* to achieve the given accuracy is needed. With patchwise techniques, we also achieve *mass balance* at each iteration step, a highly demanded feature in most of the target applications.

3.5 Safe and correct programming

Finally, we concentrate on the issue of computer implementation of scientific computing programs, noting that precise numerical simulation and guaranteed error estimation are impossible without correct computer implementation. With their increasing complexity, it becomes a major challenge to implement up-to-date scientific computing algorithms using traditional methods and languages. Fortunately, the computer science community has already encountered similar issues, and offers theoretically sound tools for *safe* and *correct programming*. We use these tools to design generic solutions for the implementation of the class of scientific computing software the project-team is dealing with. Our focus ranges from high-level programming with **OCaml** for the precious safety guards provided by its type system and for its ability to encourage *functional programming*, to proofs of correctness of numerical algorithms and programs, including bounds of the round-off errors, via *mechanical proofs* with **Coq**.

The ultimate objective of the **SERENA** project-team is to design numerical algorithms that enable to certify the **reliability** of the **overall simulation process** and its **efficiency** with respect to **computational resources** for the targeted environmental applications.

4 Application domains

4.1 Multiphase flows and transport of contaminants in the subsurface

- fractured and porous media
- flow in large-scale discrete fracture networks
- subsurface depollution after chemical leakage
- nuclear waste disposal in deep underground repositories
- geological sequestration of CO₂
- production of oil and gas

4.2 Industrial risks in energy production

- structural mechanics (friction, contact, large deformation, plasticity) mainly related to nuclear reactor operation and safety analysis
- Stokes and Navier–Stokes flows related to nuclear reactor operation
- seismic wave propagation for detection and protection
- acoustic wave propagation for non destructive evaluation
- electromagnetism for interfaces between dielectrics and negative metamaterials

5 Social and environmental responsibility

5.1 Impact of research results

Via applications with our industrial and environmental partners **EDF**, **CEA**, **IFP Energies Nouvelles**, **ANDRA**, **ITASCA**, and **BRGM**.

6 Highlights of the year

Mickael Abbas, Jérôme Bonelle, Nicolas Pignet (EDF R&D) and Alexandre Ern organized the 2023 Edition of the **CEA-EdF-Inria summer school** on Robust Polyhedral Discretizations for Computational Mechanics (June 26-30, 2023).

7 New software, platforms, open data

7.1 New software

7.1.1 DiSk++

Name: Discontinuous Skeletal C++ Library

Keywords: High order methods, Polyhedral meshes, C++

Scientific Description: Discontinuous Skeletal methods approximate the solution of boundary-value problems by attaching discrete unknowns to mesh faces (hence the term skeletal) while allowing these discrete unknowns to be chosen independently on each mesh face (hence the term discontinuous). Cell-based unknowns, which can be eliminated locally by a Schur complement technique (also known as static condensation), are also used in the formulation. Salient examples of high-order Discontinuous Skeletal methods are Hybridizable Discontinuous Galerkin methods and the recently-devised Hybrid High-Order methods. Some major benefits of Discontinuous Skeletal methods are that their construction is dimension-independent and that they offer the possibility to use general meshes with polytopal cells and non-matching interfaces. The mathematical flexibility of Discontinuous Skeletal methods can be efficiently replicated in a numerical software: by using generic programming, the DiSk++ library offers an environment to allow a programmer to code mathematical problems in a way completely decoupled from the mesh dimension and the cell shape.

Functional Description: The software provides a numerical core to discretize partial differential equations arising from the engineering sciences (mechanical, thermal, diffusion). The discretization is based on the "Hybrid high-order" or "Discontinuous Skeletal" methods, which use as principal unknowns polynomials of arbitrary degree on each face of the mesh. An important feature of these methods is that they make it possible to treat general meshes composed of polyhedral cells. The DiSk++ library, using generic programming techniques, makes it possible to write a code for a mathematical problem independently of the mesh. When a user writes the code for his problem using the basic operations offered by DiSk++, that code can be executed without modifications on all types of mesh already supported by the library and those that will be added in the future.

URL: <https://github.com/wareHHouse/diskpp>

Publication: hal-01429292

Author: Matteo Cicuttin

Contact: Matteo Cicuttin

Partner: CERMICS

7.1.2 APS-MG

Name: A-Posteriori-Steered MultiGrid

Keywords: Finite element modelling, Linear system, A posteriori error estimates, Multigrid methods, P-robustness

Scientific Description: APS-MG (a-posteriori-steered multigrid) is a geometric-type multigrid solver whose execution is steered by the associated a posteriori estimate of the algebraic error. In particular, the descent direction and the level-wise step sizes are adaptively optimized. APS-MG corresponds to a V-cycle geometric multigrid with zero pre- and solely one post-smoothing step, via block-Jacobi (overlapping additive Schwarz/local patchwise problems). Its particularity is that it is robust with respect to the polynomial degree p of the underlying finite element discretization, i.e., APS-MG contracts the error on each iteration by a factor that is independent of p . APS-MG is the implementation of the solver developed in <https://hal.science/hal-02070981> and <https://hal.science/hal-02494538>.

Functional Description: APS-MG (a-posteriori-steered multigrid) is an iterative linear solver implemented in MATLAB. It can treat systems of linear algebraic equations arising from order p conforming finite element discretization of second-order elliptic diffusion problems. APS-MG is a geometric-type multigrid method and uses a hierarchy of nested meshes. It corresponds to a V-cycle geometric multigrid solver with zero pre- and one post-smoothing step via block-Jacobi (overlapping additive Schwarz/local patchwise problems). A salient feature is the choice of the optimal step size for the descent direction on each mesh level.

URL: <https://github.com/JanPapez/APS-MG>

Publications: [hal-02070981](#), [hal-02494538](#), [hal-02498247](#)

Contact: Jan Papez

7.1.3 FEMLAB

Name: FEMLAB

Keywords: High order finite elements, Discontinuous Galerkin, Hybrid high-order methods, Adaptive algorithms, Finite element modelling

Functional Description: FEMLAB is a Matlab library for different classes of FEM code. This library is designed to use a parallel computing toolbox in Matlab to accelerate the time for assembling the linear systems. It has been tested on 48 parallel processors of the HPC nodes. Another critical point is that different FEM codes in this library are designed to support arbitrary order of the basis functions and support the adaptive mesh refinement algorithm.

Release Contributions: FEMLAB is updated in 2023 to support the adaptive algorithm.

URL: <https://gitlab.inria.fr/zdong/FEMLAB>

Publications: [hal-03109470](#), [hal-03109548](#), [hal-03322267](#), [hal-03513280](#), [hal-03185683](#), [hal-03315088](#), [hal-03695484](#), [hal-03753221](#), [hal-03889072](#)

Contact: Zhaonan Dong

7.1.4 Skwer

Keywords: Differential equations, State-oriented simulation

Scientific Description: Unlike classical approaches which discretize time a priori to determine the state, the State-Oriented Simulation (SOS) method discretizes the state to determine durations, thus following ideas from the Quantized State Systems (QSS) methods. The aim is to give rigorous interpretation of idealized or hybrid physical models, and of cosimulation. The aspect that most distinguishes us from other approaches is that we do not make use of differential-algebraic equations (DAEs). We rather solve more general multiscale numerical stiffness problems based on nonstandard ODE formulations.

