

Activity Report 2018

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.	eam, Visitors, External Collaborators	<u>1</u>			
2.	Overall Objectives	2			
3.	Research Program				
	.1. Multiphysics coupling	3			
	.2. Structure-preserving discretizations and discrete element methods	3			
	.3. Domain decomposition and Newton–Krylov (multigrid) solvers	3			
	.4. Reliability by a posteriori error control	4			
	.5. Safe and correct programming	4			
4.	Application Domains				
	.1. Multiphase flows and transport of contaminants in the subsurface	4			
	.2. Industrial risks in energy production	4			
	.3. Computational quantum chemistry	4			
5.	Highlights of the Year				
6.	New Software and Platforms				
	.1. CELIA3D	5			
	.2. DiSk++	5			
	.3. GENFIELD	6			
	.4. Mka3d	6			
	5.5. NEF-Draw	6			
	.6. NEF-Flow	6			
	7.7. ParaCirce	7			
	.8. PRune	7			
7.	ew Results				
•	.1. Unfitted hybrid-high-order methods	7			
	2. An exponential time stepping scheme for the simulation of diffusion processes	8			
	3. Localization of dual and distance norms	8			
	.4. Adaptivity with guaranteed error contraction	8			
8.	ilateral Contracts and Grants with Industry				
	artnerships and Cooperations				
<i>)</i> .	1.1. Regional Initiatives	9			
	2. National Initiatives	9			
	2.3. European Initiatives	ç			
	9.3.1. FP7 & H2020 Projects	ç			
	9.3.2. Collaborations in European Programs, Except FP7 & H2020	10			
	9.5.2. Conaborations in European Flograms, Except FF / & H2020	10			
	9.4.1. Inria International Partners	10			
	9.4.2. Participation in Other International Programs 5.5. International Research Visitors	10			
		11			
	9.5.1. Visits of International Scientists	11			
10	9.5.2. Visits to International Teams	11			
10.	Dissemination				
	0.1. Promoting Scientific Activities	11			
	10.1.1. Scientific Events Organisation	11			
	10.1.1.1. General Chair, Scientific Chair	11			
	10.1.1.2. Member of the Organizing Committees	11			
	10.1.2. Scientific Events Selection	11			
	10.1.3. Journal	12			
	10.1.3.1. Member of the Editorial Boards	12			
	10.1.3.2. Reviewer - Reviewing Activities	12			

10.1.4. Invited Talks	12
10.1.5. Leadership within the Scientific Community	12
10.1.6. Scientific Expertise	12
10.1.7. Research Administration	12
10.2. Teaching - Supervision - Juries	13
10.2.1. Teaching	13
10.2.2. Supervision	13
10.2.3. Juries	13
10.3. Popularization	14
11. Bibliography	

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]

Michel Kern [Inria, Researcher]

Géraldine Pichot [Inria, Researcher]

Pierre Weis [Inria, Senior Researcher]

Post-Doctoral Fellows

Sarah Ali Hassan [Inria, from Apr 2018 until Aug 2018]

Matteo Cicuttin [Ecole Nationale des Ponts et Chaussées, until Apr 2018]

Théophile Chaumont-Frelet [Ecole Nationale des Ponts et Chaussées, from Feb to Sep 2018]

Guillaume Delay [Ecole Nationale des Ponts et Chaussées, from Sep 2018]

Kenan Kergrene Profit [Inria, from Dec 2018]

Seyed Mohammad Zakerzadeh [Inria]

PhD Students

Amina Benaceur [EDF]

Karol Cascavita [Univ Paris-Est]

Jad Dabaghi [Inria]

Patrik Daniel [Inria]

Frédéric Marazzato [CEA]

Riccardo Milani [EDF]

Ani Miraci [Inria]

Nicolas Pignet [EDF]

Technical staff

Sébastien Furic [Inria]

Florent Hedin [Inria, from Dec 2018]

Simon Legrand [Inria]

Intern

Intissar Addali [Inria, from May 2018 until Aug 2018]

Administrative Assistants

Virginie Collette [Inria, until Oct 2018]

Meriem Henni [Inria, from Apr 2018 until Aug 2018]

Derya Gök [Inria, from Nov 2018]

Visiting Scientists

Carsten Carstensen [Humboldt University, Berlin, from Aug to Sep 2018, HDR]

Thirupathi Gudi [Indian Institute of Science, Bangalore, from Jan to Feb 2018, HDR]

Jean-Luc Guermond [Texas A&M University, from May 2018 until Jun 2018, HDR]

Christian Kreuzer [University College London, Jun 2018, HDR]

Iain Smears [University College London, Mar and Jun 2018]

External Collaborators

Hend Ben Ameur [IPEST and ENIT-Lamsin (Tunisia), Professor, HDR]

Guy Chavent [Univ Paris-Dauphine, Professor (retired), HDR]

Jérôme Jaffré [Inria, Senior Researcher (retired), HDR]

Caroline Japhet [Univ Paris-Nord, Associate Professor]

Antoine Lejay [Inria, Senior Researcher, HDR]

Lionel Lenôtre [Univ de Lorraine, IECL, Post-Doctoral Fellow]

Vincent Martin [Univ de technologie de Compiègne, Associate Professor]

Jean-Elizabeth Roberts [Inria, Senior Researcher (retired), HDR]

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.

