

IN PARTNERSHIP WITH: Ecole des Ponts ParisTech

Activity Report 2017

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

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Project-Team SERENA

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

Computer Science and Digital Science:

- A2.1.2. Object-oriented programming
- A2.1.3. 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. Personnel

Research Scientists

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Elyes Ahmed [Univ Paris-Nord, until April 2017] Thomas Boiveau [Univ Paris-Est, until September 2017] Matteo Cicuttin [Univ Paris-Est] Seyed Mohammad Zakerzadeh [Inria, from October 2017]

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Technical staff

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Khadija Talali [Inria, from March 2017 until August 2017]

Administrative Assistants

Virginie Collette [Inria, until June 2017, and from December 2017] Azzeddine Saidani [Inria, from June to August 2017] Kévin Bonny [Inria, from August to December 2017]

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] Jean-Luc Guermond [Texas A&M University, Professor, HDR] 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]

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). Our requirement is to derive *structure-preserving* methods, i.e., methods that mimic 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* for the lowest-order schemes for the Navier–Stokes equations and to the recently-devised theory of gradient schemes for discrete element methods applied to elasto-plasticity. For the schemes we develop, we study existence, uniqueness, and stability questions, and derive a priori convergence estimates. Our special interest is in higher-order methods like the hybrid high-order method, which have recently begun to receive significant attention. Even though their use in practice may not be immediate, we believe that they belong to the future generation of numerical methods for industrial simulations.

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 shall then address theoretically the question of convergence of the new algorithms and prove their numerical quasi-optimality, meaning that they need, up to a generic constant, the smallest possible number of degrees of freedom to achieve the given accuracy. We in particular seek to prove a guaranteed error reduction in terms of the number of degrees of freedom.

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
- geological sequestration of CO2
- production of oil and gas

4.2. Complex Stokes and Navier–Stokes flows

• industrial risks in energy production (fission)

4.3. Energy production, sustainable use of resources

- simulation of shock waves impinging on deformable or fragmentable structures
- use of nets of rods for sustainable construction

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

The most important results of the ERC GATIPOR are now centralized in the ERC GATIPOR Gallery.

5.1.1. Awards

Laurent Monasse was awarded an ANR JCJC (young researcher) grant.

6. New Software and Platforms

6.1. GEOFRAC

GEOFRACFLOW KEYWORDS: Hydrogeology - Numerical simulations - 3D SCIENTIFIC DESCRIPTION: GEOFRACFLOW 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 GEOFRACFLOW 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.

RELEASE FUNCTIONAL DESCRIPTION: The last version includes optimisations of the code, mainly with an efficient upload of the mesh data generated with BLSURF and vectorization of the operations.

- 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

6.2. Ref-indic

Refinement indicators

KEYWORD: Inverse problem

SCIENTIFIC DESCRIPTION: The refinement indicator algorithm is suited for the estimation of a distributed parameter occurring in a mathematical simulation model, typically a set of partial differential equations. When the numerical simulation model must be solved on a fine grid, the refinement indicator algorithm provides an adaptive parameterization of the sought parameter that avoids overparameterization difficulties. In each grid cell, the estimated parameter may be of dimension greater than one, i.e. the algorithm is able to estimate several scalar distributed parameters.

Ref-indic implements a generic version of the refinement indicator algorithm that can dock specific programs provided they conform to the generic algorithm API.

The API of Ref-indic requires four main functionalities (called tasks) for the user specific program, it must be able: * to initialize, i.e. to open all necessary data files, to perform all necessary preliminary computation, and to return an initial coarse parameterization (giving a zone number between 0 and the initial number of zones minus one for each cell of the fine grid), * to compute the gradient on the fine grid for a given fine parameterization, * to optimize the problem for a given coarse parameterization, * and to finalize, i.e. to store the resulting coarse parameterization.

Given any such user specific program, the inversion platform automatically provides a program that solves the corresponding user inverse problem using the refinement indicator algorithm.