Functional Description: Skwer aims at solving differential equations inherent to 0D physical modeling. This includes in particular standard ODEs but also differential equations with conditionals and "idealized behavior" resulting from passing to the limit over some parameters.

News of the Year: We have developed the necessary machinery to desynchronize elementary integrators making the approach fully asynchronous event in dense cases (contrary to the QSS approach, which requires synchronization of internal states in case of direct variable-equation dependency between integrators). We have finalized system rewriting aspects (various enhancement of data structures as well as algorithms). We have developed a variable order scheme where each state variable may have its own order (independent of others) thanks to the use of a formula-based technique to produce guaranteed a priori error bounds for the individual approximations. We have finally dropped the Maclaurin series code in favor of a more specialized (and lighter) approach

based on direct generation of exponential terms. We have tested the final algorithm over various systems of differential equations to validate the approach.

URL: <https://gitlab.inria.fr/skwer/skwer>

Publication: [hal-01636392](https://hal.archives-ouvertes.fr/hal-01636392)

Contact: Sebastien Furic

Participants: Sebastien Furic, François Clement, Geraldine Pichot

7.1.5 coq-num-analysis

Name: Numerical analysis Coq library

Keywords: Coq, Numerical analysis, Real analysis

Scientific Description: These Coq developments are based on the Coquelicot library for real analysis. Version 1.0 includes the formalization and proof of: (1) the Lax-Milgram theorem, including results from linear algebra, geometry, functional analysis and Hilbert spaces, (2) the Lebesgue integral, including large parts of the measure theory, the building of the Lebesgue measure on real numbers, integration of nonnegative measurable functions with the Beppo Levi (monotone convergence) theorem, Fatou's lemma, the Tonelli theorem, and the Bochner integral with the dominated convergence theorem.

Functional Description: Formal developments and proofs in Coq of numerical analysis problems. The current long-term goal is to formally prove parts of a C++ library implementing the Finite Element Method.

News of the Year: The formalization in Coq of simplicial Lagrange finite elements is almost complete. This includes the formalizations of the definitions and main properties of monomials, their representation using multi-indices, Lagrange polynomials, the vector space of polynomials of given maximum degree (about 6 kloc). This also includes algebraic complements on the formalization of the definitions and main properties of operators on finite families of any type, the specific cases of abelian monoids (sum), vector spaces (linear combination), and affine spaces (affine combination, barycenter, affine mapping), sub-algebraic structures, and basics of finite dimension linear algebra (about 22 kloc). A new version (2.0) of the opam package will be available soon, and a paper will follow.

We have also contributed to the Coquelicot library by adding the algebraic structure of abelian monoid, which is now the base of the hierarchy of canonical structures of the library.

URL: <https://lipn.univ-paris13.fr/coq-num-analysis/>

Publications: [hal-01344090](https://hal.archives-ouvertes.fr/hal-01344090), [hal-01391578](https://hal.archives-ouvertes.fr/hal-01391578), [hal-03105815](https://hal.archives-ouvertes.fr/hal-03105815), [hal-03471095](https://hal.archives-ouvertes.fr/hal-03471095), [hal-03516749](https://hal.archives-ouvertes.fr/hal-03516749), [hal-03889276](https://hal.archives-ouvertes.fr/hal-03889276)

Contact: Sylvie Boldo

Participants: Sylvie Boldo, François Clement, Micaela Mayero, Vincent Martin, Stéphane Aubry, Florian Faissole, Houda Mouhcine, Louise Leclerc

Partners: LIPN (Laboratoire d'Informatique de l'Université Paris Nord), LMAC (Laboratoire de Mathématiques Appliquées de Compiègne)

7.1.6 MODFRAC

Name: MODFRAC

Keywords: Meshing, Fracture network, Ellipses, Polygons, Meshes, Mesh

Scientific Description: The meshing methodology is based on a combined frontal-Delaunay approach in a Riemannian context.

Functional Description: The MODFRAC software automatically builds meshes of fracture networks. As an input, it takes a DFN (Discrete Fracture Network) geometric model consisting of ellipses or polygons that have been randomly generated in the tridimensional space while following experimental statistics. It completes this model by first calculating the intersections between fractures, that are straight segments. On each fracture, it computes in turn the intersections between these straight segments, subdividing them into subsegments. It then creates a conforming set of these subsegments, and selects the necessary fractures using a graph structure. It transmits this information to an “indirect” surface mesher, where the tridimensional mesh results from the construction of planar meshes of the parametric domains.

News of the Year: APP deposit, january 2023. Addition of OpenMP parallelism.

Publications: [hal-03480570](#), [hal-02102811](#)

Contact: Geraldine Pichot

Participants: Patrick Laug, Houman Borouchaki, Geraldine Pichot

Partner: Université de Technologie de Troyes

7.1.7 nef-flow-fpm

Keywords: 2D, 3D, Porous media, Fracture network, Geophysical flows

Scientific Description: The code is based on the implementation of the mixed hybrid finite element method as detailed in: An efficient numerical model for incompressible two-phase flow in fractured media Hussein Hoteit, Abbas Firoozabadi, *Advances in Water Resources* 31, 891–905, 2008. <https://doi.org/10.1016/j.advwatres.2008.02.004>

The model of fractures and the coupling between the porous flow and the flow in the network of fractures is described in: : Modeling Fractures and Barriers as Interfaces for Flow in Porous Media V. Martin, J. Jaffré, J. E. Roberts, *SIAM Journal on Scientific Computing*, 2005. <https://doi.org/10.1137/S1064827503429363>

Validation benchmark test from the publication: Inga Berre, et al., Verification benchmarks for single-phase flow in three-dimensional fractured porous media, *Advances in Water Resources*, Volume 147, 2021. <https://doi.org/10.1016/j.advwatres.2020.103759>.

Functional Description: nef-flow-fpm is a Matlab code to simulate flows in fractured porous media with the mixed-hybrid finite element methods (RT0).

Release Contributions: Implementation of the mixed hybrid method for 3D porous flows, Discrete fracture Networks (DFN) flows and the coupling between DFN and porous flows.

News of the Year: Call metis to perform the mesh partitionning. Generate data per subdomain for HPDDM solver (Neumann matrices, local sizes and indices, local second member). Simulations with PETSC/HPDDM, the largest networks contains 378k fractures.

