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Activity Report 2012

Project-Team POMDAPI

Environmental Modeling, Optimization and Programming Models

Table of contents

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

Creation of the Project-Team: January 01, 2012 .

1. Members

Research Scientists

François Clément [Researcher, Inria]
Jean Charles Gilbert [Senior Researcher, Inria]
Jérôme Jaffré [Team leader, Senior Researcher, Inria, HdR]
Michel Kern [Researcher, Inria]
Jean E. Roberts [Senior Researcher, Inria, HdR]
Martin Vohralík [since September 1 Senior Researcher, Inria, HdR]
Pierre Weis [Senior Researcher, Inria]

Faculty Members

Hend Ben Ameur [Associate Professor, IPEST and ENIT-Lamsin, HdR]
Guy Chavent [Professor Emeritus, University Paris Dauphine, HdR]
Caroline Japhet [Associate Professor, on leave from University Paris Nord]

PhD Students

Ibtihel Ben Gharbia [until August 31st University Paris Dauphine, since September 1st University Paris II]
Alice Chiche [University Pierre et Marie Curie, Cifre EDF, until February 28]
Phuong Hoang Thi Thao [University Pierre et Marie Curie, Inria fellowship, Andra contract]
Mohamed Hedi Riahi [Ecole Nationale d'Ingénieurs de Tunis et University Pierre et Marie Curie]
Fatma Cheikh [Ecole Nationale d'Ingénieurs de Tunis et University Pierre et Marie Curie]
Elyes Mohamed [Ecole Nationale d'Ingénieurs de Tunis]

Administrative Assistant

Nathalie Bonte

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 (i) 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; (ii) problems of flow and transport in porous media for hydrogeology or oil reservoir simulation; and (iii) 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 Newtonian solvers, interior point methods, decomposition methods for large scale optimization (application to the optimization of the electricity production), algebraic optimization, derivative free optimization, and semi-definite optimization (application to the global optimization of the power flow in an electricity network). *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. Software

3.1. 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/

3.2. M1cg1

– Participant: J. Ch. Gilbert.
– Version: 1.2.
– Programming language: Fortran 77.
– Solves a convex quadratic optimization problem and builds a preconditioning matrix, 8 downloads in 2012.
– https://who.rocq.inria.fr/Jean-Charles.Gilbert/modulopt/optimization-routines/m1cg1/m1cg1.html.

3.3. M1qn3

– Participants: J. Ch. Gilbert, Cl. Lemaréchal.
– Version: 3.3.
– Programming language: Fortran 77.
– Solves a very large scale differentiable optimization problem, 34 downloads in 2012.
– https://who.rocq.inria.fr/Jean-Charles.Gilbert/modulopt/optimization-routines/m1qn3/m1qn3.html.

3.4. Sklml

Participants: François Clément, Pierre Weis.

Easy coarse grain parallelization.

See also the web page http://sklml.inria.fr/.

- Version: 1.0+pl1
- Programming language: OCaml

3.5. SQPlab

– Participant: J. Ch. Gilbert.
– Version: 0.4.5.
– Programming language: Matlab.
– Solves a constrained differentiable optimization problem, 211 downloads in 2012.
– https://who.rocq.inria.fr/Jean-Charles.Gilbert/modulopt/optimization-routines/sqplab/sqplab.html.

4. Bilateral Contracts and Grants with Industry

4.1. Bilateral Contracts with Industry

Agence Nationale pour la gestion des Déchets RAdioactifs (Andra) Pomdapi takes part in 2 projects in the framework of the Andra–Inria research agreement;

- Ph. Hoang–Thi–THao is preparing a PhD (surpervised by J. E. Roberts, C. Japhet and M. Kern) on space–time domain decomposition methods for modeling transport in porous media.
- M. Kern is advising Andra in the choice of high performance linear algebra solvers for the heterogeneous problems encountered in flow simulations.

4.2. Bilateral Grants with Industry

Martin Vohralík, conjointement avec Vivette Girault (Université Pierre et Marie Curie), dirigent le projet **ERT (Equipe de Recherche Technologique)** entre le Laboratoire Jacques-Louis Lions (LJLL) et l'Institut Français du Pétrole Energies Nouvelles (IFPEN) sur la *Récupération d'huile assistée et séquestration géologique du* CO_2*: adaptation de maillage, contrôle d'erreur a posteriori et autres techniques avancées*. Projet mené en partenariat avec des industriels afin de « lever des blocages technologiques ». 9 chercheurs du LJLL, 6 chercheurs de l'IFPEN, 2 doctorants, stagiaires.

5. Partnerships and Cooperations

5.1. National Initiatives

ANR Fost: *Formal prOofs about Scientific compuTations*, with EPI Proval (Inria Saclay - Île-de-France), Laboratoire de Recherche en Informatique (University of Paris 11), and Laboratoire d'Informatique de l'Université Paris-Nord (University of Paris 13). Until May 31st.

ANR MANIF: *Problèmes mathématiques et numériques en simulation moléculaire ab initio*, with CER-MICS (Ecole Nationale des Ponts et Chaussées), and LJLL (Université Pierre et Marie Curie).

ARC Geofrac: Action de Recherche coopérative Inria "Large-scale computation of flow in complex 3D geological fractured porous media" rassemblant les équipes Inria Sage, Gamma3 et Pomdapi. From 2011.

5.2. European Initiatives

5.2.1. Collaborations in European Programs, except FP7

Program: ERC République tchèque

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, Université Charles à Prague

Other partners: Université Charles à Prague, République tchèque; Institut des mathématiques, Académie des Sciences de la République tchèque, République tchèque; Oxford Centre for Nonlinear Partial Differential Equations, UK.

