IN PARTNERSHIP WITH:
Ecole des Ponts ParisTech

Activity Report 2019

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)

RESEARCH CENTER
Paris

THEME
Earth, Environmental and Energy Sciences

Table of contents

1. Team, Visitors, External Collaborators **1**
2. Overall Objectives **2**
3. Research Program **3**
3.1. Multiphysics coupling 3
3.2. Discretization by hybrid high-order and discrete element methods 3
3.3. Domain decomposition and Newton–Krylov (multigrid) solvers 3
3.4. Reliability by a posteriori error control 4
3.5. Safe and correct programming 4
4. Application Domains **4**
4.1. Multiphase flows and transport of contaminants in the subsurface 4
4.2. Industrial risks in energy production 4
4.3. Nonlinear mechanics 4
4.4. Computational quantum chemistry 5
5. Highlights of the Year **5**
6. New Software and Platforms **5**
6.1. CELIA3D 5
6.2. DiSk++ 5
6.3. NEF-Draw 6
6.4. NEF-Flow 6
6.5. NEF++ 7
6.6. NEF-Flow-a-posteriori 7
6.7. SBM 7
7. New Results **8**
7.1. Hybrid high-order methods for nonlinear mechanics 8
7.2. A hybrid high-order method for flow simulations in discrete fracture networks 9
7.3. Analytic expressions of the solutions of advection-diffusion problems in 1D with discontinuous coefficients 9
7.4. An exponential timestepping algorithm for diffusion with discontinuous coefficients 9
7.5. Polynomial-degree-robust multilevel algebraic error estimator & solver 10
7.6. Local- and global-best equivalence, simple projector, and optimal hp approximation in $\mathbf{H}(\mathrm{div})$ 10
8. Bilateral Contracts and Grants with Industry **10**
9. Partnerships and Cooperations **11**
9.1. Regional Initiatives 11
9.2. European Initiatives 11
9.3. International Initiatives 11
9.3.1. Inria International Partners 11
9.3.2. Participation in Other International Programs 12
9.4. International Research Visitors 12
9.4.1. Visits of International Scientists 12
9.4.2. Visits to International Teams 12
10. Dissemination **13**
10.1. Promoting Scientific Activities 13
10.1.1. Scientific Events: Organisation 13
10.1.2. Scientific Events: Selection 13
10.1.2.1. Chair of Conference Program Committees 13
10.1.2.2. Member of the Conference Program Committees 13
10.1.3. Journal 13
10.1.3.1. Member of the Editorial Boards 13

10.1.3.2. Reviewer - Reviewing Activities 13
10.1.4. Invited Talks 13
10.1.5. Leadership within the Scientific Community 13
10.1.6. Research Administration 14
10.2. Teaching - Supervision - Juries 14
10.2.1. Teaching 14
10.2.2. Supervision 14
10.2.3. Juries 15
10.3. Popularization 15
11. Bibliography **15**

Project-Team SERENA

Creation of the Team: 2015 June 01, updated into Project-Team: 2017 April 01

Keywords:

Computer Science and Digital Science:

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. - Fossile energy production (oil, gas)
B4.2.1. - Fission
B5.5. - Materials

1. Team, Visitors, External Collaborators

Research Scientists

Martin Vohralík [Team leader, Inria, Senior Researcher, HDR]
François Clément [Inria, Researcher]
Alexandre Ern [Ecole Nationale des Ponts et Chaussées, Researcher, HDR]
Jean-Luc Guermond [Inria International Chair, HDR]
Michel Kern [Inria, Researcher]
Jan Papež [Inria, Starting Research Position, from Jul 2019]
Géraldine Pichot [Inria, Researcher]
Pierre Weis [Inria, Senior Researcher, until May 2019]

Post-Doctoral Fellows

Guillaume Delay [Ecole Nationale des Ponts et Chaussées, until Sep 2019]
Omar Duran [Ecole Nationale des Ponts et Chaussées, from Nov 2019]
Kenan Kergrene Profit [Inria]
Seyed Mohammad Zakerzadeh [Inria, until Jul 2019]

PhD Students

Jad Dabaghi [Inria, until Jan 2019]

Joëlle Ferzly [IFPEN, from Oct 2019]
Nicolas Pignet [EDF, until Oct 2019]
Frédéric Marazzato [CEA]
Riccardo Milani [EDF]
Idrissa Niakh [EDF, from Nov 2019]
Ani Miraci [Inria]
Stefano Piccardo [Ecole Nationale des Ponts et Chaussées, from Oct 2019]

Technical staff
Sébastien Furic [Inria, Engineer, until Jul 2019]
Florent Hédin [Inria, Engineer]

Intern and Apprentice
Théo Kaprélian [Inria, from Sep 2019]

Administrative Assistant
Derya Gök [Inria]

Visiting Scientists
Roland Becker [University of Pau, Professor, Apr 2019]
Théophile Chaumont-Frelet [Inria Sophia Antipolis, Researcher, Feb, Apr, Jun, Sep & Dec 2019]
Quaanling Deng [Curtin University, PostDoc, from May 2019 until Jun 2019]
Gregor Gantner [Vienna University of Technology, PostDoc, Feb & Sep 2019]
Thirupathi Gudi [Indian Institute of Science, Bangalore, Professor, Jun 2019]
Dirk Praetorius [Vienna University of Technology, Professor, Mar 2019]
Sergio Rojas [Curtin University, PostDoc, Sep 2019]
Ivan Yotov [University of Pittsburgh, Inria invited Professor, Sep – Dec 2019]

External Collaborators
Hend Ben Ameur [IPEST and ENIT-Lamsin (Tunisia), Professor, HDR]
Erik Burman [University College London, Professor, HDR]
Guy Chavent [Univ Paris-Dauphine, Professor (retired), HDR]
Jad Dabaghi [CEA, post-doc, from Sep 2019]
Jérôme Jaffré [Inria, Senior Researcher (retired), HDR]
Caroline Japhet [Univ Paris-Nord, Associate Professor]
Vincent Martin [Univ de technologie de Compiègne, Associate Professor]
Jean-Elizabeth Roberts [Inria, Senior Researcher (retired), HDR]
Pierre Weis [Inria, Senior Researcher (retired), from Jun 2019]

2. Overall Objectives

2.1. 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*. SERENA has taken over the project-team POMDAPI2 which ended on May 31, 2015. It has been given an authorization to become a joint project-team between Inria and ENPC at the Committee of Projects, September 1st, 2016, and was created as project-team on April 10, 2017.

3. Research Program

3.1. Multiphysics coupling

Within our project, we start from the conception and analysis of *models* based on *partial differential equations* (PDEs). Already at the PDE level, we address the question of *coupling* of different models; examples are that of simultaneous fluid flow in a discrete network of two-dimensional *fractures* and in the surrounding three-dimensional porous medium, or that of 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. At the modeling stage, we also develop model-order reduction techniques, such as the use of reduced basis techniques or proper generalized decompositions, to tackle evolutive problems, in particular in the nonlinear case, and we are also interested in developing reduced-order methods for variational inequalities such as those encountered in solid mechanics with contact and possibly also friction.

