Activity Report 2013

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.

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]
Jean Elizabeth Roberts [Inria, Senior Researcher, HdR]
Martin Vohralík [Inria, Senior Researcher, HdR]
Pierre Weis [Inria, Senior Researcher]

Faculty Member

Caroline Japhet [On leave from Université de Paris 13, Associate Professor]

External Collaborators

Hend Ben Ameur [IPEST and ENIT-Lamsin, Tunis, Tunisia, Professor]
Ibtihel Ben Gharbia [Université de Paris 9, until September 30th, 2013]
Guy Chavent [Université de Paris 9]
Zoubida Mghazli [Université Ibn Tofaïl, Kenitra, Morocco, Professor]
Vincent Martin [Université Technologique de Compiègne, Associate Professor]

Engineers

Clément Franchini [Inria, from September 1st, 2013]
Émilie Joannopoulos [Inria]

PhD Students

Elyes Ahmed [ENIT-Lamsin, Tunis, Tunisia]
Sarah Ali Hassan [Inria, from November 1st, 2013]
Nabil Birgle [Inria]
Fatma Cheikh [ENIT-Lamsin, Tunis, Tunisia and Université de Paris 6]
Thi Thao Phuong Hoang [Inria]
Cédric Josz [RTE, Cifre RTE-Inria, from March 1st, 2013]
Mohamed Hedi Riahi [ENIT-Lamsin, Tunis, Tunisia and Université de Paris 6]

Post-Doctoral Fellows

Martin Čermák [University of Ostrava, Czech Republic, from August 1st until November 30th, 2013]
Zuqi Tang [Inria, from November 1st, 2013]

Administrative Assistant

Nathalie Bonte [Inria]

Other

Markus Köppel [University of Stuttgart, Germany, until June 30th, 2013]

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 for the implementation of the coupling of numerical codes, and 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. Software and Platforms

4.1. LifeV

Participant: Michel Kern.

LifeV is a finite element (FE) library providing implementations of state of the art mathematical and numerical methods. It serves both as a research and production library. It has been used already in medical and industrial context to simulate fluid structure interaction and mass transport. LifeV is the joint collaboration between four institutions: École Polytechnique Fédérale de Lausanne (CMCS) in Switzerland, Politecnico di Milano (MOX) in Italy, Inria (Pomdapi) in France and Emory University (Sc. Comp) in the U.S.A.

Version 3.1.1

Programming language: C++

http://www.lifev.org/

4.2. M1cg1

Participant: Jean Charles Gilbert.

M1cg1 solves convex quadratic optimization problems and builds preconditioning matrices.

Version: 1.2

Programming language: Fortran 77

14 downloads in 2013

https://who.rocq.inria.fr/Jean-Charles.Gilbert/modulopt/optimization-routines/m1cg1/m1cg1.html

4.3. M1qn3

Participant: Jean Charles Gilbert.

M1qn3 solves very large scale differentiable optimization problems.

Version: 3.3

Programming language: Fortran 77

36 downloads in 2013

https://who.rocq.inria.fr/Jean-Charles.Gilbert/modulopt/optimization-routines/m1qn3/m1qn3.html

In collaboration with Claude Lemaréchal (project-team Bipop)

4.4. Oqla, Qpalm

Participants: Jean Charles Gilbert, Émilie Joannopoulos.

Oqla and Qpalm aim at solving large scale convex quadratic functions on a polyhedron by an augmented Lagrangian method.

Versions (in development): 0.1 (Oqla), 0.2 (Qpalm)

Programming languages: `C++` (Oqla), `Matlab` (Qpalm)

4.5. 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: 1.0+pl0

Programming language: OCaml

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

4.6. SQPlab

Participant: Jean Charles Gilbert.

SQPlab solves constrained differentiable optimization problems.

Version: 0.4.5

Programming language: Matlab

200 downloads in 2013

https://who.rocq.inria.fr/Jean-Charles.Gilbert/modulopt/optimization-routines/sqplab/sqplab.html

4.7. 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

Programming language: OCaml

http://sklml.inria.fr/

4.8. FreeFem++

Participants: Martin Vohralík, Martin Čermák, Zuqi Tang.

The scientific calculation code FreeFem++ is an excellent example of a complex software numerical simulation tool. It in particular encompasses all specification 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 integrate 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 are being implemented.