FUNCTIONAL DESCRIPTION: Ref-indic is an adaptive parameterization platform using refinement indicators. Slogan is "invert details only where they are worth it". Ref-indic implements a generic version of the refinement indicator algorithm that can dock specific programs provided they conform to the generic algorithm API.

NEWS OF THE YEAR: In its current implementation, the inversion platform can only build coarse parameterizations for a distributed parameter defined on a fine rectangular grid. From version 1.5+pl0, the user has the possibility to specify masked cells in the fine rectangular grid that will be ignored by the algorithm (with the use of the specific zone number -1 in the initial coarse parameterization). This allows for the treatment of inverse problems defined on unstructured meshes. The handling of both-way interpolations must be taken care of by the gradient computation and optimization tasks. The masked cells must be the same for all components of the parameter.

- Contact: François Clément
- Publications: Image Segmentation with Multidimensional Refinement Indicators The Multi-Dimensional Refinement Indicators Algorithm for Optimal Parameterization
- URL: http://refinement.inria.fr/ref-indic/

6.3. Sklml

The OCaml parallel skeleton system

KEYWORDS: Parallel programming - Functional programming

SCIENTIFIC DESCRIPTION: Writing parallel programs is not easy, and debugging them is usually a nightmare. To cope with these difficulties, the skeleton programming approach uses a set of predefined patterns for parallel computations. The skeletons are higher order functional templates that describe the program underlying parallelism.

Sklml is a new framework for parallel programming that embeds an innovative compositional skeleton algebra into the OCaml language. Thanks to its skeleton algebra, Sklml provides two evaluation regimes to programs: a regular sequential evaluation (merely used for prototyping and debugging) and a parallel evaluation obtained via a recompilation of the same source program in parallel mode.

Sklml was specifically designed to prove that the sequential and parallel evaluation regimes coincide.

FUNCTIONAL DESCRIPTION: Sklml is a functional parallel skeleton compiler and programming system for OCaml programs. Slogan is "easy coarse grain parallelization".

NEWS OF THE YEAR: Caml preprocessors are no longer needed.

- Participants: François Clément and Pierre Weis
- Contact: François Clément
- URL: http://sklml.inria.fr

6.4. GENFIELD

KEYWORDS: Hydrogeology - Algorithm - Heterogeneity

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.

RELEASE FUNCTIONAL DESCRIPTION: The new version includes: - The use of the FFTW3-mpi library for discrete Fourier transform - Non regression tests (and continuous integration through gitlab.inria.fr) - Debugging of the parallel algorithm

- Participants: Géraldine Pichot, Simon Legrand, Grégoire Lecourt, Jean-Raynald De Dreuzy and Jocelyne Erhel
- Contact: Géraldine Pichot
- Publication: Algorithms for Gaussian random field generation
- URL: https://gitlab.inria.fr/slegrand/Genfield_dev

6.5. 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.

6

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/datafl4sh/diskpp

6.6. 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/

6.7. 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/

7. New Results

7.1. A posteriori stopping criteria for domain decomposition methods

Participants: Sarah Ali Hassan, Michel Kern, Martin Vohralík.

Publication: [45]

In [45] we propose a new method for stopping iterations in a domain decomposition (DD) algorithm. The approach is based on a posteriori error estimates, and builds estimators that distinguish between the (space and time) discretization errors and that caused by the DD iterations. This enables stopping the iterations as soon as the DD error is smaller than the discretization error. In practice, numerous unnecessary iterations can be avoided, as illustrated in Figure 1 (here we stop at iteration 17 in place of the usual 61, economizing 72 % iterations). The method has been extended to global-in-time domain decomposition and to nonlinear problems. This was the topic of the Ph.D. thesis of Sarah Ali Hassan.