3.2. Discretization by hybrid high-order and discrete element methods

We consequently design *numerical methods* for the devised model. Traditionally, we have worked in the context of finite element, finite volume, mixed finite element, and discontinuous Galerkin methods. Novel classes of schemes enable the use of general *polygonal* and *polyhedral meshes* with *nonmatching interfaces*, and we develop them in response to a high demand from our industrial partners (namely EDF, CEA, and IFP Energies Nouvelles). In the lowest-order case, our focus is to design *discrete element* methods for solid mechanics. The novelty is to devise these methods to treat dynamic elastoplasticity as well as quasi-static and dynamic crack propagation. We also develop *structure-preserving* methods for the Navier–Stokes equations, i.e., methods that mimic algebraically at the discrete level fundamental properties of the underlying PDEs, such as conservation principles and preservation of invariants. In the higher-order case, we actively contribute to the development of *hybrid high-order* methods. We contribute to the numerical analysis in nonlinear cases (obstacle problem, Signorini conditions), we apply these methods to challenging problems from solid mechanics involving large deformations and plasticity, and we develop a comprehensive software implementing them. We believe that these methods belong to the future generation of numerical methods for industrial simulations; as a concrete example, the implementation of these methods in an industrial software of EDF has been completed in 2019 in the framework of the PhD thesis of Nicolas Pignet.

3.3. Domain decomposition and Newton–Krylov (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 have in the past developed *Newton–Krylov solvers* like the *adaptive inexact Newton method*, and we place a particular emphasis on *parallelization* achieved via the *domain decomposition* method. Here we traditionally specialize in *Robin transmission conditions*, where an optimized choice of the parameter has already shown speed-ups in orders of magnitude in terms of the number of domain decomposition iterations in model cases. We concentrate in the SERENA project on adaptation of these algorithms to the above novel discretization schemes, on the optimization of the free Robin parameter for challenging situations, and also on the use of the Ventcell transmission conditions. Another feature is the use of such algorithms in time-dependent problems in *space-time* domain decomposition that we have recently pioneered. This allows the use of different time steps in different parts of the computational domain and turns out to be particularly useful in porous media applications, where the amount of diffusion (permeability) varies abruptly, so that the evolution speed varies significantly from one part of the computational domain to another. Our new theme here are *Newton–multigrid solvers*, where the geometric multigrid solver is *tailored* to the specific problem under consideration and to the specific numerical method, with problem- and discretization-dependent restriction, prolongation, and smoothing. Using patchwise smoothing, we have in particular recently developed a first multigrid method whose behavior is both in theory and in practice insensitive of (robust with respect to) the approximation polynomial degree.

With patchwise techniques, we also achieve mass balance at each iteration step, a highly demanded feature in most of the target applications. The solver itself is then *adaptively steered* at each execution step by an a posteriori error estimate (adaptive stepsize, adaptive smoothing).

3.4. Reliability by a posteriori error control

The fourth part of our theoretical efforts goes towards guaranteeing 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, from the discretization scheme, from the nonlinear (Newton) solver, and from the linear algebraic (Krylov, 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 also theoretically address the question of convergence of the new fully adaptive algorithms. We identify theoretical conditions so that the error diminishes at each adaptive loop iteration by a contraction factor and we in particular derive a guaranteed error reduction factor in model cases. We have also proved a numerical optimality of the derived algorithms in model cases in the sense that, up to a generic constant, the smallest possible computational effort to achieve the given accuracy is needed.

3.5. Safe and correct programming

Finally, we concentrate on the issue of computer implementation of scientific computing programs. Increasing complexity of algorithms for modern scientific computing makes it a major challenge to implement them in the traditional imperative languages popular in the community. As an alternative, the computer science community provides theoretically sound tools for *safe* and *correct programming*. We explore here the use of these tools to design generic solutions for the implementation of the class of scientific computing software that we deal with. Our focus ranges from high-level programming via *functional programming* with OCaml through safe and easy parallelism via *skeleton parallel programming* with SklML to proofs of correctness of numerical algorithms and programs via *mechanical proofs* with Coq.

4. Application Domains

4.1. Multiphase flows and transport of contaminants in the subsurface

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

4.2. Industrial risks in energy production

- Stokes and Navier–Stokes flows related to nuclear reactor operation
- seismic wave propagation for detection and protection
- electromagnetism for interfaces between dielectrics and negative metamaterials

4.3. Nonlinear mechanics

- quasi-static and dynamic elastoplastic evolutions with small and large deformations
- quasi-static and dynamic crack propagation
- nonlinear contact and friction conditions

- application to engineering components mainly related to nuclear reactor operation and safety analysis

4.4. Computational quantum chemistry

- guaranteed bounds for ground-state energy (eigenvalues) and ground-state density matrix (eigenvectors) in first-principle molecular simulation
- application to Laplace, Gross–Pitaevskii, Kohn–Sham, and Schrödinger models

5. Highlights of the Year

5.1. Highlights of the Year

Many new results of the ERC GATIPOR project in the ERC GATIPOR Gallery.

6. New Software and Platforms

6.1. CELIA3D

KEYWORDS: Fluid mechanics - Multi-physics simulation

FUNCTIONAL DESCRIPTION: The CELIA3D code simulates the coupling between a compressible fluid flow and a deformable structure. The fluid is handled by a Finite Volume method on a structured Cartesian grid. The solid is handled by a Discrete Element method (Mka3d scheme). The solid overlaps the fluid grid and the coupling is carried out with immersed boundaries (cut cells) in a conservative way.

- Partners: Ecole des Ponts ParisTech - CEA
- Contact: Laurent Monasse
- URL: http://cermics.enpc.fr/~monassel/CELIA3D/

6.2. DiSk++

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.

- Author: Matteo Cicuttin
- Partner: CERMICS
- Contact: Matteo Cicuttin
- Publication: Implementation of Discontinuous Skeletal methods on arbitrary-dimensional, polytopal meshes using generic programming
- URL: https://github.com/wareHHOuse/diskpp

6.3. NEF-Draw

Numerical Experiments involving Fractures -Visualisation

KEYWORD: Fracture network

SCIENTIFIC DESCRIPTION: This version includes Matlab vectorization of the operations which makes it possible to load flow solution on meshes with more than one million fractures. It includes a text menu allowing the user to choose between different visualisation options (geometry, mesh together with the aspect ratio or together with the flow solution). A selective visualisation of fractures is also possible, by loading only the fractures that carry most of the flow.

FUNCTIONAL DESCRIPTION: This software is a visualization tool of discrete fractured networks. It allows the visualization of the network geometry, the mesh of the network together with several quantities of interest (mesh quality, flow solution including wells) computed with the software NEF-Flow.

NEWS OF THE YEAR: Add vizualization of new quantities (a posteriori estimators, velocity fields,...). New features for user-friendly usage of NEF-Draw.

- Participant: Géraldine Pichot
- Contact: Géraldine Pichot
- URL: https://gitlab.inria.fr/gpichot/NEF

6.4. NEF-Flow

KEYWORDS: Hydrogeology - Numerical simulations - 3D

SCIENTIFIC DESCRIPTION: NEF-Flow is a Matlab software for the simulation of steady state single phase flow in Discrete Fracture Networks (DFNs) using the Mixed Hybrid Finite Element (MHFEM) method for conforming and non conforming discretizations. It includes: wells, sink/source terms boundary conditions, implementation of RT0 and P1 non conforming finite elements, data structures to save the information local to each fracture, a set of non regression tests to check the solution on the Inria continuous integration platform, wells and sink/sources boundary conditions in the function that check the solution.