URL: <https://gitlab.inria.fr/nef/nef-flow-fpm>

Contact: Geraldine Pichot

Participants: Geraldine Pichot, Daniel Zegarra Vasquez, Michel Kern, Raphael Zanella

7.1.8 nef-transport-fpm

Keywords: 3D, Porous media, Incompressible flows, Transport model

Scientific Description: The discretization in space is performed with a cell-centered finite volume scheme. The discretization in time can be either explicit or implicit.

Functional Description: nef-transport-fpm is a Matlab code for simulating transport by advection diffusion in porous-fractured media.

News of the Year: Add transport in a network of fractures with the proper handling of the coupling conditions at the fractures intersections.

Contact: Geraldine Pichot

Participants: Geraldine Pichot, Michel Kern, Daniel Zegarra Vasquez, Alessandra Marelli, Dania Khiralla

7.1.9 ParaCirce

Name: Parallel Circulant Embedding

Keywords: 2D, 3D, Hydrogeology, Gaussian random fields, MPI

Scientific Description: ParaCirce implements the algorithm proposed by [C. R. Dietrich and G. N. Newsam. A fast and exact method for multidimensional gaussian stochastic simulations. Water Resources Research, 29(8):2861-2869, 1993] as well as an algorithm to accelerate the padding estimation [Pichot et al. SMAI Journal of Computational Mathematics, 8, pp.21, 2022].

Functional Description: ParaCirce implements a parallel Circulant Embedding method for the generation in parallel of 2D or 3D Gaussian Random Fields (second order stationary).

Release Contributions: A new GRF type has been introduced to wrap the std::vector initially returned from generate(). It contains all the characteristics of the GRE. Add API for the FFTW to select the planning strategy.

News of the Year: A new GRF type has been introduced to wrap the std::vector initially returned from generate(). It contains all the characteristics of the GRE. Add API for the FFTW to select the planning strategy.

URL: <https://gitlab.inria.fr/slegrand/paracirce>

Publication: hal-03190252

Contact: Geraldine Pichot

Participants: Geraldine Pichot, Simon Legrand

7.1.10 Pruners

Name: Pruners

Keywords: Combinatorics, Parameter studies, Automation

Functional Description: Pruners is a language aimed at automating parameter studies. It allows the specification of parameter combinations, and make them available via environment variables. Those can then be used by any specified command as input parameters.

Release Contributions: - Parameter space specification - Launching commands with each combination as parameter - File system interaction with read/write functions and Json format

News of the Year: Open source licence GPL and opening of the repository. Add skip and keep options to select particular combinations of parameters. Add configure option to replace pruners script variables into a templated file. Add asynchronous execution of combinations.

URL: <https://team.inria.fr/serena/en/research/software/pruners/>

Authors: Thierry Martinez, Simon Legrand, Geraldine Pichot

Contact: Thierry Martinez

7.2 Open data

The model proposed as part of the "Multiphase reactive transport" (see Section 8.3) has been archived on Zenodo [Reactive Multiphase Flow in Porous Media at the Darcy Scale: a Benchmark proposal](#). The results obtained by the participants have been made available on Github: [Reactive-Multiphase-Benchmark](#) to make it possible for future researchers to compare their results.

8 New results

8.1 Research axis 1: Advanced numerical discretizations and solvers

Participants: Zhaonan Dong, Alexandre Ern, Jean-Luc Guermond, Michel Kern, Stefano Piccardo, Morgane Steins, Martin Vohralik, Zuodong Wang.

Invariant-domain time-stepping for compressible flows

Participants: Alexandre Ern, Jean-Luc Guermond, Zuodong Wang.

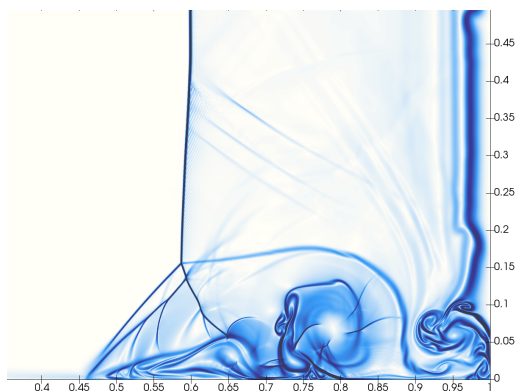


Figure 1: Compressible Navier–Stokes simulation at $Re = 1000$ (from [26])

In 2022, the authors laid the foundations of a new paradigm for invariant-domain time-stepping applied to hyperbolic problems using high-order Runge–Kutta methods. The key result achieved this year is the extension to implicit-explicit (IMEX) time-stepping and the application to the compressible Navier–Stokes equations, as described in [26]. The decisive step-forward is the satisfaction of physical bounds on the density and energy while allowing for a high-order discretization in space and in time. An example of application to the compressible Navier–Stokes equations at Reynolds $Re = 1000$ is displayed in Figure 1. This is a very challenging problem owing to the interactions between shocks and walls and the development of multiscale vortical structures. Moreover, in [49], we considered a scalar conservation law with a stiff source term having multiple equilibrium points. For this quite challenging situation, we proposed a scheme that can be asymptotic-preserving.

Polytopal discretization methods

Participants: Zhaonan Dong, Alexandre Ern, Jean-Luc Guermond, Stefano Piccardo, Morgane Steins, Zuodong Wang.

Further progress has been accomplished in the development and analysis of hybrid high-order (HHO) methods. Three topics were investigated. First, C^0 -HHO methods for the biharmonic problem in [22] leading to a competitive method in terms of error vs. computational effort with respect to established methods such as the C^0 -interior penalty discontinuous Galerkin method. Second, within the framework of the PhD Thesis of Morgane Steins ([38], defended this year), HHO methods for the wave equation using a leapfrog scheme for time discretization were studied. The contributions include a convergence analysis [50] and a time-explicit marching scheme [35]. Finally, HHO methods were used to study surface tension effects between two immiscible Stokes fluids within the PhD Thesis of Stefano Piccardo ([37], defended this year) [34].

8.2 Research axis 2: A posteriori error control, adaptivity, and safe and correct programming

Participants: François Clément, Alexandre Ern, Sébastien Furic, Gregor Gantner, André Harnist, Houda Mouhcine, Ari Rappaport, Martin Vohralík.

Error control with quality uniform in polynomial degree for the curl–curl (simplified Maxwell) problem

Participants: Martin Vohralík.