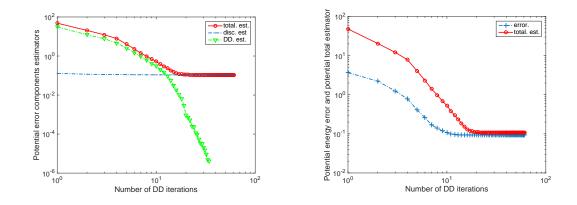


Figure 1. Error component estimates (left) and total energy error and its estimate (right), DD with GMRES solver

7.2. Finite element quasi-interpolation and best-approximation

Participant: Alexandre Ern.

Publication: [21]

In [21], we introduce a quasi-interpolation operator for scalar- and vector-valued finite element spaces constructed on affine, shape-regular meshes with some continuity across mesh interfaces. This operator gives optimal estimates of the best approximation error in any L^p -norm assuming regularity in the fractional Sobolev spaces $W^{r,p}$, where $p \in [1, \infty]$ and the smoothness index r can be arbitrarily close to zero. The operator is stable in L^1 , leaves the corresponding finite element space point-wise invariant, and can be modified to handle homogeneous boundary conditions. The theory is illustrated on H^1 -, $\mathbb{H}(\text{curl})$ -, and $\mathbb{H}(\text{div})$ -conforming spaces.

7.3. Hybrid High-Order methods for hyperelasticity

Participants: Alexandre Ern, Nicolas Pignet.

Publication: [13]

In [13], we devise and evaluate numerically Hybrid High-Order (HHO) methods for hyperelastic materials undergoing finite deformations. The HHO methods use as discrete unknowns piecewise polynomials of order $k \ge 1$ on the mesh skeleton, together with cell-based polynomials that can be eliminated locally by static condensation. The discrete problem is written as the minimization of a broken nonlinear elastic energy where a local reconstruction of the displacement gradient is used. Two HHO methods are considered: a stabilized method where the gradient is reconstructed as a tensor-valued polynomial of order k and a stabilization is added to the discrete energy functional, and an unstabilized method which reconstructs a stable higher-order gradient and circumvents the need for stabilization. Both methods satisfy the principle of virtual work locally with equilibrated tractions. We present a numerical study of the two HHO methods on test cases with known solution and on more challenging three-dimensional test cases including finite deformations with strong shear layers and cavitating voids. We assess the computational efficiency of both methods, and we compare our results to those obtained with an industrial software using conforming finite elements and to results from the literature. The two HHO methods exhibit robust behavior in the quasi-incompressible regime. In Figure 2, we present some results for a hollow cylinder under shear and compression.

7.4. A nonlinear consistent penalty method for positivity preservation

Participant: Alexandre Ern.

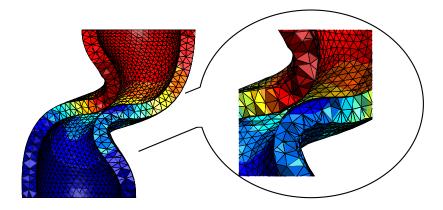


Figure 2. Euclidean displacement norm on the deformed configuration for the shear and compressed cylinder, and a zoom where the deformations are the most important. The color scale goes from 0.0 (blue) to 1.8 (red).

Publication: [16]

In [16], we devise and analyze a new stabilized finite element method to solve the first-order transport (or advection-reaction) equation. The method combines the usual Galerkin/Least-Squares approach to achieve stability with a nonlinear consistent penalty term inspired by recent discretizations of contact problems to weakly enforce a positivity condition on the discrete solution. We prove the existence and the uniqueness of the discrete solution. Then we establish quasioptimal error estimates for smooth solutions bounding the usual error terms in the Galerkin/Least-Squares error analysis together with the violation of the maximum principle by the discrete solution. A numerical example is presented in Figure 3.

