Activity Report 2014

Project-Team POMDAPI

Environmental Modeling, Optimization and Programming Models

RESEARCH CENTER
Paris - Rocquencourt

THEME
Earth, Environmental and Energy Sciences

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Project-Team POMDAPI

Keywords: Environment, Scientific Computation, Model Coupling, Porous Media, A Posteriori Error Estimates, Adaptivity

Creation of the Project-Team: 2012 January 01, end of the Project-Team: 2014 December 31.

1. Members

Research Scientists
Jérôme Jaffré [Team leader, Inria, Senior Researcher, HdR]
François Clément [Inria, Researcher]
Jean Charles Gilbert [Inria, Senior Researcher]
Michel Kern [Inria, Researcher]
Martin Vohralík [Inria, Senior Researcher, HdR]
Pierre Weis [Inria, Senior Researcher]

Engineers
Clément Franchini [Inria, granted by OSEO Innovation]
Émilie Joannopoulos [Inria, IJD]

PhD Students
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Sarah Ali Hassan [Inria]
Nabil Birgle [Inria]
Fatma Cheikh [ENIT-Lamsin, Tunis, Tunisia and Université de Paris 6]
Cédric Josz [Université de Paris 6, Cifre RTE]
Mohamed Hedi Riahi [ENIT-Lamsin, Tunis, Tunisia and Université de Paris 6]

Post-Doctoral Fellows
Martin Čermák [University of Ostrava, May–June 2014]
Zuqi Tang [Inria]

Visiting Scientist
Veerappa Gowda [TIFR-CAM,Bengalore,India, Nov-Dec 2014]

Administrative Assistant
Nathalie Bonte [Inria]

Others
Hend Ben Ameur [ENIT-Lamsin, Professor]
Guy Chavent [Université de Paris 9, Professor]
Caroline Japhet [Université de Paris 13, Associate Professor]
Jean Elizabeth Roberts [Inria, Senior Researcher, HdR]

2. Overall Objectives

2.1. Overall Objectives

The project-team Pomdapi is concerned with the construction and analysis of simulation tools for the modeling of environmental and energy problems and numerical analysis. These tools include numerical approximation schemes for partial differential equations, nonlinear solvers, numerical techniques in optimization and complementarity problems, a posteriori error estimates, and adaptivity. We are equally interested in reliable and correct programming methods for the implementation of these tools.

Our research activities are structured as follows. The axis on *numerical environmental modeling* encompasses the study of

1. coupled problems, including coupling transport with chemistry, coupling of fracture flow with matrix flow with various choices of flow in the fracture and in the matrix, and the modeling of drainage in an agricultural parcel;
2. problems of flow and transport in porous media for hydrogeology or oil reservoir simulation; and
3. approximation schemes for partial differential equations, including the use of hexahedral grids, and the problem of two-phase flow in a porous medium with a change of rock type.

The activities on *continuous optimization* deal with the development of optimization solvers for constrained problems (quadratic solvers and Newtonian solvers), interior point methods, decomposition methods for large scale optimization (application to the optimization of the electricity production), semi-definite and polynomial optimization (application to the global optimization of the power flow in an electricity network), and derivative free optimization.

Complementarity problems deal with systems of equations, in which the active equations at the solution is part of the unknowns, while inactive equations must satisfy a sign condition. We address such problems that play a major part in the modeling of geophysical systems and of chemical processes. The activities deal with numerical techniques for solving linear and nonlinear problems, in particular through the Newton-min approach.

The research on *programming models* splits into (i) high-performance computing, with the development of new algorithms as space–time domain decomposition, and reflections on parallel implementation for large scale computations; and (ii) reliable and correct programming for scientific computing, including skeleton-based programming for safe parallelization, the development of two generic platforms (one for the implementation of the coupling of numerical codes and the other for solving inverse problems), and formal proofs of correctness for numerical programs.

The research in *numerical analysis* focuses on the so-called guaranteed and robust *a posteriori error estimates*. These are fully computable quantities allowing to tightly bound the error in a numerical approximation of a partial differential equation. More precisely, we have recently focused on their usage for distinguishing different error components and conception of adaptive *stopping criteria* for iterative linear and nonlinear solvers. We are also developing *fully adaptive strategies*, combining adaptive stopping criteria with adaptive space and time mesh refinement.

3. Application Domains

3.1. Environmental sciences

Applications are in hydrogeology and water resources.

3.2. Energy sciences

Applications are in oil reservoir and sedimentary basin simulations, and in optimization of the power flow in an electricity transportation network.