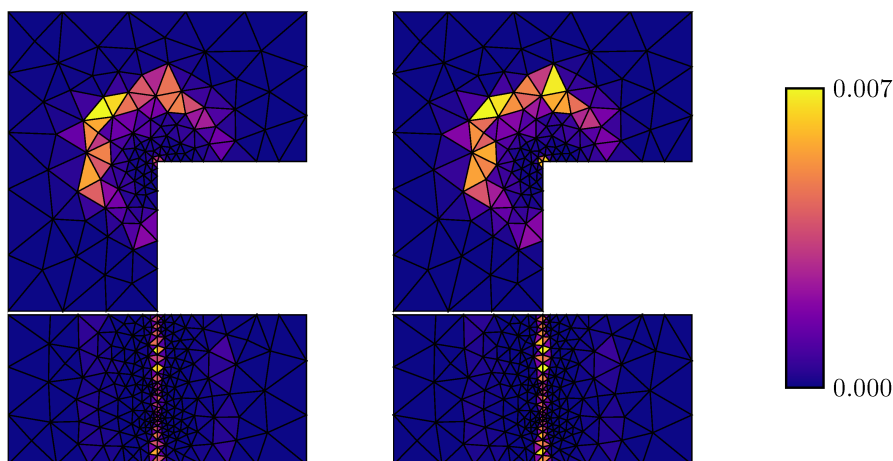


Figure 2: A posteriori estimated error (left) and actual error (right) (from [20]). Nédélec finite element approximation of the curl–curl (simplified Maxwell) problem, L-shaped 3D domain, top view (top) and side view (bottom).

In [20], we present a local construction of $\mathbf{H}(\text{curl})$ -conforming piecewise polynomials satisfying a prescribed curl constraint. We start from a piecewise polynomial not contained in the $\mathbf{H}(\text{curl})$ space but satisfying a suitable orthogonality property. The procedure employs minimizations in vertex patches and the outcome is, up to a generic constant independent of the underlying polynomial degree, as accurate as the best-approximations over the entire local versions of $\mathbf{H}(\text{curl})$. This allows to design guaranteed, fully computable, constant-free, and polynomial-degree-robust a posteriori error estimates of the Prager–Synge type for Nédélec’s finite element approximations of the curl–curl problem. A divergence-free decomposition of a divergence-free $\mathbf{H}(\text{div})$ -conforming piecewise polynomial, relying on over-constrained minimizations in Raviart–Thomas’ spaces, is the key ingredient. Numerical results confirm the theoretical developments, see Figure 2 for an illustration.

Error control with quality uniform in spline degree for isogeometric analysis

Participants: Gregor Gantner, Martin Vohralík.

In [29], we consider spline/isogeometric analysis discretizations of the Poisson model problem, focusing on high polynomial degrees and strong hierarchical refinements. We derive a posteriori error estimates by equilibrated fluxes, i.e., vector-valued mapped piecewise polynomials lying in the $\mathbf{H}(\text{div})$ space which appropriately approximate the desired divergence constraint. Our estimates are constant-free in the leading term, locally efficient, and robust with respect to the polynomial degree. They are also robust with respect to the number of hanging nodes arising in adaptive mesh refinement employing hierarchical B-splines. Two partitions of unity are designed, one with larger supports corresponding to the mapped splines, and one with small supports corresponding to mapped piecewise multilinear finite element hat basis functions. The equilibration is only performed on the small supports, avoiding the higher computational price of equilibration on the large supports or even the solution of a global system. Thus, the derived estimates are also as inexpensive as possible. An abstract framework for such a setting is developed, whose application to a specific situation only requests a verification of a few clearly identified assumptions. Numerical experiments illustrate the theoretical developments and even indicate, though not rigorously proved, robustness with respect to the smoothness of the splines.

Adaptive regularization, discretization, and linearization for nonsmooth problems

Participants: André Harnist, Ari Rappaport, Martin Vohralík.

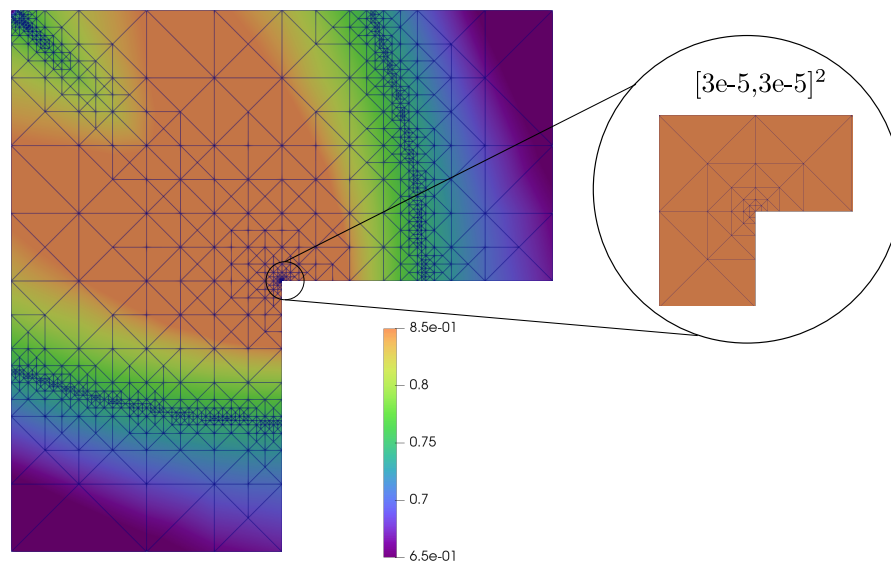


Figure 3: Adaptive mesh refinement together with adaptive regularization for a nonsmooth nonlinearity (from [28]).

In [28], we consider nonsmooth partial differential equations associated with a minimization of an energy functional. We adaptively regularize the nonsmooth nonlinearity so as to be able to apply the usual Newton linearization, which is not always possible otherwise. We apply the finite element method as a discretization. We focus on the choice of the regularization parameter and adjust it on the basis of an a posteriori error estimate for the difference of energies of the exact and approximate solutions. We prove guaranteed upper bounds for the energy difference, identify the individual error components, and design an adaptive algorithm with both adaptive regularization and adaptive mesh refinement. Efficiency and robustness of the estimates with respect to the magnitude of the nonlinearity is addressed in [52]. Numerical results confirm the theoretical developments, see Figure 3 for an illustration.

Functional software

Participants: Sébastien Furic.

See the "News of the Year" about software Skwer (Section 7.1.4).

Coq formalizations

Participants: François Clément, Houda Mouhcine.

In [36], we describe the formal definition and proof in Coq of product σ -algebras, product measures and their uniqueness, the construction of iterated integrals, up to Tonelli's theorem. We also advertise the *Lebesgue induction principle* provided by an original inductive type for nonnegative measurable functions.

See also the "News of the Year" about software coq-num-analysis (Section 7.1.5).

8.3 Research axis 3: Applications to environment and energy

Participants: Alexandre Ern, Michel Kern, Simon Legrand, Clément Maradei, Alessandra Marelli, Romain Mottier, Géraldine Pichot, Martin Vohralík, Raphaël Zanella, Daniel Zegarra Vasquez.

Flow through fractured and fractured porous media

Participants: Michel Kern, Simon Legrand, Alessandra Marelli, Géraldine Pichot, Martin Vohralík, Raphaël Zanella, Daniel Zegarra Vasquez.