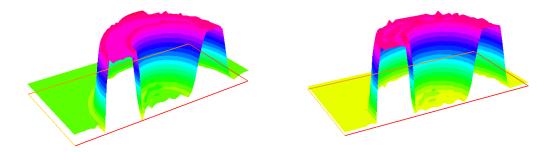


Figure 3. Elevations of solutions using piecewise quadratic elements. Left: standard method, the nodal discrete maximum principle violation is 21%. Right: consistent penalty method, violation is less than $4 \cdot 10^{-3}\%$.

7.5. A simple a posteriori estimate on general polytopal meshes

Participant: Martin Vohralík.

Publication: [30]

The recent publication [30] develops an a posteriori error estimate for lowest-order locally conservative methods on meshes consisting of general polytopal elements. We focus here on the ease of implementation and evaluation cost of the methodology based on H^1 -conforming potential reconstructions and H(div)conforming flux reconstructions that we develop in the SERENA project-team. In particular, the evaluation of our estimates for steady linear diffusion equations merely consists in some local matrix-vector multiplications, where, on each mesh element, the matrices are either directly inherited from the given numerical method, or easily constructed from the element geometry, while the vectors are the flux and potential values on the given element. This is probably the smallest computational price that one can imagine. We next extend our approach to steady nonlinear problems. We obtain a guaranteed upper bound on the total error in the fluxes that is still obtained by local matrix-vector multiplications, with the same element matrices as above. Moreover, the estimate holds true on any linearization and algebraic solver step and allows to distinguish the different error components. Finally, we apply this methodology to unsteady nonlinear coupled degenerate problems describing complex multiphase flows in porous media. It leads to an easy-to-implement and fast-torun adaptive algorithm with guaranteed overall precision, adaptive stopping criteria, and adaptive space and time mesh refinements. An example of its application to a complex porous media flow (three-phases/threecomponents black-oil problem) can be found in Figure 4.

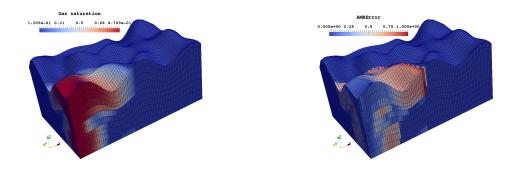


Figure 4. Simulated gas saturation after 1000 days (left) and corresponding a posteriori error estimate (right)

7.6. Sharp algebraic and total a posteriori error bounds

Participant: Martin Vohralík.

Publication: [66]

In [66], we derive guaranteed, fully computable, constant-free, and sharp upper and lower a posteriori estimates on the algebraic, total, and discretization errors of finite element approximations of the Poisson equation obtained by an arbitrary iterative solver. Though guaranteed bounds on the discretization error, when the associated algebraic system is solved exactly, are now well-known and available, this is definitely not the case for the error from the linear algebraic solver (algebraic error), and a beautiful problem arises when these two error components interact. We try to analyze it here while identifying a decomposition of the algebraic error over a hierarchy of meshes, with a global residual solve on the coarsest mesh. Mathematically, we prove equivalence of our computable total estimate with the unknown total error, up to a generic polynomial-degreeindependent constant. Numerical experiments illustrate sharp control of all error components and accurate prediction of their spatial distribution in several test problems, as we illustrate it in Figure 5 for the higherorder conforming finite element method and the conjugate gradient algebraic solver.

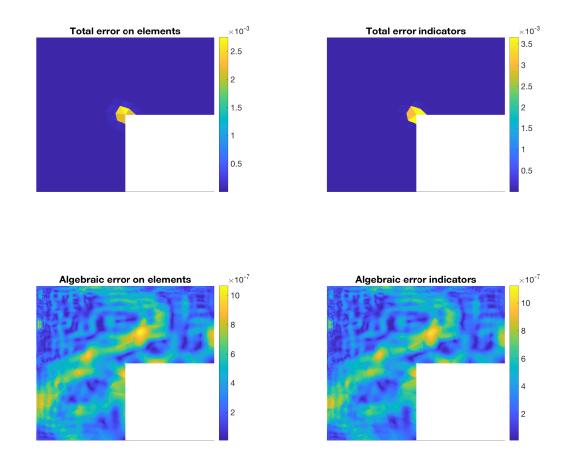


Figure 5. Actual total error (top left) and its a posteriori error estimate (top right). Actual algebraic error (bottom left) and its a posteriori error estimate (bottom right).