4. New Software and Platforms

4.1. FreeFem++

Participants: Martin Vohralík, Martin Čermák, Zuqi Tang.

The scientific calculation code FreeFem++ is an example of a complex software numerical simulation tool. It in particular encompasses all specifications of the problem, the choice and implementation of the numerical method, the choice and implementation of the linearization method (nonlinear solver), and the choice and implementation of the method of solution of the associated linear systems (linear solver). In the post-doc stays of M. Čermák and Z. Tang, we integrated there the most recent advances of the theory of a posteriori error estimation and of adaptive algorithms. In particular, adaptive stopping criteria for the linear and nonlinear solvers were implemented.

Version 3.33

Programming language: C++

http://www.freefem.org/ff++/

4.2. Oqla, Qpalm

Participants: Jean Charles Gilbert, Émilie Joannopoulos.

OQLA and QPALM aim at minimizing a large scale convex quadratic function on a polyhedron by an augmented Lagrangian method. The original features of the approach are its capacity to solve the problem without factorization, which makes them adapted to large scale problems, and to deal with unbounded and infeasible problems. In case the problem is infeasible, the codes solve the *closest feasible problem* with a global linear rate of convergence [3]. In case the problem is unbounded, the solvers build a feasible direction of unboundedness for the closest feasible problem. The solvers OQLA and QPALM only differ by their programming language; they are documented in [16], [14], [15].

Versions: 0.6 (OQLA), 0.5 (QPALM)

Programming languages: `C++` (OQLA), `Matlab` (QPALM)

4.3. Ref-image

Participants: Hend Ben Ameur, François Clément, Pierre Weis.

Ref-image is an image segmentation program using optimal control techniques. Slogan is “no gestalt inside”. Ref-image implements the refinement indicator algorithm, specialized to the case of the inversion of the identity map. It is a first step towards the implementation of a generic inversion platform using the refinement indicator algorithm.

Version: 1.1+pl0 (2014/02/28)

Programming language: OCaml

http://refinement.inria.fr/ref-image/

4.4. Ref-indic

Participants: Hend Ben Ameur, François Clément, Pierre Weis.

Ref-indic is an adaptive parameterization platform using refinement indicators. Slogan is “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.

Version: 1.4+pl0 (2014/07/01)

Programming language: OCaml

http://refinement.inria.fr/ref-indic/

4.5. Sklml

Participants: François Clément, Pierre Weis.

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

Version: 1.1+pl0 (2014/01/21)

Programming language: OCaml

http://sklml.inria.fr/

5. New Results

5.1. A posteriori error estimates

Participant: Martin Vohralík.

In [2], we have been able to derive an a posteriori error estimate for the numerical approximation of the two-phase flow problem. This is a cornerstone model problem for porous media, describing the flow of two immiscible and incompressible fluids. We take into account the capillary pressure, whence the model features such difficulties as coupling of partial differential equations with algebraic constraints, strong nonlinearities, degeneracy (disappearance of the diffusion term), advection dominance and consequent forming of sharp evolving fronts, or highly nonlinear and very badly conditioned systems of algebraic equations. Our analysis covers a large class of spatial discretizations in a unified setting, with fully implicit time stepping. We also show how the different error components, namely the spatial discretization error, the temporal discretization error, the linearization error, and the algebraic solver error can be distinguished and estimated separately. This gives rise to efficient adaptive stopping criteria, enabling to spare many useless iterations. The practical impact of our results is that even for this complicated model problem, the overall error committed in a numerical approximation can be fully controlled and, moreover, the simulation time can be reduced by factors typically of an order of magnitude. This result has then been extended in [4] to the compositional model of multiphase Darcy flow, where an arbitrary number of phases can be present, and where each phase can be composed of several components. Later, in [12], still a possible dependence on the temperature has been added. The last two references also contain convincing numerical illustrations on real-life reservoir engineering examples.

5.2. Optimization

Participants: Jean Charles Gilbert, Émilie Joannopoulos, Cédric Josz.

5.2.1. Polynomial optimization

A polynomial optimization problem (POP) consists in minimizing a multivariate real polynomial on a set K defined by polynomial inequalities and equalities. In its full generality it is a non-convex, multi-extremal, difficult global optimization problem. More than a decade ago, J. B. Lasserre proposed to solve a POP by a hierarchy of convex semidefinite programming (SDP) relaxations of increasing size and precision. Each problem in the hierarchy has a primal SDP formulation (a relaxation of a moment expression of the POP) and a dual SDP formulation (a sum-of-squares polynomial relaxation of the POP). In [18], we show that there is no duality gap between each primal and dual SDP problem in Lasserre's hierarchy, provided one of the constraints in the description of set K is a ball constraint. Our proof uses elementary results on SDP duality and it does not assume that K has a strictly feasible point.