3.2. Structure-preserving discretizations 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 requirement is to derive *structure-preserving* methods, i.e., methods that mimic algebraically at the discrete level fundamental properties of the underlying PDEs, such as conservation principles and preservation of invariants. Here, the theoretical questions are closely linked to *differential geometry* and we apply them to the Navier–Stokes equations and to elasto-plasticity. 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 begun this year.

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 spacetime 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. This in particular yields 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.

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 shall also prove the numerical optimality of the derived algorithms 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
- reduced-order models for valves related to nuclear reactor operation
- plasticity and large deformations for mechanical components related to nuclear reactor operation
- seismic wave propagation for detection and protection
- electromagnetism for interfaces between dielectrics and negative metamaterials

4.3. 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

Alexandre Ern co-edited with Daniele Di Pietro (Montpellier) and Luca Formaggia (Milano) a book on Numerical Methods for PDEs, SEMA SIMAI Springer Series, Vol. 15, Springer, 2018. ISBN 978-3-319-94675-7.

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++

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 CicuttinPartner: CERMICSContact: Matteo Cicuttin

 Publication: Implementation of Discontinuous Skeletal methods on arbitrary-dimensional, polytopal meshes using generic programming

• URL: https://github.com/wareHHOuse/diskpp

6.3. GENFIELD

KEYWORDS: Hydrogeology - Algorithm - Heterogeneity

SCIENTIFIC DESCRIPTION: GENFIELD implements a parallel version of the algorithm initially proposed by [E. Pardo-Iguzquiza and M. Chica-Olmo, Mathematical Geology, 25(2):177-217, 1993].

FUNCTIONAL DESCRIPTION: GENFIELD allows the generation of gaussian correlated fields. It is based on the circulant embedding method. Parallelism is implemented using MPI communications. GENFIELD is used in hydrogeology to model natural fields, like hydraulic conductivity or porosity fields.

NEWS OF THE YEAR: In 2018, we have performed scaling tests on ADA cluster. They have revealed that the symmetry of the phases required by this algorithm penalized a lot the parallel efficiency of GENFIELD (cf poster hal-01960444, version 1). We have decided to stop the development of GENFIELD. In 2018, we have developed a complete new software (cf BIL Inria ParaCIRCE) based on another algorithm initially 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].

- Participants: Géraldine Pichot, Simon Legrand, Grégoire Lecourt, Jean-Raynald De Dreuzy and Jocelyne Erhel
- Contact: Géraldine Pichot
- Publications: GENFIELD: A parallel software for the generation of stationary Gaussian random fields Algorithms for stationary Gaussian random field generation
- URL: https://gitlab.inria.fr/slegrand/Genfield_dev

6.4. Mka3d

KEYWORDS: Scientific computing - Elasticity - Elastodynamic equations

FUNCTIONAL DESCRIPTION: The Mka3d method simulates an elastic solid by discretizing the solid into rigid particles. An adequate choice of forces and torques between particles allows to recover the equations of elastodynamics.

Partners: Ecole des Ponts ParisTech - CEA

• Contact: Laurent Monasse

• URL: http://cermics.enpc.fr/~monassel/Mka3D/

6.5. NEF-Draw

Numerical Experiments involving Fractures -Visualisation

KEYWORD: Fracture network

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: This version includes Matlab vectorization of the operations which makes it possible to load flow solution on meshes with more than one million of 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, loading only the fractures that carry most of the flow.

Participant: Géraldine PichotContact: Géraldine Pichot

• URL: https://gitlab.inria.fr/gpichot/NEF

6.6. 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.

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 feature: - wells, sink/source terms boundary conditions - Implementation of P1 non conforming finite elements - New data structures to save the information local to each fracture - New tests per fracture have been added to check the solution - Add wells and sink/sources boundary conditions in the function that check the solution.

- 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

6.7. ParaCirce

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].

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

NEWS OF THE YEAR: - MPI implementation - Dedicated C++ classes to allow a user-friendly and safe usage of the library - Efficient use of the external library RngStream (L'Ecuyer) for a guarantee of independent realizations and reproductibility. - Splitting of the domain along one direction. The repartition of the field is automatic or defined by the user. - Automatic computation of the padding

- Participants: Géraldine Pichot and Simon Legrand
- Contact: Géraldine Pichot
- URL: https://gitlab.inria.fr/slegrand/paracirce

6.8. PRune

ParserRUNnEr KEYWORD: Test

FUNCTIONAL DESCRIPTION: Python tool to parse single or multi configurations parameters files and to automatically run a program and store the results in a predefined tree.

- Participants: Simon Legrand and Géraldine Pichot
- Contact: Simon Legrand

7. New Results

7.1. Unfitted hybrid-high-order methods

Participants: Alexandre Ern, Guillaume Delay.