We have experimented with the domain decomposition preconditioner **HPDDM**, developed by the **ALPINES** team [55, 56] to solve the linear system obtained from `nef-flow-fpm`. The improvement over the more classical preconditioners used until then (mainly algebraic multigrid) are significant as can be seen on Figure 4.

Thanks to the gmres solver and the **HPDDM** preconditioner, we are now able to solve flow problem in large scale fractured porous media that are out of reach with direct solvers like MUMPS Cholesky or with gmres preconditioned by multigrid like BoomerAMG. As example, solving the linear system of size 1.41×10^8 for a network containing 378k fractures takes in parallel, with gmres preconditioned with **HPDDM**, only 2 minutes and 40 iterations with 4096 MPI processes.

Another goal is to simulate the transport by advection of an inert tracer. The transport is described by the conservation of mass and gives rise to an equation with partial derivatives of the first order in which

Test case	Frac- tures	Tetra DoF NNZ	# sub-dom DoF/sbdom	Cholesky MUMPS	gmres Boomer AMG	gmres HPDDM Neumann
L20 geo	1 810	$3.27 \cdot 10^5$ $7.72 \cdot 10^5$ $5.55 \cdot 10^6$	24 $3.22 \cdot 10^4$	9s	2m 46s	9s
				-	4034 it.	34 it.
				0.21 GB	0.50 GB	1.66 GB
L130 geo	377 725	$5.99 \cdot 10^7$ $1.41 \cdot 10^8$ $2.09 \cdot 10^8$	4096 $3.45 \cdot 10^4$	Out of memory	11m 37s	2m 7s
				Out of memory	gmres did not converge (max it reached)	40 it.
				Out of memory	94 GB	336 GB

Figure 4: Performances of the domain decomposition preconditioner HPDDM to solve flow in fractured porous media

the velocity, computed with the software nef-flow-fpm, is heterogeneous. The discretization in space is performed with a cell-centered finite volume scheme. The discretization in time can be either explicit or implicit.

As part of Alessandra Marelli's internship, we were able to simulate the transport in a network of fractures. The main challenge was the correct handling of the coupling conditions at the fracture intersections. An example is shown in Figure 5. The method is implemented in nef-transport-fpm.

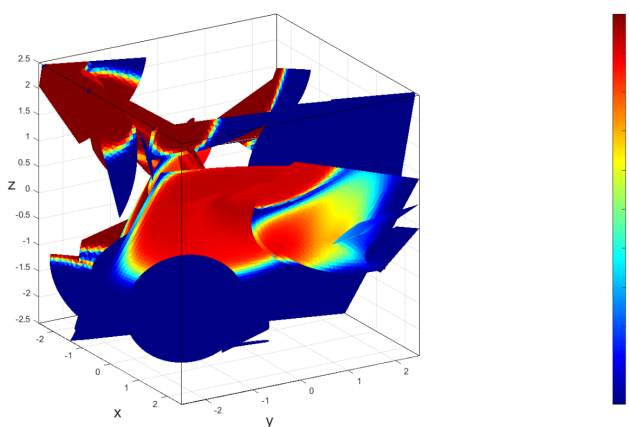


Figure 5: Snapshot of the concentration in a discrete fracture network with 28 fractures.

Multiphase reactive flow

Participants: Michel Kern.

Michel Kern was part of a group with Etienne Ahusborde, Brahim Amaziane (University of Pau), Stephen de Hoop and Denis Voskov (Delft University of Technology) that proposed a benchmark targeted towards the simulation of *reactive two-phase flow*. Six teams participated in the benchmark. The results

showed good agreements between most groups on the simpler test cases, but also that the interaction between complex chemistry and two-phase flow with phase exchanges still remains a challenge for simulation software. The model is presented in [30], while the results are presented in [14], see Figure 6.

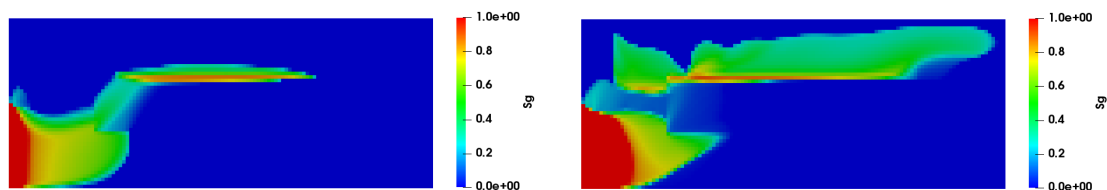


Figure 6: Evolution of the gas saturation (at 200 and 600 days). Gas is injected from the bottom left. The middle section has a lower permeability, which forces the gas to rise above it.

Wave propagation in geophysical media

Participants: Alexandre Ern, Michel Kern, Clément Maradei, Romain Mottier.

As part of the internship of Clément Maradei, we studied a model for the wave equations that includes both a diffusive (first order derivative in time) and a so-called "viscous" term (first order time derivative of the Laplacian). The model has been proposed to represent frequency-dependent attenuation. Thanks to finite element simulations (using FreeFem++), we were able to compare the respective contributions of the two terms, and use a scaling analysis to better understand the influence of the two parameters. The results have been presented at the [15th FreeFem Days](#).

Within the PhD Thesis of Romain Mottier, we developed HHO methods to simulate coupled acoustic-elastodynamic waves in geophysical media. One goal is to highlight the role of sedimentary basins in energy transfer from the bedrock to the atmosphere.

Data assimilation

Participants: Alexandre Ern.

Our work on data assimilation was pursued this year by addressing the heat equation. Our first contribution is on the theoretical side and concerns a Carleman estimate [18]. The second contribution deals with the devising and numerical analysis of a high-order method (based on a dG method in time and a hybrid dG method in space) [17].

8.4 Research axis 4: PDE and numerical analysis foundations

Participants: Zhaonan Dong, Alexandre Ern, Jean-Luc Guermond, Géraldine Pichot, Martin Vohralík.

A stable local commuting projector and optimal hp approximation estimates in $H(\text{curl})$

Participants: Théophile Chaumont-Frelet, Martin Vohralík.

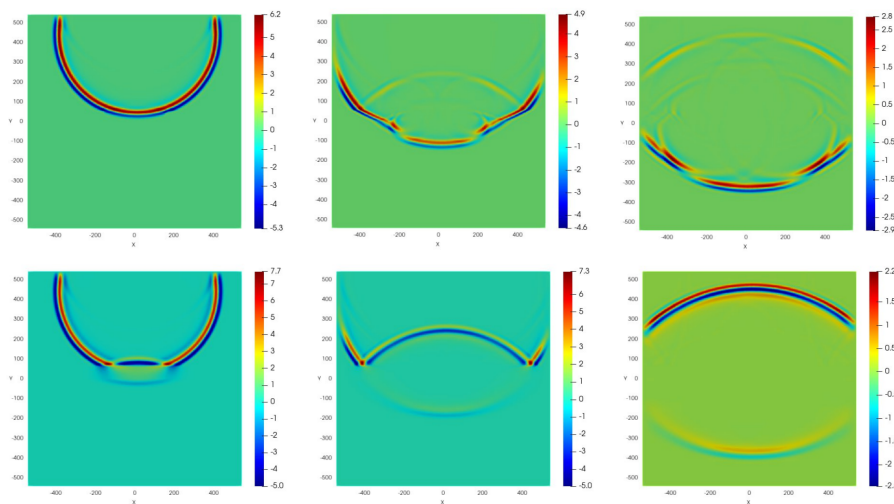


Figure 7: Comparison of the wavefield for the diffusive damping (top) and the viscous damping (bottom) at three different times, showing the expected phase reversal.