5.2.2. *Convex quadratic optimization*

Convex quadratic optimization deals with problems consisting in minimizing a convex quadratic function on a polyhedron. In [3], we analyzed the behavior of the augmented Lagrangian algorithm when it deals with an *infeasible* convex quadratic optimization problem; this situation is important to master in order to be able to solve correctly the QPs that are generated by the SQP (or Newton-like) algorithm to solve a nonlinear optimization problem, QPs whose feasibility is not guaranteed. It is shown that the algorithm finds a point that, on the one hand, satisfies the constraints shifted by the smallest possible shift that makes them feasible and, on the other hand, minimizes the objective on the corresponding shifted constrained set. The speed of convergence to such a point is globally linear, with a rate that is inversely proportional to the augmentation parameter. This suggests a rule for determining the augmentation parameter that aims at controlling the speed of convergence of the shifted constraint norm to zero; this rule has the advantage of generating bounded augmentation parameters even when the problem is infeasible. The approach has also been implemented in the pieces of software OQLA and QPALM during the ADT MINOQS (see section 4.2 and [16], [14], [15]).

6. Bilateral Contracts and Grants with Industry

6.1. Bilateral Contracts with Industry

RTE (Réseau de Transport de l'Électricité) and ANRT (Association Nationale de la Recherche et de la Technologie) are funding the PhD thesis of C. Josz (Cifre agreement).

Andra is funding the PhD thesis of S. Ali Hassan (an agreement that is part of an *accord Cadre* between Inria and Andra).

IFP Énergies Nouvelles (*Institut Français du Pétrole Énergies Nouvelles*) supports a collaboration on numerical methods for the flow simulation in porous media with fractures for modeling sedimentary basins or oil reservoirs. This collaboration concerns J. E, Roberts and J. Jaffré on the Inria side and I. Faille and A. Fumagalli on the IFPEN side.

7. Partnerships and Cooperations

7.1. Regional Initiatives

GT Elfic (Labex DigiCosme, 2014–2016): "Programmes d'éléments finis formellement vérifiés", with TOCCATA (Inria Saclay - Île-de-France), LIX (École Polytechnique), CEA LIST, LIPN (Université de Paris 13), and LMAC (Université de Technologie de Compiègne).

7.2. National Initiatives

ANR DEDALES (2014–2017): "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. The project will specifically target 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, Maison de la Simulationand Andra. The coordinator of the project is M. Kern.

ANR GEOPOR (2014–2017): "Geometrical approach for porous media flows: theory and numerics", with Laboratoire Jacques-Louis Lions (Université de Paris 6).

ANR MANIF (2011–2014): "Mathematical and numerical issues in first-principle molecular simulation", with CERMICS (École Nationale des Ponts et Chaussées), and Laboratoire Jacques-Louis Lions (Université de Paris 6).

C2S@Exa (Computer and Computational Sciences at Exascale, 2011–2015) is an Inria Project Lab (IPL). This national initiative aims at the development of numerical modeling methodologies that fully exploit the processing capabilities of modern massively parallel architectures in the context of a number of selected applications related to important scientific and technological challenges for the quality and the security of life in our society. This project supports in particular the PhD of N. Birgle, supervised by. J. Jaffré, which is part of an Inria-Andra collaboration.

Projet P (2011–2015) is funded by the French FUI (*Fonds Unique Interministériel*). Project P aims at supporting the model-driven engineering of high-integrity embedded real-time systems by providing an open code generation framework. The contribution of project-team Pomdapi is in the domain of language translation and block-schema modelization semantics. This project supports the work of C. Franchini, under the supervision of P. Weis.

7.3. European Initiatives

7.3.1. Collaborations in European Programs, except FP7 & H2020

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

Other partners: Institute of Mathematics, Academy of Sciences of the Czech Republic; Oxford Centre for Nonlinear Partial Differential Equations, Great Britain.

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, see http://more.karlin.mff.cuni.cz/.