Our team contributes actively to the development of hybrid high-order (HHO) methods. Such methods support polyhedral meshes with hanging nodes, but one requirement is that the mesh cells have planar faces. This is difficult when it comes to solving with high accuracy a problem posed on a domain with curved boundaries or a problem involving a curved interface separating two materials with different properties. One key idea to treat these problems is to use an unfitted mesh, so that the curved boundary or the curved interface freely cuts through the mesh cells. This greatly simplifies the meshing process, but at the same time poses the question on how the HHO method can address the approximation of functions that are not smooth within some mesh cells. The major idea in our approach, which is inspired from similar approaches developed in the context of the more classical finite element method, is to double the discrete unknowns attached to the cut mesh faces and to introduce a consistent Nitsche-type formulation to enforce either the boundary condition or the jump conditions across the interface in a weak manner. In this context, we started a collaboration with Erik Burman (University College London) and we elaborated in [20] the numerical analysis of HHO methods in an unfitted context; further analysis for Stokes and Helmholtz equations has started recently within the postdoc of Guillaume Delay and a collaboration on the subject with CEA is on the way.

7.2. An exponential time stepping scheme for the simulation of diffusion processes

Participant: Géraldine Pichot.

We present in [56] 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.

7.3. Localization of dual and distance norms

Participants: Martin Vohralík, Patrick Ciarlet Jr., Jan Blechta, Josef Málek.

Dual norms like the dual norm of the residual and the distance norm to the Sobolev space H_0^1 seem to be fundamentally global over the entire computational domain. In [23], together with P. Ciarlet, we prove, in extension of some older results, that they are both equivalent to the Hilbertian sums of their localizations over patches of elements. Together with J. Blechta and J. Málek, we extend in [45] this result from the space H_0^1 with Hilbertian structure to the Sobolev space $H_0^{1,p}$, with the exponent P_0^1 bigger than or equal to one, and to an arbitrary bounded linear functional on $H_0^{1,p}$.

7.4. Adaptivity with guaranteed error contraction

Participants: Martin Vohralík, Alexandre Ern, Patrik Daniel, Iain Smears.

In [26], we conceive novel adaptive refinement strategies which automatically decide between mesh refinement and polynomial degree increase. We numerically observe that the error decreases exponentially as a function of the number of degrees of freedom, for smooth as well as for singular numerical solutions. The salient feature of our approach is, however, that we ensure that the error on the next hp-refinement step will be reduced at least by a factor that is given. We then extend in [53] this result to the case where the underlying algebraic solver is inexact. To the best of our knowledge, these results, obtained in the framework of the Ph.D. thesis of Patrik Daniel, is the first ever where such an error contraction bound is computable and guaranteed. Numerically, its precision turns out to be very high (overestimation by a factor very close to the optimal value of one). It immediately implies convergence of the adaptive method, and we would like to use it in the near future for optimality proofs.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

Three two-part contracts with EDF accompanying the PhD theses of Amina Benaceur, Nicolas Pignet, and Riccardo Milani.

Two two-part contract with CEA accompanying the PhD thesis of Frédéric Marazzato and the postdoc of Guillaume Delay.

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

AMIES NEF-PEPS1 (Dec. 2018–Feb. 2020) Collaboration with the joint laboratory LabCom fractory (ITASCA, Géosciences Rennes). SERENA representants are F. Clément, Sébastien Furic, Florent Hédin, M. Kern and G. Pichot (Coordinator).

Two-part contract with IFP Energies Nouvelles for co-supervision of the post-doc of G. Mallik.

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. National Initiatives

9.2.1. ANR

ANR HHOMM: "Hybrid high-order methods on polyhedral meshes", Theoretical foundations and applications (up to software development) for the recently-devised Hybrid high-order methods. Coordinated by D. Di Pietro, University of Montpellier. SERENA representant is A. Ern, period 2015–2019.

ANR DEDALES: "Algebraic and geometric domain decomposition for subsurface flow". The project aims at developing high performance software for the simulation of two phase flow in porous media. It specifically targets parallel computers where each node is itself composed of a large number of processing cores, such as are found in new generation many-core architectures.

The partners are HIEPACS, Laboratoire Analyse, Géométrie et Application, University Paris 13, Maison de la Simulation, and ANDRA. SERENA representants are M. Kern (grant leader) and M. Vohralík, period 2014–2018. The project ended in October 2018.

9.3. European Initiatives

9.3.1. FP7 & H2020 Projects

• EoCoE: "Energy Oriented Center of Excellence" This project is coordinated by Maison de la Simulation and gathers 23 partners from 13 countries to use the tremendous potential offered by the ever-growing computing infrastructure to foster and accelerate the European transition to a reliable low carbon energy supply using HPC (High Performance Computing). SERENA representant M. Kern, period 2015–2018.

- 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), period 2015–2020.
- PRACE: "Partnership for Advanced Computing in Europe" The mission of PRACE is to enable high-impact scientific discovery and engineering research and development across all disciplines to enhance European competitiveness for the benefit of society. PRACE has an extensive education and training effort for effective use of the Research Infrastructure. M. Kern is the French representative for training, and is in charge of the French node of the Prace training network, organizing 10-12 courses each year (period 2017-2019).