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

Participant: Géraldine Pichot.

Publication: [64]

Grants: H2MN04 3

In [64], we provide a general methodology to compute the resolvent kernel as well as the density when available for a one-dimensional second-order differential operators with discontinuous coefficients. In a sequel, the computed resolvent kernel will be used to set-up an efficient and accurate simulation scheme.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

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

One contract with CEA accompanying the PhD thesis of Frédéric Marazzato.

One contract with ANDRA accompanying the PhD thesis of Sarah Ali Hassan (ended, Ph.D. defended in June 2017).

One contract with IFP Energies Nouvelles, in the framework of the Inria–IFP Energies Nouvelles "contrat cadre".

Three-parts contract Inria–EDF–Sciworks Technologies (from April 2017) on "Form-L for the formalization of constraints of complex systems".

9. Partnerships and Cooperations

9.1. Regional Initiatives

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 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 project had its intermediate review in December 2016, and received excellent marks from the expert panel.

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 2014–2017.

ANR GEOPOR: "Geometrical approach for porous media flows: theory and numerics". A new approach to numerical methods for multiphase simulations based on the concept of gradient flows is investigated. With Laboratoire Jacques-Louis Lions, University Pierre and Marie Curie. SERENA representant is M. Vohralík, period 2013–2017.

- ANR H2MNO4: "Original optimized object-oriented numerical model for heterogeneous hydrogeology". The project H2MNO4 develops numerical models for reactive transport in heterogeneous media. The objective is to design both Eulerian and Lagrangian models. Three applications are concerned: freshwater supply, remediation of mine drainage, and waste geological disposal. The project relies on a consortium of six partners, involving four public research laboratories (Inria, Geosciences Rennes, University of Lyon 1, University of Poitiers, Pprime Institute), one public institution (ANDRA), and one enterprise (ITASCA). International collaborations are pursued with University of San Diego (USA) and UPC (Spain). SERENA representant is G. Pichot, period 2012–2016.
- 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.

9.3. European Initiatives

9.3.1. FP7 & H2020 Projects

- **ERC GATIPOR:** "Guaranteed fully adaptive algorithms with tailored inexact solvers for complex porous media flows". The subject of this project 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.
- **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 evergrowing 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.

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.

MoRe

Program: Research, Development and Innovation Council of the Czech Republic

Project acronym: MoRe

Project title: Implicitly constituted material models: from theory through model reduction to efficient numerical methods

Duration: September 2012 - September 2017

Coordinator: Josef MÁLEK, Charles University in Prague. SERENA representant is M. Vohralík. Other partners: Institute of Mathematics, Czech Academy of Sciences; University of Oxford

Abstract: A multidisciplinary project on nonlinear Navier–Stokes flows with implicit constitutive laws. It focuses on development of accurate, efficient, and robust numerical methods for simulations of the new class of implicit models.

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 medial applications.

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

9.5. International Research Visitors

9.5.1. Visits of International Scientists

Lars Diening, Professor at University of Bielefeld, Germany, February 17-23, 2017.

Christian Kreuzer, Professor at University of Dortmund, Germany, February 19–25, 2017.

Joscha Gedicke, post-doc at University Vienna, Austria, May 29-June 2, 2017.

Martin Eigel, post-doc at Weierstrass Institute Berlin, Germany, May 29–June 2, 2017.

Carsten Carstensen, Professor at Humboldt University Berlin, Germany, August 15–September 15, 2017.

Peter Minev, Professor at the University of Alberta, Canada, September 15–October 15, 2017.

Hend Ben Ameur, Professor at IPEST and member of ENIT-Lamsin, Tunis, Tunisia, October 23–November 3, 2017.