7.4. International Initiatives

7.4.1. Participation In other International Programs

Pomdapi is part of the EuroMediterranean 3+3 program with the project HYDRINV (2012–2015): Direct and inverse problems in subsurface flow and transport. Besides Inria, institutions participating in this project are: Universitat Politècnica de Catalunya (Barcelona, Spain), Universidad de Sevilla (Spain), École Mohamedia d'Ingénieurs (Rabat, Morocco), Université Ibn Tofaïl (Kenitra, Morocco), University Centre of Khemis Miliana (Algeria), École Nationale d'Ingénieurs de Tunis (Tunisia).

7.5. International Research Visitors

7.5.1. Visits of International Scientists

Todd Arbogast, professor, Center for Subsurface Modeling, The University of Texas at Austin. September 2014.

Peter Bastian, professor, Interdisciplinary Center for Scientific Computing, University of Heidelberg. June 2014.

H. Ben Ameur, professor at IPEST and member of ENIT-Lamsin, Tunis, Tunisia. June and December 2014.

G. D. Veerappa Gowda, professor, Tata Institute for Fundamental Research, Center for Applicable Mathematics, Bengalore. November-December 2014.

7.5.1.1. Internships

E. Ahmed, from École Nationale d'Ingénieurs de Tunis (Tunisia), has visited Pomdapi for nine months on the subject *Modélisation d'écoulements diphasiques dans un milieu poreux fracturé*.

F. Cheikh, from École Nationale d'Ingénieurs de Tunis (Tunisia), has visited Pomdapi for six months on the subject *Identification de failles dans un milieu poreux par une méthode d'indicateurs*.

M. H. Riahi, from École Nationale d'Ingénieurs de Tunis (Tunisia), has visited Pomdapi for six months on the subject *Identification de paramètres hydrogéologiques dans un milieu poreux*.

7.5.2. Visits to International Teams

7.5.2.1. Research stays abroad

M. Vohralík, April 1st–May 9th. Research stay in the framework of the project MORE "Implicitly constituted material models: from theory through model reduction to efficient numerical methods", Charles University in Prague, see http://more.karlin.mff.cuni.cz/.

8. Dissemination

8.1. Promoting Scientific Activities

8.1.1. Scientific events organization

M. Kern, with H. Ben Ameur (ENIT-Lamsin, Tunis), I. Ben Gharbia (IFPEN) and V. Martin (Université de Technologie de Compiègne) organized the Conference *Modeling and simulation in porous media*, 8-9 Dec 2014, Rocquencourt. The conference was held in honor of Jean Roberts and Jérôme Jaffré, and gathered 14 internationally recognized scientists. It was attended by about 60 participants. Talks can be found on the event web page http://mspm-jrjj2014.sciencesconf.org/.

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

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

M. Kern is a member of the Scientific Board of GDR Calcul.

M. Kern is a member of the jury and executive board of Label C3I.

J. E. Roberts is a member of the External Advisory Board for CFSES (Center for Frontiers of Subsurface Energy Security), University of Texas at Austin and SANDIA National Laboratories, Albuquerque, New Mexico.

J. E. Roberts is a member of the prize committee for the Interpore society.

J. E. Roberts is a member of the selection committee for recruiting professors in the department of maths of the University of Bergen, and a member of the national Norwegian committee for the promotion of professors.

M. Vohralík started to co-organize, from September 2013, together with Irène Vignon-Clementel from the project-team REO, the monthly *Modeling and Scientific Calculation Seminar* of the Inria Paris-Rocquencourt research center, see the web page https://iww.inria.fr/modelisation_et_calcul_scientifique/en/.

8.1.1.1. member of the editorial board

M. Vohralík is a member (from December 2013) of the editorial board of *SIAM Journal on Numerical Analysis*, see http://www.siam.org/journals/sinum/board.php.

8.1.1.2. reviewer

M. Kern was reviewer for the journals *Transport in Porous Media*, *Computational Geosciences* and *Mathematics and Computers in Simulation*.

8.2. Teaching - Supervision - Juries

8.2.1. Teaching

Training: F. Clément, *Mise en œuvre de techniques numériques d'inversion de paramètres distribués*, 12 h, M2, LEME, Université de Paris 10, France.

Master: J. Ch. Gilbert, *Optimisation différentiable — Théorie et algorithmes*, 42 h, M1, Ensta ParisTech, France.

Master: C. Josz, *Optimisation différentiable — Théorie et algorithmes*, 30 h, M1, Ensta ParisTech, France.

Master: C. Josz, *Analyse convexe et optimisation non différentiable*, 6 h, M2, Ensta ParisTech, France.

Licence: C. Josz, *Analyse hilbertienne*, 24 h, L3, Université de Paris 1, France.

Master: M. Kern, *Éléments finis*, 30 h, M1, Mines ParisTech, France.