9.3.2. Collaborations in European Programs, Except FP7 & H2020

OPENCPS

Program: ITEA 3

Project acronym: OPENCPS

Project title: Open cyber-physical system model-driven certified development

Duration: Dec 2015–Dec 2018 Coordinator: Magnus Eek

Other partners: AB SKF, CEA, ELTE-Soft Kft., ESI Group, EDF, Wqua Simulation AB, Ericsson, IncQuery Labs Kft., KTH, Linköping University, RTE, SICS, SIREHNA, Saab AB, Sherpa Engineering, Siemens Industrial Torbumachinery AB, VTT Technical Research Center of Finland Ltd.

Abstract: Cyber-physical systems put increasing demands on reliability, usability, and flexibility while, at the same time, lead time and cost efficiency are essential for industry competitiveness. Tools and environments for model-based development of cyber-physical systems are becoming increasingly complex and critical for the industry: tool interoperability, vendor lock-ins, and tool life-cycle support are some of the challenges. The project focuses on interoperability between the standards Modelica/UML/FMI, improved execution speed of (co-)simulation, and certified code generation.

SERENA representants are Sébastien Furic and Pierre Weis.

9.4. International Initiatives

9.4.1. Inria International Partners

9.4.1.1. Informal International Partners

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

Jean-Luc Guermond, Professor at Texas A&M University, USA, finite element methods.

Ulrich Rüde, Professor at Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany, multigrid methods.

Mary Wheeler, professor, University of Texas at Austin, USA, porous media applications.

Barbara Wohlmuth, Professor at Technical University of München, Germany, mixed finite element methods.

9.4.2. Participation in Other International Programs

Alexandre Ern participated for two weeks in Jul 2018 as an invited scientist in the ESI Program on Numerical Analysis on Complex PDE in the Sciences, Vienna, Austria (https://www.esi.ac.at/activities/events/2018/numerical-analysis-of-complex-pde-models-in-the-sciences).

9.5. International Research Visitors

9.5.1. Visits of International Scientists

Iain Smears, lecturer at University College London, March 26–30.

Thirupathi Gudi, Professor at Indian Institute of Science, Bangalore, India, January 15-February 28.

Jean-Luc Guermond, Professor at Texas A&M University, College Station, Texas, May 1-June 15.

Iain Smears, lecturer at University College London, June 18–27, and Christian Kreuzer, Professor at University Dortmund, June 18–29.

Carsten Carstensen, Professor at Humboldt University, Berlin, August 20-September 20.

Roland Becker, Professor at University of Pau, September 17–20.

Hend Ben Ameur, Professor at IPEST and member of ENIT-Lamsin, Tunis, Tunisia, November 19-30.

Théophile Chaumont-Frelet, junior researcher at Inria Sophia Antipolis, November 22–23.

9.5.1.1. Internships

Intissar Addali, 2nd year internship at ENSTA ParisTech, from May to Aug 2018, supervised by Karol Cascavita and Alexandre Ern.

9.5.2. Visits to International Teams

9.5.2.1. Research Stays Abroad

Alexandre Ern visited the research group of Prof. Victor Calo, Curtin University, Perth, Australia, in November 2018.

Martin Vohralík was invited for two weeks stay to Charles University, Prague for collaboration with J. Málek, April 2018.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

10.1.1.1. General Chair, Scientific Chair

Géraldine Pichot was the co-chair of the Computational Methods in Water Resources 2018 conference.

Ibtihel Ben Gharbia and Martin Vohralík have organized a 1-day workshop Journée contrat cadre IFP Energies Nouvelles/Inria.

10.1.1.2. Member of the Organizing Committees

Michel Kern was the member of the local organizing committee of the Computational Methods in Water Resources 2018 conference.

10.1.2. Scientific Events Selection

10.1.2.1. Member of the Conference Program Committees

Alexandre Ern is a member of the Scientific Committee for the European Finite Element Fair.

Michel Kern was a member of the program committee for the JCAD 2018 (Journées Calcul et Données, Lyon October 2018).

Géraldine Pichot co-organized a mini-symposium, entitled "Numerical methods for processes in fractured media" at the InterPore 2018 - 10th Annual Meeting and Jubilee, New Orleans, United States, June 2018.

10.1.3. Journal

10.1.3.1. Member of the Editorial Boards

François Clément was a member of the editorial board of Matapli until June 2018.

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 served as reviewer for dozens of papers in different journals.

Michel Kern was a reviewer for OGST, BIT, Mathematics and Computers in Simulation, Computers and Geosciences.

Martin Vohralík served as reviewer for dozens of papers in different journals.

10.1.4. Invited Talks

Alexandre Ern gave an invited lecture at the BAIL 2018 conference in Glasgow (*International conference on Boundary and Interior Layers*).