Version 3.26-2

Programming language: C++

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

5. Bilateral Contracts and Grants with Industry

5.1. Bilateral Contracts with Industry

RTE (*Réseau de Transport de l'Électricité*) financially supports the supervision of the PhD thesis of C. Josz, through a convention that is part of the Cifre, which also partly finances the thesis. J. Ch. Gilbert is the thesis advisor.

Andra (*Agence Nationale pour la gestion des Déchets Radioactifs*) has sponsored the PhD of T. T. P. Hoang, (surpervised by J. E. Roberts, C. Japhet and M. Kern) on space–time domain decomposition methods for modeling ransport in porous media. This work was part of the Andra–Inria research agreement. The thesis was defended in December 2013 [1].

This work will be continued in the PhD of S. Ali Hassan (supervised by M. Vohralík), to integrate a posteriori error estimated, and adaptive stopping criteria for the iterative methods.

IFPEN (*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.

5.2. Bilateral Grants with Industry

M. Vohralík, together with Vivette Girault (Université de Paris 6), have led the ERT (*Équipe de Recherche Technologique*) project between the Laboratoire Jacques-Louis Lions (LJLL) and IFPEN on "enhanced oil recovery and geological sequestration of CO_2: mesh adaptivity, a posteriori error control, and other advanced techniques". Project with an industrial partner designed to *overcome a technological issue*.

6. Partnerships and Cooperations

6.1. National Initiatives

ANR GEOPOR: "Geometrical approach for porous media flows: theory and numerics", with LJLL (Université de Paris 6).

ANR MANIF: "Mathematical and numerical issues in first-principle molecular simulation", with Cermics (École Nationale des Ponts et Chaussées), and LJLL (Université de Paris 6).

ARC Geofrac: (*Action de Recherche Coopérative*, Inria) "Large-scale computation of flow in complex 3D geological fractured porous media" with Inria project-teams Sage and Gamma3. From 2011.

C2S@Exa (Computer and Computational Sciences at Exascale) is an Inria Porject 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: Project P is a four-year research project funded by the French FUI (*Fonds Unique Interministériel*) that started in 2011. 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 modelisation semantics. This project supports the work of C. Franchini (under the supervision of P. Weis).

6.2. European Initiatives

6.2.1. FP7 Projects

Program: ERC Czech Republic

Project acronym: MORE

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

Duration: September, 2012–August, 2017

Coordinator: Josef Málek, Charles University in Prague

Other partners: Charles University in Prague, Czech Republic; Institute of Mathematics, Academy of Sciences of the Czech Republic, Czech Republic; Oxford Centre for Nonlinear Partial Differential Equations, United Kingdom

www: http://more.karlin.mff.cuni.cz/

6.3. International Initiatives

Pomdapi is associated with LIRNE-Équipe d'Ingéniérie Mathématiques, Université Ibn Tofaïl (Kenitra, Morocco) (PHC Volubilis) in the project "Techniques multi-échelles adaptatives pour la résolution des problèmes d'écoulement et de transport en milieux poreux hétérogènes". From 2010.

Pomdapi is part of the EuroMediterranean 3+3 program with the project HYDRINV (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). From 2012.

6.4. International Research Visitors

6.4.1. Visits of International Scientists

Laïla Amir, professor at FSTG in Marrakech, Morocco, was invited for one week.

H. Ben Ameur, professor at IPEST and member of the ENIT-Lamsin laboratory, Tunis, Tunisia, was invited for three months.

Lamia Guellouz, associate professor at Ecole Nationale d'Ingénieurs de Tunis, Tunisia, was invited for two weeks.

Z. Mghazli, professor at university Ibn Tofaïl, Kenitra, Morocco, was invited for one week.

6.4.2. 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*.

6.4.3. Visits to International Teams

M. Vohralík has visited from March 29th till May 15th Charles University in Prague, Czech Republic, Departement of Numerical Analysis (collaboration on the project MORE, teaching a Master 2nd year course).

7. Dissemination

7.1. Scientific Animation

J. Jaffré organized (with P. Knabner) the mini symposium "Complementarity Problems for Flow in a Porous Medium" at the SIAM Geosciences conference, June 17–20, 2013, Padova, Italy.

C. Japhet and M. Kern organized the mini symposium "Coupled Models and Domain Decomposition in Geosciences" at the SIAM Geosciences conference, June 17–20, 2013, Padova, Italy.

M. Kern was co-chair of the Scientific Committee of the SIAM Conference on Mathematical and Computational Issues in the Geosciences http://www.siam.org/meetings/gs13/, June 17–20, Padova, Italy.