We design an operator from the infinite-dimensional Sobolev space $\mathbf{H}(\text{curl})$ to its finite-dimensional subspace formed by the Nédélec piecewise polynomials on a tetrahedral mesh that has the following properties: 1) it is defined over the entire $\mathbf{H}(\text{curl})$, including boundary conditions imposed on a part of the boundary; 2) it is defined locally in a neighborhood of each mesh element; 3) it is based on simple piecewise polynomial projections; 4) it is stable in the L^2 -norm, up to data oscillation; 5) it has optimal (local-best) approximation properties; 6) it satisfies the commuting property with its sibling operator on $\mathbf{H}(\text{div})$; 7) it is a projector, i.e., it leaves intact objects that are already in the Nédélec piecewise polynomial space. This operator can be used in various parts of numerical analysis related to the $\mathbf{H}(\text{curl})$ space. We in particular employ it here to establish the two following results: i) equivalence of global-best, tangential-trace- and curl-constrained, and local-best, unconstrained approximations in $\mathbf{H}(\text{curl})$ including data oscillation terms; and ii) fully h - and p - (mesh-size- and polynomial-degree-) optimal approximation bounds valid under the minimal Sobolev regularity only requested elementwise.

Some novel results concerning Maxwell's equations

Participants: Alexandre Ern, Jean-Luc Guermond.

In [43], we established the asymptotic optimality of the edge finite element approximation of the time-harmonic Maxwell's equations. This fundamental result, which is the counterpart of a known result concerning the Helmholtz equation and conforming finite elements, was still lacking in the literature. A second novel result, that was also lacking in the literature, concerns the spectral correctness (no spurious eigenvalues) of the dG approximation of Maxwell's equations in first-order form (the result was known for Maxwell's equations in second-order form), thereby confirming numerical observations by various authors made over the last two decades. We proved this result first with constant coefficients [27] and then in the more challenging case of discontinuous coefficients [48].

Solutions to 1D advection-diffusion problems with discontinuous coefficients

Participants: Géraldine Pichot.

Diffusive transport in media with discontinuous properties is a challenging problem that arises in many applications. In [39], we focus on one-dimensional discontinuous media with generalized permeable boundary conditions at the discontinuity interface. The paper presents novel analytical expressions from the method of images to simulate diffusive processes, such as mass or thermal transport. The analytical expressions are used to formulate a generalization of the existing Skew Brownian Motion, HYMLA and Uffink's method, here named as GSBM, GHYMLA and GUM respectively, to handle generic interface conditions. The algorithms rely upon the random walk method and are tested by simulating transport in a bimaterial and in a multilayered medium with piece-wise constant properties. The results indicate that the GUM algorithm provides the best performance in terms of accuracy and computational cost. The methods proposed can be applied for simulation of a wide range of differential problems, like heat transport problem [40].

Model-order reduction

Participants: Alexandre Ern, Abbas Kabalan.

One important topic has been the development of reduced-order methods to handle variational inequalities such as those encountered when studying contact problems (with friction) in computational mechanics. In [33], we introduce an efficient algorithm to guarantee inf-sup stability for saddle-point problems with parameter-dependent constraints. In [54], we pursued a different, and complementary, approach, where the constraints are taken into account by a nonlinear Nitsche's method, thereby allowing one to use a primal formulation. Finally, within the PhD Thesis of Abbas Kabalan, we are investigating shape variability within the context of reduced-order models.

Best-approximation errors for fields with low regularity

Participants: Zhaonan Dong, Alexandre Ern, Jean-Luc Guermond.

In [23], we established optimal decay rates on the best-approximation errors using vector-valued finite elements (of Nédélec or Raviart–Thomas type) for fields with low regularity but having an integrable curl or divergence.

hp -optimal error estimates of dG methods

Participants: Zhaonan Dong.

In [25], we derived hp -optimal error estimates for dG methods for the biharmonic problem with homogeneous essential boundary conditions, which removed the 1.5 suboptimal rate in term of p in the classical error analysis of dG methods. The main ingredient in the analysis is the construction of a global H^2 piecewise polynomial approximants with hp -optimal approximation properties over the meshes. Moreover recently, we derived hp -optimal error estimates for the upwind dG method when approximating solutions to first-order hyperbolic problems with constant convection fields in the L_2 and DG norms in [47]. The main novelty in the analysis are novel hp -optimal approximation properties of the special projector introduced in [Cockburn, Dong, Guzman, SINUM, 2008].

These works were performed in collaboration with L. Mascotto.

9 Bilateral contracts and grants with industry

9.1 Bilateral contracts with industry

Participants: Alexandre Ern, Martin Vohralík.

- Two-part contract with **CEA** accompanying the PhD thesis of Nicolas Hugot.
- Two-part contract with Safran Tech accompanying the PhD thesis of Abbas Kabalan (co-supervised with V. Ehrlacher).
- Two-part contract with **CEA** accompanying the PhD thesis of Romain Mottier.
- Two-part contract with **ANDRA** accompanying the PhD thesis of Ari Rappaport.
- Two-part contract with **CEA** accompanying the PhD thesis of Morgane Steins.

10 Partnerships and cooperations

10.1 International research visitors

10.1.1 Visits of international scientists

Inria International Chair Prof. Jean-Luc Guermond (Texas A&M University) visited the SERENA team for a comprehensive duration of 15 weeks in 2023 in the framework of his INRIA International Chair. He mainly interacted with Alexandre Ern on invariant-domain preserving high-order time-stepping and on the spectral correctness of discontinuous Galerkin methods for the Maxwell eigenvalue problem, and also with Zhaonan Dong and Zuodong Wang on transport equations with stiff source terms having multiple stable equilibrium points.

Other international visits to the team

Dirk Praetorius

Status researcher

Institution of origin: **TU Wien**

Country: Austria

Dates: june 2023

Context of the visit: Dirk Praetorius visited us in June 2023. He is a world-leading expert on adaptive mesh refinement, adaptive solvers, and proofs of convergence and optimality. He mainly interacted with Martin Vohralík. He has by now also applied for the Inria International Chair.