Géraldine Pichot was an invited speaker at the InterPore 2018 - 10th Annual Meeting and Jubilee, New Orleans, United States, June 2018 and at the Workshop Reactive Flows in Deformable, Complex Media, Oberwolfach, Germany, August 2018.

Martin Vohralík was an invited speaker at the workshop FEEC and High Order Methods, Oslo, Norway, the Seventh Conference on Finite Difference Methods: Theory and Applications, Lozenetz, Bulgaria, and the Workshop Reactive Flows in Deformable, Complex Media, Oberwolfach, Germany, August 2018.

10.1.5. Leadership within the Scientific Community

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

M. Kern is a member of the Scientific Committee of Orap (ORganisation Associative du Parallélisme), of the steering committee of Géosciences franciliennes of the Scientific Board of GDR Calcul, and of the jury and executive board of Label C3I.

M. Vohralík is a member of the steering committees of Géosciences franciliennes and Summer schools CEA-EDF-Inria.

M. 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. Scientific Expertise

M. Kern is a reviewer for the German Supercomputing Center JARA program.

10.1.7. 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.

François Clément was the *AMIES facilitator* of the Inria Research Center of Paris until June 2018.

M. Kern is Deputy Director of Maison de la Simulation, a joint project between CEA, CNRS, Inria, Université de Paris 11, and Université de Versailles, focused on applications of high end computing.

M. Kern is a member of the *Comité de site* of the Inria center of Paris.

Géraldine Pichot was a member of the *Comité local d'hygiène, de sécurité et des conditions de travail* of the Inria Research Center of Paris until Sep 2018.

Géraldine Pichot was a member of the *Commission de développement technologique* of the Inria Research Center of Paris until March 2018.

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, Optimal Control, 20h, L3, Ecole Polytechnique, France.

Licence : Alexandre Ern, Partial differential equations, 10h, L3, Ecole nationale des ponts et chaussées, France.

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

Master: Michel Kern, Inverse Problems, 26h, M1, Mines-ParisTech, France

Master: Michel Kern, Advanced Numerical Analysis, 30h, M2, Institut Galilée, Université Paris 13, France

Master: Michel Kern, Subsurface flows, 30h (with E. Mouche), M2, Université Paris Saclay, France

Master: Martin Vohralík, A posteriori error estimates for efficiency and error control in numerical simulations, 36h, M2, Charles University, Prague, Czech Republic.

10.2.2. Supervision

PhD: Amina Benaceur, Model reduction for nonlinear thermics and mechanics, 21 Dec 2018, Alexandre Ern.

PhD: Karol Cascavita, Hybrid discretization methods for Signorini contact and Bingham flow problems, 18 Dec 2018, Alexandre Ern and Xavier Chateau.

PhD in progress: Jad Dabaghi, A posteriori error estimates and adaptive stopping criteria for formulations with complementarity constraints, 01 November 2015, Martin Vohralík and Vincent Martin.

PhD in progress: Patrik Daniel, Adaptive *hp*-finite elements with guaranteed error contraction and inexact multilevel solvers, 01 October 2015, Martin Vohralík and Alexandre Ern.

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

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

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

PhD in progress: Nicolas Pignet, Hybrid High-Order methods for nonlinear mechanics, 01 November 2016, Alexandre Ern.

10.2.3. Juries

Alexandre Ern, Referee, PhD A. Bensalah, ENSTA ParisTech, Jul 2018.

Alexandre Ern, Examiner, PhD G. Morel, Sorbonne University, Sep 2018.

Alexandre Ern, Referee, PhD P. Vega, University of Concepcion, Chile, Nov 2018.

Alexandre Ern, Referee, PhD G. Pennesi, Politecnico Milano, Italy, Dec 2018.

Michel Kern, Examiner, HDR J. Carrayrou, University of Strasbourg, 21 March 2018.

Martin Vohralík, Referee, PhD O. Gorynina, Université de Bourgogne Franche-Comté, Besançon, Feb 2018.

Martin Vohralík, Examiner, PhD M. Botti, Université de Montpellier, Nov 2018.

10.3. Popularization

10.3.1. Interventions

- M. Kern: présentation "Des mathématiques pour modéliser et simuler le monde", Lycée des Pierres-Vives (Terminale S), Carrières-sur-Seine, May 2018.
- M. Vohralík: "Advancing scientific knowledge together to support innovation", dissemination video, IFP Energies Nouvelles. Available here. February 2018.