9.5.1.1. Internships

K. Talali, université de Fez, Morocco, April 1-August 31 (Master degree).

9.5.2. Visits to International Teams

9.5.2.1. Research Stays Abroad

Alexandre Ern participated as Invited Professor to the HIM Program on Multiscale Problems: Algorithms, Numerical Analysis and Computation, in Bonn, Germany, January 2017.

Martin Vohralík was invited for two weeks stay to Charles University in Prague collaboration with J. Málek, April 2017.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

10.1.1.1. General Chair, Scientific Chair

Alexandre Ern, Iain Smears, and Martin Vohralík have organized a 2-day workshop on **A posteriori** error estimates, adaptivity, and advanced applications, in the framework of the ERC GATIPOR project. 40 participants from the whole world.

Soleiman Yousef 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

Géraldine Pichot and Michel Kern are members of the local organizing committee of the Computational Methods in Water Resources 2018 conference.

Martin Vohralík was a member of the organizing committee of the *Finite Volumes for Complex Applications* conference.

10.1.2. Scientific Events Selection

10.1.2.1. Member of the Conference Program Committees

Alexandre Ern and Martin Vohralík were members of the scientific committee of the ENUMATH 2017 conference.

Martin Vohralík was a member of the scientific committee of the *Finite Volumes for Complex Applications* conference.

10.1.3. Journal

10.1.3.1. Member of the Editorial Boards

François Clément is a member of the editorial board of Matapli from September 2017.

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, Computational Methods in Applied Mathematics, and Journal de l'Ecole polytechnique, Mathématiques.

M. Vohralík is a member of the editorial boards of SIAM Journal on Numerical Analysis and of Acta Polytechnica.

10.1.3.2. Reviewer - Reviewing Activities

Thomas Boiveau was a reviewer for the Journal of Scientific Computing and the journal Geometrically Unfitted Finite Element Method and Applications (Proceedings of the UCL Workshop 2016).

Matteo Cicuttin was a reviewer for the journal Journal of Computational and Applied Mathematics. Alexandre Ern served as reviewer for tens of papers in different journals.

Frédéric Marazzato was a reviewer for the journal Modelling and Simulation in Materials Science and Engineering.

Laurent Monasse was a reviewer for the Journal of Computational Physics, the European Journal of Mechanics B Fluids, and the International Journal for Numerical Methods in Engineering.

Michel Kern was a reviewer for Computers and Geosciences, Advances in Computational Mathematics, ESAIM: proceedings, ARIMA, and Applicable Analysis.

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

10.1.4. Invited Talks

Alexandre Ern, plenary speaker, SIAM Conference on Mathematical and Computational Issues in the Geosciences 2017, Erlangen, Germany.

Alexandre Ern, invited speaker, POEMS 2017, Milano, Italy.

Alexandre Ern, invited speaker, Inauguration workshop of the French-German-Italian LIA COPDESC on Applied Analysis.

Michel Kern, plenary speaker, 6th Workshop on Parallel-in-Time methods, Locarno, Switzerland.

Martin Vohralík, plenary speaker, TamTam 2017, Hammamet, Tunisia, May 2017.

Martin Vohralík, plenary speaker, International Conference on Approximation Methods and Numerical Modelling in Environment and Natural Resources, Oujda, Morocco, May 2017.

Martin Vohralík, plenary speaker, Czech workshop on complex systems, Prague, Czech Republic, September 2017.

10.1.5. Leadership within the Scientific Community

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

M. Kern is a member of the Scientific Committee of Orap (ORganisation Associative du Parallélisme), 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.

10.1.6. Research Administration

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

F. Clément is the AMIES facilitator of the Inria Research Center of Paris.

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.

G. Pichot is a member of the *Comité local d'hygiène, de sécurité et des conditions de travail* of the Inria center of Paris.