Mobility program/type of mobility: research stay

Fabio Vicini

Status researcher

Institution of origin: Politecnico di Torino

Country: Italy

Dates: december 2022 - january 2023

Context of the visit: Fabio works in the GEOSCORE group of Politecnico di Torino. GEOSCORE and SERENA have a common research topic that is the development of efficient and robust numerical methods to solve large-scale subsurface flows. To this end, during the past years, our respective teams have developed different meshing and numerical strategies. During Fabio's stay, he mainly interacted with Géraldine Pichot to compare these different approaches: matching vs non-matching meshes, Virtual Element Method vs Hybrid High Order method, direct vs iterative solvers, adaptive mesh refinement strategies based on a posteriori error estimates.

Mobility program/type of mobility: research stay

Lina Zhao

Status Assistant Professor

Institution of origin: City University of Hong Kong

Country: China

Dates: June 2023 - June 2023

Context of the visit: Dr. Lina Zhao (City University of Hong Kong) visited the SERENA team for 4 weeks in June 2023. She mainly interacted with Zhaonan Dong and Alexandre Ern on minimum regularity of Staggered DG methods for the flow problems, and a posteriori error analysis for the coupled problems.

Mobility program/type of mobility: research stay

10.1.2 Visits to international teams**Research stays abroad****Martin Vohralík**

Visited institution: University of Texas at Austin

Country: USA

Dates: 9 - 25 Jan 2023

Context of the visit: scientific collaboration with Prof. Leszek Demkowicz on commuting projects

Mobility program/type of mobility: research stay

10.2 European initiatives

10.2.1 H2020 projects

EMC2 [EMC2 project on cordis.europa.eu](https://cordis.europa.eu)

Title: Extreme-scale Mathematically-based Computational Chemistry

Duration: From September 1, 2019 to February 28, 2026

Partners:

- INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET AUTOMATIQUE (INRIA), France
- ECOLE NATIONALE DES PONTS ET CHAUSSEES (ENPC), France
- CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE CNRS (CNRS), France
- SORBONNE UNIVERSITE, France

Inria contact: Laura GRIGORI (Alpines)

Coordinator:

Summary: Molecular simulation has become an instrumental tool in chemistry, condensed matter physics, molecular biology, materials science, and nanosciences. It will allow to propose de novo design of e.g. new drugs or materials provided that the efficiency of underlying software is accelerated by several orders of magnitude.

The ambition of the EMC2 project is to achieve scientific breakthroughs in this field by gathering the expertise of a multidisciplinary community at the interfaces of four disciplines: mathematics, chemistry, physics, and computer science. It is motivated by the twofold observation that, i) building upon our collaborative work, we have recently been able to gain efficiency factors of up to 3 orders of magnitude for polarizable molecular dynamics in solution of multi-million atom systems, but this is not enough since ii) even larger or more complex systems of major practical interest (such as solvated biosystems or molecules with strongly-correlated electrons) are currently mostly intractable in reasonable clock time. The only way to further improve the efficiency of the solvers, while preserving accuracy, is to develop physically and chemically sound models, mathematically certified and numerically efficient algorithms, and implement them in a robust and scalable way on various architectures (from standard academic or industrial clusters to emerging heterogeneous and exascale architectures).

EMC2 has no equivalent in the world: there is nowhere such a critical number of interdisciplinary researchers already collaborating with the required track records to address this challenge. Under the leadership of the 4 PIs, supported by highly recognized teams from three major institutions in the Paris area, EMC2 will develop disruptive methodological approaches and publicly available simulation tools, and apply them to challenging molecular systems. The project will strongly strengthen the local teams and their synergy enabling decisive progress in the field.

10.3 National initiatives

Participants: Michel Kern.

The team is part of the recently created GDR [HydroGEMM](#) ("Hydrogène du sous-sol: étude intégrée de la Genèse... à la Modélisation Mathématique"). One of the thematic axes of the GDR is the mathematical analysis and the numerical simulation hydrogen storage in geological reservoirs.

11 Dissemination

Participants: François Clément, Zhaonan Dong, Alexandre Ern, Gregor Gantner, Jean-Luc Guermond, Michel Kern, Martin Vohralík.

11.1 Promoting scientific activities

11.1.1 Scientific events: organisation

Member of the organizing committees Alexandre Ern is a member of the Scientific Committee of the European Finite Element Fair.

Mickaël Abbas, Jérôme Bonelle, Nicolas Pignet (EDF R&D) and Alexandre Ern organized the 2023 Edition of the [CEA-EdF-Inria summer school](#) on Robust Polyhedral Discretizations for Computational Mechanics (June 26-30, 2023).

Alexandre Ern co-organized with Samir Adly (SMAI), R. Herbin (Aix-Marseille University), Nina Aguillon, Xavier Claeys, Bruno Després, Yvon Maday, Ayman Moussa (Sorbonne University) the Month of Applied and Industrial Mathematics (M2AI) held at IHP on November 2023. Four large-audience lectures were given with the goal to show to undergraduate (and college) students how applied mathematics can (and do) shape our world.

Michel Kern was a member of the organizing committee of the [annual meeting](#) of GDR HydroGEMM, held at University of Pau in November 2023.

Pierre Rousselin, Sylvie Boldo ([TOCCATA](#)), François Clément and Micaela Mayero ([LIPN](#)) organized the [kickoff meeting](#) of the task devoted to the creation of content (math library, exercises, interactive classes) within [Inria Challenge LiberAbaci](#) for the teaching of mathematics using [Coq](#).

Martin Vohralík (with Guillaume Enchéry and Ibtihel Ben Gharbia, [IFP Energies Nouvelles](#)) organized the regular 1-day workshop [Journée contrat cadre IFP Energies Nouvelles – Inria](#).

11.1.2 Scientific events: selection

Member of the conference program committees Martin Vohralík was a member of the scientific committee of the European Conference on Numerical Mathematics and Advanced Applications [ENUMATH 2023](#).

Reviewer François Clément served as reviewer for [NFM23](#).

11.1.3 Journal

Member of the editorial boards Alexandre Ern is a member of the Editorial Board of SIAM Journal on Scientific Computing, ESAIM Mathematical Modeling and Numerical Analysis, IMA Journal of Numerical Analysis, Journal of Scientific Computing, and Computational Methods in Applied Mathematics.

Martin Vohralík is a member of the editorial boards of [Acta Polytechnica](#), [Applications of Mathematics](#), and [Computational Geosciences](#).

Reviewer - reviewing activities Zhaonan Dong, Alexandre Ern, Michel Kern, Géraldine Pichot, and Martin Vohralík reviewed numerous papers for leading journals in numerical analysis and computational methods in geosciences.

11.1.4 Invited talks

Zhaonan Dong and Géraldine Pichot were invited to organize a mini-tutorial at the [SIAM Conference on Mathematical & Computational Issues in the Geosciences 2023](#), Bergen, Norway, June 2023.

Alexandre Ern gave a plenary lecture at the ECCOMAS Meeting on [Modern Finite Element Technologies](#), Mühlheim an der Ruhr, Germany, August, 2023.