Major publications by the team in recent years:

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, no 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, no 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, no 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.
- [5] A. ERN, J.-L. GUERMOND. Finite element quasi-interpolation and best approximation, in "ESAIM Math. Model. Numer. Anal.", 2017, vol. 51, no 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, no 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^o 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, no 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^o 1, pp. B86–B105, http://dx.doi.org/10.1137/100804383

Publications of the year

Doctoral Dissertations and Habilitation Theses

[11] A. BENACEUR. *Réduction de modèles en thermique et mécanique non-linéaires*, Université Paris-Est Marne la Vallée, December 2018, https://hal.archives-ouvertes.fr/tel-01958278

Articles in International Peer-Reviewed Journals

- [12] M. ABBAS, A. ERN, N. PIGNET. *Hybrid High-Order methods for finite deformations of hyperelastic materials*, in "Computational Mechanics", January 2018, vol. 62, n^o 4, pp. 909-928 [*DOI*: 10.1007/s00466-018-1538-0], https://hal.archives-ouvertes.fr/hal-01575370
- [13] 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.archivesouvertes.fr/hal-01768411
- [14] E. AHMED, A. BEN ABDA. *The sub-Cauchy Stokes Problem: Solvability Issues and Lagrange Multiplier Methods with Artificial Boundary Conditions*, in "Journal of Computational and Applied Mathematics", January 2018, https://hal.archives-ouvertes.fr/hal-01467425
- [15] S. ALI HASSAN, C. JAPHET, M. KERN, M. VOHRALÍK. A posteriori stopping criteria for optimized Schwarz domain decomposition algorithms in mixed formulations, in "Computational Methods in Applied Mathematics", June 2018, vol. 18, n^o 3, pp. 495-519 [DOI: 10.1515/CMAM-2018-0010], https://hal.inria.fr/hal-01529532
- [16] S. ALI HASSAN, C. JAPHET, M. VOHRALÍK. A posteriori stopping criteria for space-time domain decomposition for the heat equation in mixed formulations, in "Electronic Transactions on Numerical Analysis", 2018, vol. 49, pp. 151–181, [DOI: 10.1553/ETNA_VOL49s151], https://hal.inria.fr/hal-01586862
- [17] L. AMIR, M. KERN. *Preconditioning a coupled model for reactive transport in porous media*, in "International Journal of Numerical Analysis and Modeling", 2018, vol. 16, n^o 1, pp. 1-30, https://arxiv.org/abs/1710.01483, https://hal.inria.fr/hal-01327307
- [18] H. BEN AMEUR, G. CHAVENT, F. CHEIKH, F. CLÉMENT, V. MARTIN, J. E. ROBERTS. First-order indicators for the estimation of discrete fractures in porous media, in "Inverse Problems in Science and Engineering", 2018, vol. 26, n^o 1, pp. 1–32, https://arxiv.org/abs/1602.08304 [DOI: 10.1080/17415977.2017.1290087], https://hal.inria.fr/hal-01279503

- [19] A. BENACEUR, V. EHRLACHER, A. ERN, S. MEUNIER. A progressive reduced basis/empirical interpolation method for nonlinear parabolic problems, in "SIAM Journal on Scientific Computing", 2018, vol. 40, n^o 5, pp. A2930-A2955, https://arxiv.org/abs/1710.00511, https://hal.archives-ouvertes.fr/hal-01599304
- [20] E. BURMAN, A. ERN. An unfitted Hybrid High-Order method for elliptic interface problems, in "SIAM Journal on Numerical Analysis", 2018, vol. 56, no 3, pp. 1525-1546, https://hal.archives-ouvertes.fr/hal-01625421
- [21] E. CANCÈS, G. DUSSON, Y. MADAY, B. STAMM, M. VOHRALÍK. Guaranteed and robust a posteriori bounds for Laplace eigenvalues and eigenvectors: a unified framework, in "Numerische Mathematik", July 2018, vol. 140, no 4, pp. 1033-1079 [DOI: 10.1007/s00211-018-0984-0], https://hal.inria.fr/hal-01483461
- [22] K. L. CASCAVITA, J. BLEYER, X. CHATEAU, A. ERN. *Hybrid discretization methods with adaptive yield surface detection for Bingham pipe flows*, in "Journal of Scientific Computing", June 2018, vol. 77, n^o 3, pp. 1424-1443 [DOI: 10.1007/s10915-018-0745-3], https://hal.archives-ouvertes.fr/hal-01698983
- [23] P. CIARLET, M. VOHRALÍK. Localization of global norms and robust a posteriori error control for transmission problems with sign-changing coefficients, in "Modelisation Mathématique et Analyse Numérique", December 2018, vol. 52, n^o 5, pp. 2037-2064 [DOI: 10.1051/M2AN/2018034], https://hal.inria.fr/hal-01148476
- [24] M. CICUTTIN, D. A. DI PIETRO, A. ERN. Implementation of Discontinuous Skeletal methods on arbitrary-dimensional, polytopal meshes using generic programming, in "Journal of Computational and Applied Mathematics", 2018, vol. 344, pp. 852–874 [DOI: 10.1016/J.CAM.2017.09.017], https://hal.archives-ouvertes.fr/hal-01429292
- [25] M. CICUTTIN, A. ERN, S. LEMAIRE. A Hybrid High-Order method for highly oscillatory elliptic problems, in "Computational Methods in Applied Mathematics", 2018 [DOI: 10.1515/CMAM-2018-0013], https://hal.archives-ouvertes.fr/hal-01467434
- [26] P. DANIEL, A. ERN, I. SMEARS, M. VOHRALÍK. *An adaptive hp-refinement strategy with computable guar-anteed bound on the error reduction factor*, in "Computers and Mathematics with Applications", September 2018, vol. 76, n^o 5, pp. 967-983, https://arxiv.org/abs/1712.09821 [DOI: 10.1016/J.CAMWA.2018.05.034], https://hal.inria.fr/hal-01666763
- [27] A. ERN, J.-L. GUERMOND. Abstract nonconforming error estimates and application to boundary penalty methods for diffusion equations and time-harmonic Maxwell's equations, in "Computational Methods in Applied Mathematics", 2018, vol. 18, no 3, pp. 451-475 [DOI: 10.1515/CMAM-2017-0058], https://hal.archives-ouvertes.fr/hal-01563594
- [28] 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", June 2018 [DOI: 10.1093/IMANUM/DRY035], https://hal.inria.fr/hal-01489721
- [29] M. KÖPPEL, V. MARTIN, J. JAFFRÉ, J. E. ROBERTS. A Lagrange multiplier method for a discrete fracture model for flow in porous media, in "Computational Geosciences", September 2018, https://hal.archives-ouvertes.fr/hal-01700663