Master: M. Kern, *Problèmes inverses*, 26 h, M1, Mines ParisTech, France.

Master: M. Kern, *Écoulements dans la géosphère*, 18 h, M2, Master Modélisation et Simulation, Fondation de coopération scientifique du campus du plateau de Saclay.

Master: M. Vohralík, *A posteriori error estimates for efficiency and error control in numerical simulations*, 36 hours/year, M2, Laboratoire Jacques-Louis Lions (Université de Paris 6), France.

Master: M. Vohralík, *A posteriori error estimates for efficiency and error control in numerical simulations*, 36 hours/year, M2, Department of Numerical Mathematics, Charles University in Prague, Czech Republic.

8.2.2. Supervision

PhD: Viatcheslav Vostrikov, *Numerical simulation of two-phase multicomponent flow with reactive transport in porous media*, Université de Pau et des Pays de l'Adour, defended on December 15th, 2014, B. Amaziane and M. Kern.

PhD in progress: Sarah Ali Hassan, *A posteriori error estimates and stopping criteria for domain decomposition solvers with local time stepping*, November 2013, M. Vohralík.

PhD in progress: N. Birgle, *Écoulements souterrains, méthodes numériques, et calcul haute performance*, October 2012, J. Jaffré.

PhD in progress: F. Cheikh, *Identification de failles dans un milieu poreux par une méthode d'indicateurs*, December 2011, J. E. Roberts and H. Ben Ameur.

PhD in progress: C. Josz, *Optimisation globale des flux d'énergie dans un réseau de transport d'électricité*, May 2013, J. Ch. Gilbert.

PhD in progress: M. H. Riahi, *Identification de paramètres hydrogéologiques dans un milieu poreux*, December 2011, J. Jaffré and H. Ben Ameur.

8.2.3. Juries

M. Kern was part of the PhD thesis committee of *Feng Xing*, Université de Lille (December 2014).

M. Vohralík has been in the PhD thesis committee of *Karel Tůma*, Charles University in Prague, Czech Republic (April 4th, 2014).

8.3. Popularization

J. Ch. Gilbert has written the following page on Wikipedia.fr in 2014: Optimisation quadratique.

M. Kern participated in a meeting with high school students during the "Fête de la Science" (CNAM, Paris, October 3rd, 2014), and gave presentations on the theme "Mathematics and Simulation for Underground Water" to middle school and high school students.

9. Bibliography

Publications of the year

Articles in International Peer-Reviewed Journals

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[2] C. CANCÈS, I. S. POP, M. VOHRALÍK. *An a posteriori error estimate for vertex-centered finite volume discretizations of immiscible incompressible two-phase flow*, in "Mathematics of Computation", 2014, vol. 83, n° 285, pp. 153-188, https://hal.archives-ouvertes.fr/hal-00623209

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Invited Conferences

[10] G. PICHOT, P. LAUG, J. ERHEL, J. E. ROBERTS, J. JAFFRÉ, J.-R. DE DREUZY. *Meshing Strategies and the Impact of Finite Element Quality on the Velocity Field in Fractured Media*, in "SIAM Annual Meeting", Chicago, United States, July 2014, https://hal.inria.fr/hal-01074807

Research Reports

[11] A. CHICHE, J. C. GILBERT. *How the augmented Lagrangian algorithm can deal with an infeasible convex quadratic optimization problem*, Inria Paris-Rocquencourt, 2015, n^o RR-8583, 31 p. , https://hal.inria.fr/hal-01057577

Scientific Popularization

[12] D. A. DI PIETRO, M. VOHRALÍK, S. YOUSEF. *An a posteriori-based, fully adaptive algorithm with adaptive stopping criteria and mesh refinement for thermal multiphasecompositional flows in porous media*, in "Computer and mathematics with applications", December 2014, vol. Volume 68, n° Issue 12, Part B, pp. 2331-2347 [*DOI :* 10.1016/J.CAMWA.2014.08.008], https://hal.archives-ouvertes.fr/hal-00856437

Other Publications

[13] E. CANCÈS, G. DUSSON, Y. MADAY, B. STAMM, M. VOHRALÍK. *A perturbation-method-based a posteriori estimator for the planewave discretization of nonlinear Schrödinger equations*, May 2014, https://hal.archives-ouvertes.fr/hal-00994568

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[18] C. JOSZ, D. HENRION. *Strong duality in Lasserre's hierarchy for polynomial optimization*, December 2014, https://hal.archives-ouvertes.fr/hal-00997726

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