FUNCTIONAL DESCRIPTION: The software NEF-Flow solves the problem of an incompressible fluid flowing through a network of fractures. The software is interfaced with different mesh generators, among which BLSURF from the GAMMA3 team. A mixed hybrid finite element method is implemented.

NEWS OF THE YEAR: The last version includes new features (new APP v1.1): a full documentation of the code, new 2D test cases with analytical solutions to study the convergence of the non-conforming (Mortar) method, new organization of the non regression tests and automatic run on the Inria continuous integration platform, a refactoring of the solver parts, new developments of an iterative solver to solve flow in fractures networks (research work with Pr. Ludmil Zikatanov, PennState University), the computation of the velocity fields with P1 non conforming FE.

- Participants: Géraldine Pichot, Jean-Raynald De Dreuzy and Jocelyne Erhel
- Contact: Géraldine Pichot
- Publication: A mixed hybrid Mortar method for solving flow in discrete fracture networks
- URL: https://gitlab.inria.fr/gpichot/NEF

6.5. NEF++

KEYWORDS: Fracture network - Finite element modelling - High order methods

SCIENTIFIC DESCRIPTION: NEF++ is able to solve in a very efficient way flow in large scale fractures networks using the HHO method.

FUNCTIONAL DESCRIPTION: The software NEF++ allows to solve flow problems in fractured rocks. It is based on a hybrid high order (HHO) method. It is based on the C++17 standard. It relies on the Eigen library, which is a C++ template library for linear algebra and on the DiSk++ library for HHO https://bil.inria.fr/fr/software/view/3143/tab. The linear systems can be solved with direct solvers or with iterative solvers like the preconditioned conjugate gradient or multigrid solvers.

RELEASE FUNCTIONAL DESCRIPTION: Work in progress, no production release yet.

NEWS OF THE YEAR: NEF++ has been successfully tested on networks that contain up to 500,000 fractures. The following two direct solvers can be called: Pardiso from Intel MKL library or SuiteSparse. Both solvers support tasks parallelism, either using OpenMP or Intel TBB and support SIMD (Single Instruction, Multiple Data) vectorization. The input parameters are JSON files. The mesh data are in .vector files (see Appendix A, publication hal-00735675). The outputs are written in HDF5 files.

- Participants: Florent Hedin, Géraldine Pichot, Alexandre Ern and Nicolas Pignet
- Contact: Géraldine Pichot
- Publication: A hybrid high-order method for flow simulations in discrete fracture networks.
- URL: https://gitlab.inria.fr/nef/NEFpp

6.6. NEF-Flow-a-posteriori

KEYWORD: A posteriori error estimates

SCIENTIFIC DESCRIPTION: The a posteriori error estimates that are implemented are the ones described in the publication https://hal.archives-ouvertes.fr/hal-00019800/document.

FUNCTIONAL DESCRIPTION: Compute a posteriori estimators for diffusion problems.

NEWS OF THE YEAR: New software: implementation of the estimators, management of input files with Json.

- Participants: Géraldine Pichot and Martin Vohralík
- Contact: Géraldine Pichot
- Publication: A posteriori error estimates for lowest-order mixed finite element discretizations of convection-diffusion-reaction equations
- URL: https://gitlab.inria.fr/gpichot/nef-flow-a-posteriori

6.7. SBM

Skew Brownian Motion

KEYWORDS: Monte-Carlo methods - Skew Brownian Motion

FUNCTIONAL DESCRIPTION: SBM is a code allowing exact or approximated simulations of the Skew Brownian Motion. This code is used for the simulation, with a Monte-Carlo approach, of a 1D diffusion process with a discontinuous diffusion coefficient. Several benchmark tests are also implemented.

NEWS OF THE YEAR: - Refactoring and Cmake compilation - Automatic non regression tests on ci-inria.fr - Full documentation - Open source project on gitlab-inria

- Authors: Antoine Lejay and Géraldine Pichot
- Contact: Antoine Lejay
- Publication: Simulating diffusion processes in discontinuous media: Benchmark tests
- URL: https://gitlab.inria.fr/lejay/sbm

7. New Results

7.1. Hybrid high-order methods for nonlinear mechanics

Participants: Alexandre Ern, Nicolas Pignet.

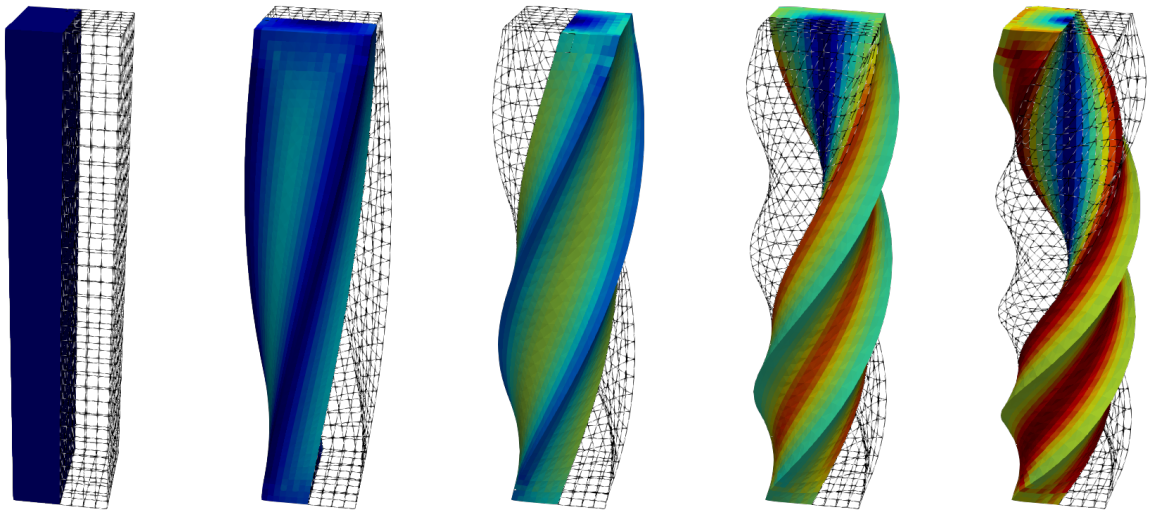

Figure 1. Torsion of a square-section bar: Equivalent plastic strain p (values between 0 (blue) to 0.49 (red)) for HHO with polynomial degree $k = 1$ at the quadrature points for different rotation angles Θ. From left to right: $\Theta = 0°$, $\Theta = 90°$, $\Theta = 180°$, $\Theta = 270°$, *and* $\Theta = 360°$

Our team contributes actively to the development of hybrid high-order (HHO) methods for nonlinear solid mechanics. Within the PhD of Nicolas Pignet in collaboration with EDF we have addressed several nonlinearities, including plasticity, large deformations, contact, and (Tresca) friction [15], [14], [49]. The advantage with respect to conforming finite elements is the robustness with respect to volumetric locking. The advantage with respect to mixed approaches is computational efficiency avoiding saddle-point formulations and additional unknowns. The advantage with respect to discontinuous Galerkin methods is avoiding the integration of the nonlinear behavior law at face quadrature nodes and the use of symmetric tangent matrices within Newton's method. The torsion of a square-section elastoplastic bar is presented in Figure 1. The color filling reports the equivalent plastic strain. The solution is obtained with the HHO method using the polynomial degree $k = 1$ for the face and the cell unknowns.