[30] F. MARAZZATO, A. ERN, C. MARIOTTI, L. MONASSE. An explicit pseudo-energy conserving timeintegration scheme for Hamiltonian dynamics, in "Computer Methods in Applied Mechanics and Engineering", 2019 [DOI: 10.1016/J.CMA.2019.01.013], https://hal-enpc.archives-ouvertes.fr/hal-01661608

- [31] J. PAPEŽ, Z. STRAKOŠ, M. VOHRALÍK. *Estimating and localizing the algebraic and total numerical errors using flux reconstructions*, in "Numerische Mathematik", February 2018, vol. 138, n^o 3, pp. 681-721 [DOI: 10.1007/s00211-017-0915-5], https://hal.inria.fr/hal-01312430
- [32] M. VOHRALÍK, S. YOUSEF. A simple a posteriori estimate on general polytopal meshes with applications to complex porous media flows, in "Computer Methods in Applied Mechanics and Engineering", April 2018, vol. 331, pp. 728-760 [DOI: 10.1016/J.CMA.2017.11.027], https://hal.archives-ouvertes.fr/hal-01532195
- [33] M. ČERMÁK, F. HECHT, Z. TANG, M. VOHRALÍK. Adaptive inexact iterative algorithms based on polynomial-degree-robust a posteriori estimates for the Stokes problem, in "Numerische Mathematik", February 2018, vol. 138, n^o 4, pp. 1027-1065 [DOI: 10.1007/s00211-017-0925-3], https://hal.inria.fr/hal-01097662

Invited Conferences

- [34] H. BARUCQ, H. CALANDRA, G. CHAVENT, F. FAUCHER. Stability and convergence analysis for seismic depth imaging using FWI, in "Reconstruction Methods for Inverse Problems", Rome, Italy, Reconstruction Methods for Inverse Problems, May 2018, https://hal.archives-ouvertes.fr/hal-01807980
- [35] G. PICHOT, P. LAUG, J. ERHEL, R. LE GOC, C. DARCEL, P. DAVY, J.-R. DE DREUZY. *Flow simulations in geology-based Discrete Fracture Networks*, in "2018 Reactive Flows in Deformable, Complex Media", Oberwolfach, Germany, August 2018, pp. 1-3, https://hal.inria.fr/hal-01900605
- [36] G. PICHOT, P. LAUG, R. LE GOC, C. DARCEL, P. DAVY, J.-R. DE DREUZY. *Computation of flow properties of large scale fractured media*, in "InterPore 2018 10th Annual Meeting and Jubilee", New Orleans, United States, June 2018, https://hal.inria.fr/hal-01900599

International Conferences with Proceedings

[37] S. LOPEZ, R. MASSON, L. BEAUDE, N. BIRGLE, K. BRENNER, M. KERN, F. SMAÏ, F. XING. *Geothermal Modeling in Complex Geological Systems with the ComPASS Code*, in "Stanford Geothermal Workshop 2018 - 43rd Workshop on Geothermal Reservoir Engineering", Stanford, United States, Stanford University, February 2018, https://hal-brgm.archives-ouvertes.fr/hal-01667379

Conferences without Proceedings

- [38] P. LAUG, G. PICHOT, R. LE GOC, C. DARCEL, P. DAVY. Automatic meshing of Discrete Fracture Networks, in "Computational Methods in Water Resources XXII (CMWR 2018)", Saint-Malo, France, June 2018, https:// hal.inria.fr/hal-01896927
- [39] P. LAUG, G. PICHOT. Simulations in large tridimensional Discrete Fracture Networks (DFN): I. Geometric modeling and mesh generation, in "MASCOT 2018 15th IMACS/ISGG meeting on applied scientific computing and tools", Rome, Italy, October 2018, pp. 1-2, https://hal.inria.fr/hal-01896881