Alexandre Ern gave an invited lecture within the special activity organized by IIT Roorkee, India on **Differential equations: analysis, computation and applications**.

Géraldine Pichot gave a plenary lecture at the Large-Scale Scientific Computations international conference **LSSC23**, Sozopol, Bugaria, June 2023.

Martin Vohralík gave an plenary talk at the **SIAM Conference on Mathematical and Computational Issues in the Geosciences** Bergen, Norway (June 2023), a plenary talk at **Congrès international sur l'analyse numérique des EDP**, Meknès, Morocco (October 2023), and an invited talk at **HOFEIM 2023**, Larnaca, Cyprus (May 2023).

11.1.5 Leadership within the scientific community

Alexandre Ern served within the Administration Board of SMAI and was Vice-President in charge of relations with industry.

Michel Kern is a member of

- the Scientific Board of ORAP, Organisation Associative du Parallélisme;
- the board of *École Doctorale Galilée* at University Sorbonne Paris-Nord;
- the steering committee of GDR **HydroGEMM**
- Martin Vohralík served as the president/member of the scientific committee of **Summer schools CEA-EDF-INRIA**.
- Martin Vohralík served as a member of the scientific board of the **IFP Energies Nouvelles – Inria joint strategic partnership laboratory**.

11.1.6 Scientific expertise

Michel Kern is a reviewer for the Allocation of Computing Time located at the Juelich Supercomputing Centre in Germany.

11.1.7 Research administration

François Clément is a member of the *Commission des usagers de la rue Barrault* (CURB) for the next relocation of the Inria Paris Center.

Michel Kern is the chair of the Commission de Développement Technologique of the Inria Paris Center.

Géraldine Pichot is the president of the *Commission des utilisateurs des moyens informatiques de Paris* (CUMI Paris).

Géraldine Pichot is a member of the *Comité de Suivi Doctoral de Paris* (CSD).

Géraldine Pichot is the contact person at Inria Paris for the *Agence pour les Mathématiques en Interaction avec l'Entreprise et la Société* (AMIES).

11.2 Teaching - Supervision - Juries

11.2.1 Teaching

- Master : Alexandre Ern, Discontinuous Galerkin methods, 20h, M2, Sorbonne University, France.
- Master: Alexandre Ern, Finite Elements, 15h, M1, ENPC, France.
- Master: Alexandre Ern, Hyperbolic equations, 6h, M2, Sorbonne University, France.
- Master: Michel Kern, Models and numerical methods for subsurface flow, 30h, M2, Université Paris Saclay, France.
- Master: Michel Kern, Advanced numerical analysis, 30h, M1, Institut Galilée, Université Paris-Nord, France.
- Master: Martin Vohralík, Advanced finite elements, 21h, M1, ENSTA (Ecole nationale supérieure de techniques avancées), Paris, France.

11.2.2 Supervision

- PhD defended: Stefano Piccardo, Simulation of two-fluid immiscible Stokes flows using hybrid nonconforming methods and geometrically unfitted meshes, 04 December 2023, Alexandre Ern and Antonio Huerta (UPC Barcelone), [37].
- PhD defended: Morgane Steins, An explicit hybrid high-order method for structural dynamics, 05 December 2023, Alexandre Ern and Olivier Jamond (CEA), [38].
- PhD in progress: Nicolas Hugot, A posteriori error estimates for the wave equation, started November 2023, Martin Vohralík.
- PhD in progress: Abbas Kabalan, Model order reduction for nonparametrized geometrical variability, started October 2022, Virginie Ehrlacher (Matherials) and Alexandre Ern.
- PhD in progress: Clément Maradei, Parallel adaptive hp -FEM, started October 2023, Zhaonan Dong and Martin Vohralík.
- PhD in progress: Romain Mottier, Unfitted hybrid high-order methods for geophysical wave propagation, started October 2021, Alexandre Ern and Laurent Guillot (CEA).
- PhD in progress: Houda Mouhcine, Formal proofs in applied mathematics: verification of a generator for quadrature formulas, started October 2021, Sylvie Boldo (TOCCATA), François Clément, and Micaela Mayero (LIPN).
- PhD in progress: Ari Rappaport, A posteriori error estimates and adaptivity in numerical approximation of PDEs: regularization, linearization, discretization, and floating point precision, started January 2021, Martin Vohralík.
- PhD in progress: Daniel Zegarra Vasquez, High-performance simulation of single-phase flows in a fractured porous medium, started October 2021, Géraldine Pichot, Michel Kern, and Martin Vohralík.
- PhD in progress: Zuodong Wang, Finite element methods for hyperbolic and degenerate parabolic problems, started October 2021, Zhaonan Dong and Alexandre Ern.
- Internship: Nicolas Hugot (ENSTA), Flux reconstruction for the wave equation, April-September 2023, Martin Vohralík.
- Internship: Clément Maradei (Sup Galilée), Finite element simulation of the viscous wave equation, February-March 2023, Michel Kern.
- Internship: Clément Maradei (Sup Galilée), Parallel adaptive hp -FEM, April-September 2023, Zhaonan Dong and Martin Vohralík.
- Internship: Alessandra Marelli (Politecnico di Milano), Simulation of advective transport in fracture networks, April-September 2023, Géraldine Pichot and Michel Kern.

11.2.3 Juries

- Alexandre Ern was external reviewer for the PhD of Matthieu Barré (IPP), Simon Le Berre (CEA Cadarache and Mines ParisTech), and Kenneth Assogba (IPP) and committee member for the HDR of Laurent Monasse (Cote d'Azur University) and for the PhD of Julien Moatti (Lille University).
- Martin Vohralík was a referee and committee president for the PhD thesis of Hussein Albazzal (Université de Bourgogne Franche-Comté), committee president for the PhD thesis of Georges Seeman (Université Saint-Joseph de Beyrouth), and committee member for the PhD thesis of Sarah Perez (Université de Pau et des Pays Adour) and Yipeng Wang (Sorbonne Université).

11.3 Popularization

11.3.1 Internal or external Inria responsibilities

Martin Vohralík served in the scientific committee of [Summer schools CEA–EDF–INRIA](#).

11.3.2 Interventions

Michel Kern gave a presentation on "Modeling and simulation: applications to subsurface water" to a "classe de seconde" at Lycée Lucie Aubrac (Courbevoie) as part of the *1 scientifique, 1 classe : chiche!* project.

12 Scientific production

12.1 Major publications

- [1] E. Ahmed, S. Ali Hassan, C. Japhet, M. Kern and M. Vohralík. 'A posteriori error estimates and stopping criteria for space-time domain decomposition for two-phase flow between different rock types'. In: *SMAI Journal of Computational Mathematics* 5 (Dec. 2019), pp. 195–227. DOI: [10.5802/smai-jcm.47](https://doi.org/10.5802/smai-jcm.47). URL: <https://hal.inria.fr/hal-01540956>.
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