7.2. A hybrid high-order method for flow simulations in discrete fracture networks

Participants: Florent Hédin, Géraldine Pichot, Alexandre Ern.

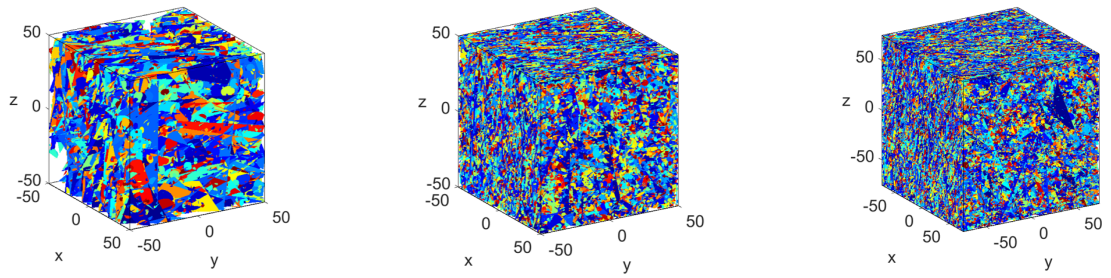

Figure 2. Examples of DFN: (left) B1: 19,007 fractures; (center) B2: 152,399 fractures ; (right) B3: 508,338 fractures.

In [36], we are interested in solving flow in large trimensional Discrete Fracture Networks (DFN) (cf Figure 2) with the hybrid high-order (HHO) method. The objectives of this paper are: (1) to demonstrate the benefit of using a high-order method for computing macroscopic quantities, like the equivalent permeability of fracture rocks; (2) to present the computational efficiency of our C++ software, `NEF++`, which implements the solving of flow in fractures based on the HHO method.

7.3. Analytic expressions of the solutions of advection-diffusion problems in 1D with discontinuous coefficients

Participants: Antoine Lejay, Lionel Lenôtre, Géraldine Pichot.

In [30], we provide a method to compute analytic expressions of the resolvent kernel of differential operators of the diffusion type with discontinuous coefficients in one dimension. Then we apply it when the coefficients are piecewise constant. We also perform the Laplace inversion of the resolvent kernel to obtain expressions of the transition density functions or fundamental solutions. We show how these explicit formula are useful to simulate advection-diffusion problems using particle tracking techniques.

7.4. An exponential timestepping algorithm for diffusion with discontinuous coefficients

Participants: Antoine Lejay, Lionel Lenôtre, Géraldine Pichot.

In [29], we present a new Monte Carlo algorithm to simulate diffusion processes in presence of discontinuous convective and diffusive terms. The algorithm is based on the knowledge of close form analytic expressions of the resolvents of the diffusion processes which are usually easier to obtain than close form analytic expressions of the density. In the particular case of diffusion processes with piecewise constant coefficients, known as Skew Diffusions, such close form expressions for the resolvent are available. Then we apply our algorithm to this particular case and we show that the approximate densities of the particles given by the algorithm replicate well the particularities of the true densities (discontinuities, bimodality, ...) Besides, numerical experiments show a quick convergence.

7.5. Polynomial-degree-robust multilevel algebraic error estimator & solver

Participants: Ani Miraci, Jan Papež, Martin Vohralík.

In [58], we devise a novel multilevel a posteriori estimator of the algebraic error. It delivers a fully computable, guaranteed lower bound on the error between an unknown exact solution of a system of linear algebraic equations and its approximation by an algebraic solver. The bound is also proved to be efficient, i.e., it also gives an upper bound on the algebraic error. Remarkably, the quality of these bounds is independent of the approximation polynomial degree. The derived estimates give immediately rise to a multilevel iterative algebraic solver whose contraction factor is independent of the polynomial degree of the approximation. We actually prove an equivalence between efficiency of the estimator and contraction of the solver. The estimator/solver are based on a global coarsest-level solve of lowest-order ($p = 1$), followed by local patchwise p-degree problems solved on the other levels. It corresponds to a V-cycle geometric multigrid solver with zero pre- and one post-smoothing step via block-Jacobi. A salient feature is the choice of the optimal step size for the descent direction.

7.6. Local- and global-best equivalence, simple projector, and optimal hp approximation in $\mathbf{H}(\mathrm{div})$

Participants: Alexandre Ern, Thirupathi Gudi, Iain Smears, Martin Vohralík.

$$\min_{\substack{\boldsymbol{v}_{\mathcal{T}} \in \boldsymbol{RTN}_p(\mathcal{T}) \cap \boldsymbol{H}_{0,\Gamma_{\mathrm{N}}}(\mathrm{div},\Omega) \\ \nabla\cdot\boldsymbol{v}_{\mathcal{T}} = \Pi^p_{\mathcal{T}}(\nabla\cdot\boldsymbol{v})}} \|\boldsymbol{v} - \boldsymbol{v}_{\mathcal{T}}\|^2_\Omega$$
$$\approx \sum_{K\in\mathcal{T}} \min_{\boldsymbol{v}_K \in \boldsymbol{RTN}_p(K)} \|\boldsymbol{v} - \boldsymbol{v}_K\|^2_K$$

Figure 3. Equivalence between global-best and local-best approximation for any $\mathbf{H}(\mathrm{div})$ function $\mathbf{v}$ with zero normal flux over part of the boundary and piecewise polynomial divergence

In [53], we prove that a global-best approximation in $\mathbf{H}(\mathrm{div})$, with constraints on normal component continuity and divergence, is equivalent to the sum of independent local-best approximations, without any constraints, as illustrated in Figure 3. This may seem surprising on a first sight since the right term in Figure 3 is seemingly much smaller (since the minimization set is unconstrained and thus much bigger). This result leads to optimal a priori hp-error estimates for mixed and least-squares finite element methods, which were missing in the literature until 2019. Additionally, the construction we devise gives rise to a simple stable local commuting projector in $\mathbf{H}(\mathrm{div})$, which delivers approximation error equivalent to the local-best approximation and applies under the minimal necessary Sobolev $\mathbf{H}(\mathrm{div})$ regularity, which is another result that has been sought for a very long time.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

One new two-part contract with EDF accompanying the PhD thesis of Idrissa Niakh.

One new two-part contract with CEA accompanying the postdoc of Guillaume Delay.

One new two-part contract with IFP Energies Nouvelles accompanying the PhD thesis of Joëlle Ferzly.

Three-part contract Inria–EDF–Sciworks Technologies (2017–2020) on "Form-L for the formalization of constraints of complex systems". SERENA representants are François Clément, Sébastien Furic and Pierre Weis.

AMIES contract with ITASCA, January 10, 2019 - March 10, 2020. SERENA representants are François Clément, Sébastien Furic, Florent Hédin, Michel Kern, Géraldine Pichot.

9. Partnerships and Cooperations

9.1. Regional Initiatives

MILC (DMI RFSI, 2018–2019): "Mesure et Intégrale de Lebesgue en Coq", with LIPN (Université de Paris 13), and TOCCATA (Inria Saclay - Île-de-France). SERENA representants are François Clément and Vincent Martin (UTC).