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

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 organized (with A. Scotti and L. Formaggia) the mini symposium "Discrete-fracture Models for Porous Media Flow" at the SIAM Geosciences conference, June 17–20, 2013, Padova, Italy.

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 was member of the ENUMATH 2013 scientific committee, see http://enumath2013.epfl.ch/.

M. Vohralík organized a workshop on "A posteriori error estimates and mesh adaptivity for porous medium problems", on November 13th, 2013, see https://who.rocq.inria.fr/Martin.Vohralik/A_posteriori/13/.

7.2. Teaching - Supervision - Juries

7.2.1. Teaching

Licence : I. Ben Gharbia, *Mathématiques 4*, 54 h, L2, Université de Paris 2, France.

Licence : I. Ben Gharbia, *Statistiques 4*, 54 h, L2, Université de Paris 2, France.

Master : J. Ch. Gilbert, *Optimisation différentiable – Théorie et algorithmes*, 42 h, M1, ENSTA ParisTech, 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. Vohralík, A posteriori error estimates for efficiency and error control in numerical simulations, 36 h, M2, Université de Paris 6, France.

Master : M. Vohralík, A posteriori error estimates for efficiency and error control in numerical simulations, 21 h, M2, Charles University, Czech Republic.

7.2.2. Supervision

PhD : T. T. P. Hoang, *Méthodes de décomposition de domaine espace-temps pour la formulation mixte de problèmes d'écoulement et de transport en milieu poreux*, Université de Paris 6, December 11th, 2013, J. E. Roberts, C. Japhet, M. Kern.

PhD : Carole Widmer-Heinry, Adaptive finite volume method based on a posteriori error estimators for solving two phase flow in porous media, Université de Paris 6, November 21st, 2013, M. Vohralík, Vivette Girault (LJLL), Huy Tran (IFPEN).

PhD : Soleiman Yousef, A posteriori error estimates and adaptivity based on stopping criteria and adaptive mesh refinement for multiphase and thermal flows. Application to steam-assisted gravity drainage, Université de Paris 6, December 10th, 2013, M. Vohralík, Vivette Girault (LJLL), Éric Flauraud (IFPEN).

PhD in progress : E. Ahmed, *Modélisation d'écoulements diphasiques dans un milieu poreux fracturé*, January 2012, J. E. Roberts and A. Ben Abda.

PhD in progress : S. Ali Hassan, *Estimations d'erreur a posteriori et critères d'arrêt pour des solveurs par décomposition de domaine et avec des pas de temps locaux*, November 1st, 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 1st, 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.

7.2.3. Juries

J. Ch. Gilbert was a member of the Selection Commity for a Maître de Conférence position at both Université Joseph Fourier (Grenoble 1) and ENSEEIHT (INP Toulouse).

M. Vohralík was the referee of the PhD thesis of Simon Lemaire (Université de Paris 12, December 12th, 2013) and examiner of the HdR thesis of Ludovic Chamoin (ENS Cachan, October 11th, 2013).

7.3. Popularization

J. Ch. Gilbert has written the following pages on Wikipedia.fr in 2013: Algorithme des directions alternées, Borne d'erreur, Complémentarité, Cône dual, Ensemble de sous-niveau, Gradient projeté, Inéquation variationnelle, Lagrangien (optimisation), Lemme de Hoffman, Matrice complètement positive, Matrice copositive, Méthode de Gauss-Seidel, Optimisation complètement positive, Optimisation conique, Optimisation convexe, Optimisation copositive, Optimisation SDP.

M. Kern gave a talk on "Mathematics and Simulation" at the *Palmarès académique des Olympiades de mathématiques de l'Académie de Paris*, on May 29th, 2013.

M. Kern gave a talk on "Mathematics and Subsurface Water", as part of the *Promenades mathématiques* program for students in Terminale S and 1ère S, at Lycée Émilie du Châtelet (Serris), on May 22nd, 2013.

8. Bibliography

Publications of the year

Doctoral Dissertations and Habilitation Theses

[1] T. T. P. HOANG. , *Méthodes de décomposition de domaine espace-temps pour la formulation mixte de problèmes d'écoulement et de transport en milieu poreux*, Université Pierre et Marie Curie - Paris VI, December 2013, http://hal.inria.fr/tel-00922325

Articles in International Peer-Reviewed Journals

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