G. Pichot is member of the Conseil de département MAM of Polytech Lyon.

G. Pichot is member of the Commission de developpement technologique (CDT) of the Inria center of Paris.

G. Pichot is a member of the CES commission of the Inria center of Paris.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

Licence : Amina Benaceur, Eléments d'arithmétique, 19h15, L2, University Pierre et Marie Curie, France.

Licence : Thomas Boiveau, Equations aux dérivées partielles et éléments finis 15h, L3, Ecole des ponts ParisTech, France

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.

Licence : Frédéric Marazzato, Analyse et Calcul Scientifique, 15h, L3, Ecole Nationale des Ponts et Chaussées, France.

Master : Alexandre Ern, Discontinuous Galerkin methods, 20h, M2, University Pierre et Marie Curie, France.

Master : Alexandre Ern is the leader of the Master Mathématiques et applications of ENPC.

Master : Frédéric Marazzato, Remise à niveau en Mécanique des Milieux Continus, 9h, M2, Ecole Nationale des Ponts et Chaussées, France.

Master : Frédéric Marazzato, Reliability of Materials and Structures, 15h, M1, Ecole Nationale des Ponts et Chaussées, France.

Master : Frédéric Marazzato, Projet de Département Génie Mécanique et Matériaux, 20h, M1, Ecole Nationale des Ponts et Chaussées, 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, 30 h (with E. Mouche), M2, Université Paris Saclay, France Martin Vohralík, CIMPA Summer School on Multiscale Computational Methods and Error Control, Kanpur, India, July 2017, 10h.

10.2.2. Supervision

PhD: Sarah Ali Hassan, A posteriori error estimates and stopping criteria for solvers using the domain decomposition method and with local time stepping, University Pierre and Marie Curie, 26 June 2017, Martin Vohralík, Caroline Japhet, and Michel Kern.

PhD: Yannick Masson, Tchebyshev nets and application to Grid Shells, University Paris-Est, 09 June 2017, Alexandre Ern and Olivier Baverel.

PhD: Rita Riedlbeck, Adaptive algorithms for poromechanics and poroplasticity, University of Montpellier, 27 November 2017, Daniele di Pietro and Alexandre Ern.

PhD in progress: Amina Benaceur, Model reduction in thermo-mechanics, 01 January 2016, Alexandre Ern.

PhD in progress: Karol Cascavita, Discontinuous skeletal methods for yield fluids, 01 October 2015, Alexandre Ern and Xavier Chateau.

PhD in progress: Jad Dabaghi, Adaptive modeling via complementarity of phase appearance and disappearance in fractured and porous media, 01 November 2015, Martin Vohralík Vincent Martin.

PhD in progress: Patrik Daniel, Adaptive multilevel solvers with a posteriori error control for porous media flows, 01 October 2015, Martin Vohralík and Alexandre Ern.

PhD in progress: Frédéric Marazzato, Fracture and fragmentation simulated by the discrete element method, 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, Examiner, HDR C. Le Potier, University Paris Est, 15 November 2017.

Laurent Monasse, Examiner, PhD J. Ridoux, University Pierre and Marie Curie, 4 October 2017. Martin Vohralík, President of the committee, PhD R. Riedelbeck, University of Montpellier, 27 November 2017.

Martin Vohralík, Examiner, HDR P. Gosselet, ENS Cachan, 10 February 2017.

10.3. Popularization

F. Clément was the coordinator of the Maths-Enterprises booth for AMIES and Labex mathématiques Hadamard at the *18e Salon Culture & Jeux Mathématiques*, held in Paris, 27–30 May, 2017. F. Clément coordinated an article for AMIES in Interstices ([42]).

Major publications by the team in recent years: [1], [2], [3], [4], [5], [6], [7], [8], [9], [10].

11. Bibliography

Major publications by the team in recent years

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- [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
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- [12] R. RIEDLBECK. Adaptive algorithms for poro-mechanics and poro-plasticity, Université de Montpellier, November 2017, https://hal.inria.fr/tel-01676709

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