GiS: scientific collaboration network between ten public institutions from the Paris (Ile-de-France) region, focused on natural resources and environment. The project-team SERENA is a member.

9.2. European Initiatives

9.2.1. FP7 & H2020 Projects

- ERC GATIPOR: "Guaranteed fully adaptive algorithms with tailored inexact solvers for complex porous media flows". The subject of this consolidator grant are new approaches to porous media multiphase flows: inexact Newton-multigrid solvers, local stopping criteria, adaptivity, and a posteriori error control. The goal is to guarantee the overall simulation error and to speed-up importantly the present-day simulations. SERENA representant is M. Vohralík (grant leader, 75% commitment), period 2015–2020.
- ERC EMC2: " Extreme-scale Mathematically-based Computational Chemistry". The goal of this project is to develop physical and chemical models in chemistry, condensed matter physics, molecular biology, materials science, and nanosciences, altogether with mathematically-certified and numerically-efficient algorithms, and to implement them in a scalable way on various computer architectures. There are 4 principal investigators and a little more than 10 co-investigators. SERENA representant is M. Vohralík (co-investigator, 10% commitment), period 2019–2025.

9.3. International Initiatives

9.3.1. Inria International Partners

9.3.1.1. Informal International Partners

Erik Burman, Professor, University College London, unfitted methods.

Ulrich Rüde, Professor, University of Erlangen-Nürnberg, multigrid methods.

Iain Smears, Lecturer, University College London, local-global approximations.

Benjamin Stamm, Professor, RTWH Aachen University, eigenvalue problems (first-principle molecular simulation).

Barbara Wohlmuth, professor, Technical University Munich, multigrid methods.

9.3.2. Participation in Other International Programs

9.3.2.1. Inria International Chairs

IIC GUERMOND Jean-Luc

Title: Curved H(div), H(curl) elements, and magnetohydrodynamics & Approximation of hyperbolic systems

International Partner (Institution - Laboratory - Researcher):

Texas A&M University (United States) - Department of Mathematics - Jean-Luc Guermond

Duration: 2019 - 2023

Start year: 2019

See also: https://www.math.tamu.edu/~guermond/

The program is articulated around two themes: (1) Theoretical aspects in finite elements and applications to multi-physics magneto-hydrodynamics; (2) Finite element approximation of hyperbolic systems and applications. The results from this research will have applications in problems related to porous media flows, magnetohydrodynamics, water management, and compressible and incompressible fluid flows.

9.4. International Research Visitors

9.4.1. Visits of International Scientists

Hend Ben Ameur, Professor at IPEST and member of ENIT-Lamsin, Tunis, Tunisia, November 4–15.

Gregor Gantner, Vienna University of Technology. Collaboration on IGA methods. September 23–27.

Thirupathi Gudi, Indian Institute of Science, Bangalore. Collaboration on local-global approximations. June 10–17.

Dirk Praetorius, Vienna University of Technology. Collaboration on cost-optimality of fully adaptive algorithms. March 21–23.

Ivan Yotov, Professor, University of Pittsburgh. Inria Paris invited professor, September 1–December 15, 2019. Collaboration on multilevel and space-time domain decomposition methods.

9.4.1.1. Internships

Théo Kaprélian, internship at Ecole Centrale de Lyon, from September 2019 to February 2020, supervised by Martin Vohralík.

9.4.2. Visits to International Teams

9.4.2.1. Research Stays Abroad

+ Géraldine Pichot was invited for a one week stay at Pennstate University, USA for a collaboration with Pr. Ludmil Zikatanov.
+ Géraldine Pichot was invited for a one week stay at University of Bergen, Norway for a collaboration with Pr. Florin Radu.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events: Organisation

10.1.1.1. Member of the Organizing Committees

Michel Kern was co-organizer of the SITRAM19 workshop (Advances in the SImulation of reactive flow and TRAnsport in porous Media), December 2–3, Pau, France.

10.1.2. Scientific Events: Selection

10.1.2.1. Chair of Conference Program Committees

Guillaume Enchéry and Martin Vohralík have organized a 1-day workshop Journée contrat cadre IFP Energies Nouvelles/Inria.

10.1.2.2. Member of the Conference Program Committees

Alexandre Ern is a member of the Scientific Committee of the European Finite Element Fair (EFEF) and of the European Numerical Mathematics and Advanced Applications Conference (ENUMATH).

Géraldine Pichot is a member of the Scientific Commitee of FRAME2020 - FRActured MEdia: Numerical methods for fluid flow and mechanics, September 21-24, 2020.

Michel Kern and Martin Vohralík were members of the Scientific Committee of the SimRace 2019 conference.

Michel Kern was a member of the Program Comittee of JCAD2019, Journées Calcul et Données .

10.1.3. Journal

10.1.3.1. Member of the Editorial Boards

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

Martin Vohralík is a member of the editorial boards of SIAM Journal on Numerical Analysis, Acta Polytechnica, and Applications of Mathematics.

10.1.3.2. Reviewer - Reviewing Activities

Alexandre Ern and Martin Vohralík served as reviewers for dozens of papers in different journals.

Michel Kern serrved as reviewer for BIT, Numerical Mathematics, Computational Geosciences, SIAM Journal on Scientific Computing, Applicable Analysis, and Journal of Mathematical Study.

Géraldine Pichot served as reviewer for Computational Geosciences.

10.1.4. Invited Talks

Alexandre Ern was invited as one of the two keynote lecturers at the Workshop on Computational Modeling and Numerical Analysis, Petropolis, Brésil, Feb 2019.

Michel Kern was invited as one of the keynote speakers at the HPC TerrSys fall school, Bonn, Germany, Sep. 2019.

Martin Vohralík was an invited speaker at GAMM section on Numerical methods of differential equations, Vienna, Austria, February 2019, Modern Finite Element Technologies 2019, Bad Honnef, Germany, July 2019, and Reliable Methods of Mathematical Modeling, Vienna, Austria, Sep 2019.

10.1.5. Leadership within the Scientific Community

Alexandre Ern is the coordinator of the Master Mathématiques et applications, Ecole nationale des ponts et chaussées.

Michel Kern is a member of the SIAM "Committee on Committees and Appointments".

Michel Kern is a member of the Scientific Board of ORAP (Organisation Associative du Parallélisme).

Michel Kern is a member of the Scientific Advisory Board of GDR CNRS Groupe Calcul.

Michel Kern is a member of the steering committee of Géosciences franciliennes.

Martin Vohralík is a member of the steering committee of Summer schools CEA–EDF–Inria.

Martin Vohralík is in charge of the topic "Numerical schemes, mesh generation algorithms, and error control" in the ANDRA, BRGM, CEA, EDF, IFP Energies Nouvelles, and Total working group on *High-Performance Numerical Simulation in the Geosciences* (identification of common challenges and collaboration opportunities).

10.1.6. Research Administration

François Clément is a member of the *Comité local d'hygiène, de sécurité et des conditions de travail* of the Inria Research Center of Paris.

Michel Kern is a member of the *Comité de Centre* of the Inria Research Center of Paris.

Martin Vohralík is a member of the Inria Paris *Committee on scientific positions* (evaluation of applications for Ph.D. theses (CORDI-S), post-docs, and délégations).

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

Licence : Alexandre Ern, Numerical analysis, 77h, L3/M1, Ecole Polytechnique, France.