- [40] A. LEJAY, G. PICHOT, L. LENÔTRE. Diffusion processes in discontinuous media: numerical algorithms and benchmark tests, in "Workshop Validation approaches for multiscale porous media models", Nottingham, United Kingdom, July 2018, https://hal.inria.fr/hal-01900609
- [41] S. LOPEZ, R. MASSON, F. XING, L. BEAUDE, F. SMAÏ, M. KERN, A. ARMANDINE LES LANDES, G. AMIEZI, K. BRENNER, G. COURRIOUX, S. CARITG-MONNOT. *Modélisation hydrothermale des systèmes géothermiques profonds fracturés avec le code ComPASS*, in "26ème Réunion des Sciences de la Terre RST", Lille, France, October 2018, https://hal-brgm.archives-ouvertes.fr/hal-01890182
- [42] G. PICHOT, P. LAUG, J. ERHEL, R. LE GOC, C. DARCEL, P. DAVY, J.-R. DE DREUZY. Simulations in large tridimensional Discrete Fracture Networks (DFN): II. Flow simulations, in "MASCOT 2018 -15th IMACS/ISGG meeting on applied scientific computing and tools", Rome, Italy, October 2018, https://hal.inria.fr/hal-01896900

Other Publications

- [43] M. ABBAS, A. ERN, N. PIGNET. A Hybrid High-Order method for finite elastoplastic deformations within a logarithmic strain framework, January 2019, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01978385
- [44] 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, November 2018, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01919067
- [45] J. BLECHTA, J. MÁLEK, M. VOHRALÍK. Localization of the $W^{-1,q}$ norm for local a posteriori efficiency, July 2018, working paper or preprint, https://hal.inria.fr/hal-01332481
- [46] T. BOIVEAU, V. EHRLACHER, A. ERN, A. NOUY. Low-rank approximation of linear parabolic equations by space-time tensor Galerkin methods, October 2018, https://arxiv.org/abs/1712.07256 working paper or preprint, https://hal.archives-ouvertes.fr/hal-01668316
- [47] V. M. CALO, M. CICUTTIN, Q. DENG, A. ERN. Spectral approximation of elliptic operators by the Hybrid High-Order method, July 2018, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01628698
- [48] E. CANCÈS, G. DUSSON, Y. MADAY, B. STAMM, M. VOHRALÍK. *Post-processing of the planewave approximation of Schrödinger equations. Part I: linear operators*, November 2018, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01908039
- [49] C. CANCÈS, F. NABET, M. VOHRALÍK. Convergence and a posteriori error analysis for energy-stable finite element approximations of degenerate parabolic equations, October 2018, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01894884
- [50] J.-P. CHANCELIER, S. FURIC, P. WEIS. *Translating Simulink Models to Modelica using the Nsp Platform*, December 2018, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01948681
- [51] M. CICUTTIN, A. ERN, T. GUDI. *Discontinuous-Skeletal methods with linear and quadratic reconstructions for the elliptic obstacle problem*, February 2018, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01718883

[52] J. DABAGHI, V. MARTIN, M. VOHRALÍK. Adaptive inexact semismooth Newton methods for the contact problem between two membranes, October 2018, working paper or preprint, https://hal.inria.fr/hal-01666845

- [53] P. DANIEL, A. ERN, M. VOHRALÍK. An adaptive hp-refinement strategy with inexact solvers and computable guaranteed bound on the error reduction factor, November 2018, working paper or preprint, https://hal.inria. fr/hal-01931448
- [54] A. ERN, J.-L. GUERMOND. *Quasi-optimal nonconforming approximation of elliptic PDES with contrasted coefficients and minimal regularity*, December 2018, working paper or preprint, https://hal.archives-ouvertes.fr/hal-01964299
- [55] A. ERN, M. VOHRALÍK. Stable broken H1 and H(div) polynomial extensions for polynomial-degree-robust potential and flux reconstruction in three space dimensions, August 2018, working paper or preprint, https://hal.inria.fr/hal-01422204
- [56] A. LEJAY, L. LENÔTRE, G. PICHOT. An exponential timestepping algorithm for diffusion with discontinuous coefficients, June 2018, working paper or preprint, https://hal.inria.fr/hal-01806465
- [57] G. MALLIK, M. VOHRALÍK, S. YOUSEF. Goal-oriented a posteriori error estimation for conforming and nonconforming approximations with inexact solvers, December 2018, working paper or preprint, https://hal.inria.fr/hal-01964733
- [58] G. PICHOT, S. LEGRAND, J. ERHEL, M. OUMOUNI. *GENFIELD: A parallel software for the generation of stationary Gaussian random fields*, May 2018, 1 p., InterPore 2018 10th Annual Meeting and Jubilee, Poster, https://hal.inria.fr/hal-01960444
- [59] M. RIAHI, H. BEN AMEUR, J. JAFFRÉ, R. BOUHLILA. *Refinement indicators for estimating hydrogeologic parameters*, January 2018, working paper or preprint, https://hal.inria.fr/hal-01674486
- [60] I. SMEARS, M. VOHRALÍK. Simple and robust equilibrated flux a posteriori estimates for singularly perturbed reaction-diffusion problems, 2018, working paper or preprint, https://hal.inria.fr/hal-01956180