Licence : Alexandre Ern, Optimal control, 10h, L3, Ecole nationale des ponts et chaussées, France.

Master : Alexandre Ern, Discontinuous Galerkin methods, 20h, M2, Sorbonne University, France.

Master: Michel Kern, Models and numerical methods for subsurface flow, 30h, M2, Université Paris Saclay, France

Master: Michel Kern, Inverse Problems, 24h, M1, Mines-ParisTech, France

Master: Michel Kern, Introduction to Partial Differential Equations, 30h, & Advanced numerical analysis, 30h, M1, Institut Galilée, Université Paris-Nord, France.

10.2.2. Supervision

PhD defended on June 3, 2019: Jad Dabaghi, A posteriori error estimates and adaptive stopping criteria for formulations with complementarity constraints, Martin Vohralík and Vincent Martin.

PhD defended on March 22, 2019: Patrik Daniel, Adaptive hp-finite elements with guaranteed error contraction and inexact multilevel solvers, Martin Vohralík and Alexandre Ern.

PhD in progress: Joëlle Ferzly, A posteriori error estimates and adaptivity for complementarity problems, started 15 October 2019, Martin Vohralík.

PhD in progress: Frédéric Marazzato, Discrete element methods for fracture and fragmentation, started 01 October 2016, Alexandre Ern.

PhD in progress: Riccardo Milani, Compatible Discrete Operator schemes for Navier–Stokes equations, started 01 October 2017, Alexandre Ern.

PhD in progress: Ani Miraci, Robust a posteriori error control and adaptivity with inexact solvers, started 01 October 2017, Martin Vohralík and Alexandre Ern.

PhD in progress: Idrissa Niakh, Reduced models for variational inequalities in computational mechanics, started 01 November 2019, Alexandre Ern and Virginie Ehrlacher (ENPC).

PhD in progress: Stefano Piccardo, High-fidelity simulation of droplets in complex shear flows, started 01 October 2019, Alexandre Ern and Antonio Huerta (UPC).

PhD defended on October 22, 2019: Nicolas Pignet, Hybrid high-order methods for nonlinear solid mechanics, Alexandre Ern.

10.2.3. Juries

Alexandre Ern, Examiner and Chairman, PhD V. Mamet, INP Grenoble, Jan 2019.

Alexandre Ern, Referee, PhD A. Rupp, Erlangen FA University, Mar 2019.

Alexandre Ern, Examiner, HDR C. Millet, University Paris-Sud, Mar 2019.

Michel Kern, Examiner, PhD Daniel Salas, Université de Strasbourg, Sep. 2019.

Michel Kern, Examiner, PhD Kevish Napal, Université Paris Saclay, Dec. 2019.

Géraldine Pichot, Referee, PhD Fabio Vicini, Politecnico di Torino, April 2019.

Martin Vohralík, Examiner and Chairman, PhD Hoang Phuong Thai, ENS Paris-Saclay, Jun 2019.

10.3. Popularization

10.3.1. Internal or external Inria responsibilities

+ Géraldine Pichot is a member of the editorial committee of Interstices since November 2019.

11. Bibliography

Major publications by the team in recent years

[1] S. BOLDO, F. CLÉMENT, J.-C. FILLIÂTRE, M. MAYERO, G. MELQUIOND, P. WEIS. *Wave equation numerical resolution: a comprehensive mechanized proof of a C program*, in "Journal of Automated Reasoning", April 2013, vol. 50, n^{o} 4, pp. 423–456, http://dx.doi.org/10.1007/s10817-012-9255-4

[2] S. BOLDO, F. CLÉMENT, J.-C. FILLIÂTRE, M. MAYERO, G. MELQUIOND, P. WEIS. *Trusting computations: A mechanized proof from partial differential equations to actual program*, in "Computers and Mathematics with Applications", August 2014, vol. 68, n^{o} 3, pp. 325–352, http://dx.doi.org/10.1016/j.camwa.2014.06.004

[3] E. CANCÈS, G. DUSSON, Y. MADAY, B. STAMM, M. VOHRALÍK. *Guaranteed and robust a posteriori bounds for Laplace eigenvalues and eigenvectors: conforming approximations*, in "SIAM J. Numer. Anal.", 2017, vol. 55, n^{o} 5, pp. 2228–2254, http://dx.doi.org/10.1137/15M1038633

[4] D. A. DI PIETRO, A. ERN. *A hybrid high-order locking-free method for linear elasticity on general meshes*, in "Comput. Methods Appl. Mech. Engrg.", 2015, vol. 283, pp. 1–21, http://dx.doi.org/10.1016/j.cma.2014.09.009

[5] A. ERN, J.-L. GUERMOND. *Finite element quasi-interpolation and best approximation*, in "ESAIM Math. Model. Numer. Anal.", 2017, vol. 51, n^{o} 4, pp. 1367–1385, https://doi.org/10.1051/m2an/2016066

[6] A. ERN, M. VOHRALÍK. *Polynomial-degree-robust a posteriori estimates in a unified setting for conforming, nonconforming, discontinuous Galerkin, and mixed discretizations*, in "SIAM J. Numer. Anal.", 2015, vol. 53, n^{o} 2, pp. 1058–1081, http://dx.doi.org/10.1137/130950100

[7] T.-T.-P. HOANG, J. JAFFRÉ, C. JAPHET, M. KERN, J. E. ROBERTS. *Space-time domain decomposition methods for diffusion problems in mixed formulations*, in "SIAM J. Numer. Anal.", 2013, vol. 51, n^{o} 6, pp. 3532–3559, http://dx.doi.org/10.1137/130914401

[8] T.-T.-P. HOANG, C. JAPHET, M. KERN, J. E. ROBERTS. *Space-time domain decomposition for reduced fracture models in mixed formulation*, in "SIAM J. Numer. Anal.", 2016, vol. 54, n° 1, pp. 288–316, http://dx.doi.org/10.1137/15M1009651

[9] A. LEJAY, G. PICHOT. *Simulating diffusion processes in discontinuous media: a numerical scheme with constant time steps*, in "J. Comput. Phys.", 2012, vol. 231, n° 21, pp. 7299–7314, http://dx.doi.org/10.1016/j.jcp.2012.07.011

[10] G. PICHOT, J. ERHEL, J.-R. DE DREUZY. *A generalized mixed hybrid mortar method for solving flow in stochastic discrete fracture networks*, in "SIAM J. Sci. Comput.", 2012, vol. 34, n° 1, pp. B86–B105, http://dx.doi.org/10.1137/100804383

Publications of the year

Doctoral Dissertations and Habilitation Theses

[11] J. DABAGHI. *A posteriori error estimates for variational inequalities: application to a two-phase flow in porous media*, Sorbonne Université, Université Pierre et Marie Curie, Paris 6, June 2019, https://hal.archives-ouvertes.fr/tel-02151951

[12] P. DANIEL. *Adaptive hp-finite elements with guaranteed error contraction and inexact multilevel solvers*, Sorbonne Université ; Inria Paris, March 2019, https://hal.inria.fr/tel-02104982

[13] N. PIGNET. *Hybrid High-Order methods for nonlinear solid mechanics*, Université Paris-Est Marne la Vallée, October 2019, https://tel.archives-ouvertes.fr/tel-02318157

Articles in International Peer-Reviewed Journals

[14] M. ABBAS, A. ERN, N. PIGNET. *A Hybrid High-Order method for finite elastoplastic deformations within a logarithmic strain framework*, in "International Journal for Numerical Methods in Engineering", June 2019 [*DOI :* 10.1002/NME.6137], https://hal.archives-ouvertes.fr/hal-01978385

[15] M. ABBAS, A. ERN, N. PIGNET. *A Hybrid High-Order method for incremental associative plasticity with small deformations*, in "Computer Methods in Applied Mechanics and Engineering", April 2019, vol. 346, pp. 891-912, https://arxiv.org/abs/1804.06129 [*DOI :* 10.1016/J.CMA.2018.08.037], https://hal.archives-ouvertes.fr/hal-01768411

[16] E. AHMED, S. ALI HASSAN, C. JAPHET, M. KERN, 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", December 2019, vol. 5, pp. 195-227, https://hal.inria.fr/hal-01540956

[17] L. AMIR, M. KERN. *Preconditioning a coupled model for reactive transport in porous media*, in "International Journal of Numerical Analysis and Modeling", 2019, vol. 16, n° 1, pp. 18-48, https://arxiv.org/abs/1710.01483 , https://hal.inria.fr/hal-01327307

[18] H. BARUCQ, G. CHAVENT, F. FAUCHER. *A priori estimates of attraction basins for nonlinear least squares, with application to Helmholtz seismic inverse problem*, in "Inverse Problems", 2019, forthcoming [*DOI :* 10.1088/1361-6420/AB3507], https://hal.archives-ouvertes.fr/hal-02194212

[19] I. BEN GHARBIA, J. DABAGHI, V. MARTIN, M. VOHRALÍK. *A posteriori error estimates and adaptive stopping criteria for a compositional two-phase flow with nonlinear complementarity constraints*, in "Computational Geosciences", December 2019 [*DOI :* 10.1007/S10596-019-09909-5], https://hal.archives-ouvertes.fr/hal-01919067

[20] A. BENACEUR, A. ERN, V. EHRLACHER. *A reduced basis method for parametrized variational inequalities applied to contact mechanics*, in "International Journal for Numerical Methods in Engineering", October 2019 [*DOI :* 10.1002/NME.6261], https://hal.archives-ouvertes.fr/hal-02081485

[21] J. BLECHTA, J. MÁLEK, M. VOHRALÍK. *Localization of the $W^{-1,q}$ norm for local a posteriori efficiency*, in "IMA Journal of Numerical Analysis", March 2019 [*DOI :* 10.1093/IMANUM/DRZ002], https://hal.inria.fr/hal-01332481

[22] S. BLIUDZE, S. FURIC, J. SIFAKIS, A. VIEL. *Rigorous Design of Cyber-Physical Systems : Linking Physicality and Computation*, in "Software and Systems Modeling", 2019, vol. 18, n^{o} 3, pp. 1613–1636, forthcoming [*DOI :* 10.1007/S10270-017-0642-5], https://hal.inria.fr/hal-01636392

[23] T. BOIVEAU, V. EHRLACHER, A. ERN, A. NOUY. *Low-rank approximation of linear parabolic equations by space-time tensor Galerkin methods*, in "ESAIM: Mathematical Modelling and Numerical Analysis", May 2019, vol. 53, n^{o} 2, pp. 635-658, https://arxiv.org/abs/1712.07256 [*DOI :* 10.1051/M2AN/2018073], https://hal.archives-ouvertes.fr/hal-01668316

[24] V. M. CALO, M. CICUTTIN, Q. DENG, A. ERN. *Spectral approximation of elliptic operators by the Hybrid High-Order method*, in "Mathematics of Computation", 2019, vol. 88, n^{o} 318, pp. 1559-1586, https://hal.archives-ouvertes.fr/hal-01628698

[25] M. CICUTTIN, A. ERN, S. LEMAIRE. *A Hybrid High-Order method for highly oscillatory elliptic problems*, in "Computational Methods in Applied Mathematics", 2019, vol. 19, n^{o} 4, pp. 723-748 [*DOI :* 10.1515/CMAM-2018-0013], https://hal.archives-ouvertes.fr/hal-01467434

[26] P. DANIEL, A. ERN, M. VOHRALÍK. *An adaptive hp-refinement strategy with inexact solvers and computable guaranteed bound on the error reduction factor*, in "Computer Methods in Applied Mechanics and Engineering", November 2019, vol. 359, 112607 p. [*DOI :* 10.1016/J.CMA.2019.112607], https://hal.inria.fr/hal-01931448

[27] A. ERN, I. SMEARS, M. VOHRALÍK. *Equilibrated flux a posteriori error estimates in $L^2(H^1)$-norms for high-order discretizations of parabolic problems*, in "IMA Journal of Numerical Analysis", 2019, vol. 39, n^{o} 3, pp. 1158-1179 [*DOI :* 10.1093/IMANUM/DRY035], https://hal.inria.fr/hal-01489721

[28] A. ERN, M. VOHRALÍK. *Stable broken H1 and H(div) polynomial extensions for polynomial-degree-robust potential and flux reconstruction in three space dimensions*, in "Mathematics of Computation", October 2019 [*DOI :* 10.1090/MCOM/3482], https://hal.inria.fr/hal-01422204

[29] A. LEJAY, L. LENÔTRE, G. PICHOT. *An exponential timestepping algorithm for diffusion with discontinuous coefficients*, in "Journal of Computational Physics", November 2019, vol. 396, pp. 888-904 [*DOI :* 10.1016/J.JCP.2019.07.013], https://hal.inria.fr/hal-01806465

[30] A. LEJAY, L. LENÔTRE, G. PICHOT. *Analytic expressions of the solutions of advection-diffusion problems in 1D with discontinuous coefficients*, in "SIAM Journal on Applied Mathematics", September 2019, vol. 79, n° 5, pp. 1823-1849 [*DOI :* 10.1137/18M1164500], https://hal.inria.fr/hal-01644270

[31] G. MALLIK, M. VOHRALÍK, S. YOUSEF. *Goal-oriented a posteriori error estimation for conforming and nonconforming approximations with inexact solvers*, in "Journal of Computational and Applied Mathematics", August 2019, vol. 366, 112367 p. [*DOI :* 10.1016/J.CAM.2019.112367], https://hal.inria.fr/hal-01964733

[32] F. MARAZZATO, A. ERN, C. MARIOTTI, L. MONASSE. *An explicit pseudo-energy conserving time-integration scheme for Hamiltonian dynamics*, in "Computer Methods in Applied Mechanics and Engineering", April 2019, vol. 347, pp. 906-927 [*DOI :* 10.1016/J.CMA.2019.01.013], https://hal-enpc.archives-ouvertes.fr/hal-01661608

International Conferences with Proceedings

[33] E. BURMAN, A. ERN. *A cut-cell Hybrid High-Order method for elliptic problems with curved boundaries*, in "ENUMATH 2017", Bergen, Norway, EnuMath 2019 - European Numerical Mathematics and Advanced Applications Conference, 2019 [*DOI :* 10.1007/978-3-319-96415-7_14], https://hal.archives-ouvertes.fr/hal-01653685

[34] T. CHAUMONT-FRELET, A. ERN, M. VOHRALÍK. *Asymptotically constant-free, p-robust and guaranteed a posteriori error estimates for the Helmholtz equation*, in "EnuMath 2019 - European Numerical Mathematics and Advanced Applications Conference", Egmond aan Zee, Netherlands, September 2019, https://hal.inria.fr/hal-02321140

[35] M. CICUTTIN, A. ERN, S. LEMAIRE. *On the implementation of a multiscale Hybrid High-Order method*, in "ENUMATH 2017", Bergen, Norway, I. BERRE, K. KUMAR, J. M. NORDBOTTEN, I. S. POP, F. A. RADU (editors), Numerical Mathematics and Advanced Applications - ENUMATH 2017, Springer, Cham, 2019, vol. 126, pp. 509-517 [*DOI :* 10.1007/978-3-319-96415-7_46], https://hal.archives-ouvertes.fr/hal-01661925

[36] F. HÉDIN, G. PICHOT, A. ERN. *A hybrid high-order method for flow simulations in discrete fracture networks*, in "ENUMATH - European Numerical Mathematics and Advanced Applications Conference 2019", Egmond aan Zee, Netherlands, September 2019, https://hal.inria.fr/hal-02315491

Research Reports

[37] H. BARUCQ, H. CALANDRA, G. CHAVENT, F. FAUCHER. *A priori estimates of attraction basins for velocity model reconstruction by time-harmonic Full Waveform Inversion and Data Space Reflectivity formulation*, Magique 3D ; Inria Bordeaux Sud-Ouest ; Université de Pau et des Pays de l'Adour, February 2019, n° RR-9253, Material under review by journal Geophysics, https://hal.archives-ouvertes.fr/hal-02016373

Other Publications

[38] E. AHMED, C. JAPHET, M. KERN. *Space-time domain decomposition for two-phase flow between different rock types*, January 2020, working paper or preprint, https://hal.inria.fr/hal-02275690

[39] A. BENACEUR. *A time-dependent Parametrized Background Data-Weak approach*, October 2019, working paper or preprint, https://hal.archives-ouvertes.fr/hal-02330408

[40] A. BENACEUR. *An inexpensive Parametrized Background Data-Weak approach for time-dependent problems*, August 2019, working paper or preprint, https://hal.archives-ouvertes.fr/hal-02265533

[41] E. BURMAN, M. CICUTTIN, G. DELAY, A. ERN. *An unfitted Hybrid High-Order method with cell agglomeration for elliptic interface problems*, September 2019, working paper or preprint, https://hal.archives-ouvertes.fr/hal-02280426

[42] E. BURMAN, G. DELAY, A. ERN. *The unfitted HHO method for the Stokes problem on curved domains*, January 2020, working paper or preprint, https://hal.archives-ouvertes.fr/hal-02438622

[43] V. M. CALO, A. ERN, I. MUGA, S. ROJAS. *An adaptive stabilized conforming finite element method via residual minimization on dual discontinuous Galerkin norms*, 2019, https://arxiv.org/abs/1907.12605 - working paper or preprint, https://hal.archives-ouvertes.fr/hal-02196242

[44] E. CANCÈS, G. DUSSON, Y. MADAY, B. STAMM, M. VOHRALÍK. *Guaranteed a posteriori bounds for eigenvalues and eigenvectors: multiplicities and clusters*, May 2019, working paper or preprint, https://hal.archives-ouvertes.fr/hal-02127954

[45] E. CANCÈS, G. DUSSON, Y. MADAY, B. STAMM, M. VOHRALÍK. *Post-processing of the planewave approximation of Schrödinger equations. Part I: linear operators*, January 2020, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01908039

[46] C. CANCÈS, F. NABET, M. VOHRALÍK. *Convergence and a posteriori error analysis for energy-stable finite element approximations of degenerate parabolic equations*, January 2019, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01894884

[47] J.-P. CHANCELIER, S. FURIC, P. WEIS. *Translating Simulink Models to Modelica using the Nsp Platform*, February 2019, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01948681

[48] T. CHAUMONT-FRELET, A. ERN, M. VOHRALÍK. *On the derivation of guaranteed and p-robust a posteriori error estimates for the Helmholtz equation*, July 2019, working paper or preprint, https://hal.inria.fr/hal-02202233

[49] F. CHOULY, A. ERN, N. PIGNET. *A Hybrid High-Order discretization combined with Nitsche's method for contact and Tresca friction in small strain elasticity*, September 2019, working paper or preprint, https://hal.archives-ouvertes.fr/hal-02283418

[50] M. CICUTTIN, A. ERN, T. GUDI. *Hybrid high-order methods for the elliptic obstacle problem*, May 2019, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01718883

[51] J. DABAGHI, V. MARTIN, M. VOHRALÍK. *A posteriori estimates distinguishing the error components and adaptive stopping criteria for numerical approximations of parabolic variational inequalities*, August 2019, working paper or preprint, https://hal.archives-ouvertes.fr/hal-02274493

[52] J. ERHEL, M. OUMOUNI, G. PICHOT, F. SCHOEFS. *Analysis of continuous spectral method for sampling stationary Gaussian random fields*, April 2019, working paper or preprint, https://hal.archives-ouvertes.fr/hal-02109037

[53] A. ERN, T. GUDI, I. SMEARS, M. VOHRALÍK. *Equivalence of local-and global-best approximations, a simple stable local commuting projector, and optimal hp approximation estimates in H(div)*, August 2019, https://arxiv.org/abs/1908.08158 - working paper or preprint, https://hal.inria.fr/hal-02268960

[54] A. ERN, M. VOHRALÍK, M. ZAKERZADEH. *Guaranteed and robust L^2-norm a posteriori error estimates for 1D linear advection problems*, April 2019, working paper or preprint, https://hal.archives-ouvertes.fr/hal-02105418

[55] A. ERN, P. ZANOTTI. *A quasi-optimal variant of the hybrid high-order method for elliptic PDEs with H^{-1} loads*, April 2019, working paper or preprint, https://hal.archives-ouvertes.fr/hal-02114715

[56] F. MARAZZATO, A. ERN, L. MONASSE. *A consistent discrete element method for quasi-static and dynamic elasto-plasticity*, November 2019, https://arxiv.org/abs/1911.00738 - working paper or preprint, https://hal.archives-ouvertes.fr/hal-02343280

[57] R. MILANI, J. BONELLE, A. ERN. *Compatible Discrete Operator schemes for the steady incompressible Stokes and Navier-Stokes equations*, December 2019, working paper or preprint, https://hal.archives-ouvertes.fr/hal-02417514

[58] A. MIRAÇI, J. PAPEŽ, M. VOHRALÍK. *A multilevel algebraic error estimator and the corresponding iterative solver with p-robust behavior*, July 2019, working paper or preprint, https://hal.archives-ouvertes.fr/hal-02070981

[59] J. PAPEŽ, U. RÜDE, M. VOHRALÍK, B. WOHLMUTH. *Sharp algebraic and total a posteriori error bounds for h and p finite elements via a multilevel approach. Recovering mass balance in any situation*, December 2019, working paper or preprint, https://hal.inria.fr/hal-01662944

[60] J. PAPEŽ, M. VOHRALÍK. *Inexpensive guaranteed and efficient upper bounds on the algebraic error in finite element discretizations*, January 2020, working paper or preprint, https://hal.inria.fr/hal-02422851