5.3. International Initiatives

5.3.1. Participation In International Programs

- Pomdapi is associated with LIRNE-Equipe d'ingéniérie mathématiques, université Ibn Tofaïl, Kenitra, Maroc (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, Universidad de Sevilla, université Ibn Tofaïl (Kenitra, Maroc), University Centre of Khemis Miliana (Algeria), Ecole Nationale d'Ingénieurs de Tunis.

5.4. International Research Visitors

5.4.1. Internships

Mohamed Hedi Riahi (from May 2012 until Aug 2012)

 Subject: Implémentation d'un algorithme d'estimation de paramètres

 Institution: Ecole Nationale d'Ingénieurs de Tunis (Tunisia)

Fatma Cheikh (from Sep 2012 until Nov 2012)

 Subject: Implémentation d'indicateurs de localisation de failles en milieux poreux

 Institution: Ecole Nationale d'Ingénieurs de Tunis (Tunisia)

Emna Mejri (from Jun 2012 until Jul 2012)

 Subject: Ecoulements eau-air en milieu poreux

 Institution: Ecole Nationale d'Ingénieurs de Tunis (Tunisia)

5.4.2. Visits to International Teams

J. Jaffré and J. E. Roberts were invited by Rainer Helmig to visit the Department of Hydromechanics and Modelling of Hydrosystems (March 14 – April 6 2012).

6. Dissemination

6.1. Scientific Animation

C. Japhet was in the local organization committee for the 21st International Conference on Domain Decomposition Methods, Rennes, 25-29 June 2012.

C. Japhet and M. Kern have organized a minisymposia on Domain decomposition for porous media flow and transport at the 21st International Conference on Domain Decomposition Methods, Rennes, 25-29 June 2012.

C. Japhet and Y. Maday (UPMC-Paris 6) have organized a minisymposia on Domain decomposition with mortars at the 21st International Conference on Domain Decomposition Methods, Rennes, 25-29 June 2012.

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

M. Kern is Program Director of the SIAM Activity Group on Geosciences, and is co-chair (with M. Putti, University of Padova) of the SIAM Conference on Mathematical and Computational Issues in the Geosciences (to be held June 17-20, 2013 in Padova, Italy).

M. Kern was part of the program committee for the 21st International Conference on Domain Decomposition Methods, Rennes, 25-29 June 2012.

J. E. Roberts is a member of the External Advisory Board for CFSES (Center for Frontiers of Subsurface Energy Security).

J. E. Roberts organized (with Z. Mghazli and H. Ben Ameur) the mini symposium "Problems in porous media: modeling and solving techniques" at the SM2A conference, 10-13 September 2012, Marrakech, Morrocco.

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.

J. E. Roberts was a member of the Scientific Committee and the Prize Committee for the Interpore 2012 conference, May 14-16, West Lafayette, Indiana. USA. For this conference she also organized the 3 session mini-symposium "Numerical modeling for flow in fractured and other heterogeneous porous media".

J. E. Roberts was a member of the Nominating Committee for Officers of the SIAM Activity Group Geosciences.

6.2. Teaching - Supervision - Juries

6.2.1. Teaching

Licence : I. Ben Gharbia, *Analyse numérique et calcul scientifique*, 78 h, L2, Université Paris–Dauphine, France.

Licence : I. Ben Gharbia, *Mathématiques 5*, 54 h, L3, Université Panthéon–Assas, France.

Licence : I. Ben Gharbia, *Mathématiques 1*, 18 h, L1, Université Panthéon–Assas, France.

Licence : I. Ben Gharbia, *Statistiques 1*, 18 h, L1, Université Panthéon–Assas, France.

Licence : F. Clément, *Calcul différentiel*, 17 h, L3, Mines ParisTech, 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: J. Jaffré et J. E. Roberts, *Volumes finis et éléments finis mixtes*, 20 h, M2, École Nationale d'Ingénieurs de Tunis (ENIT), Tunisia.

Master: J. E. Roberts, *Approximation methods*, 20 h, M1, École Supérieure d'Ingénieurs Léonard de Vinci, France.

6.2.2. *Supervision*

PhD: Ibtihel Ben Gharbia, *Résolution de Problèmes de Complémentarité – Application à un Écoulement Diphasique Dans un Milieu Poreux*, Université Paris-Dauphine, 5th of December 2012, supervision J. Ch. Gilbert and J. Jaffré.

PhD : Nancy Chalhoub, Estimations a posteriori pour l'équation de convection–diffusion–réaction instationnaire et applications aux volumes finis, Université Paris-Est, 17 décembre 2012, Alexandre Ern (Université Paris-Est), Toni Sayah (Université Saint Joseph, Liban), Martin Vohralík.

PhD: Alice Chiche, *Théorie et Algorithmes Pour la Résolution de Problèmes d'Optimisation de Grande Taille – Application à la Gestion de Production d'Électricité*, Université Pierre et Marie Curie, 28th of June 2012, supervision J. Ch. GILBERT.

PhD in progress: Soleiman Yousef, *Estimations d'erreur a posteriori et adaptativité pour le problème de Stefan*, septembre 2009, Vivette Girault (Université Pierre et Marie Curie), Martin Vohralík.

PhD in progress: Carole Heinry, *Adaptation de maillage et contrôle d'erreur a posteriori pour récupération d'huile assistée*, septembre 2009, Vivette Girault (Université Pierre et Marie Curie), Martin Vohralík.

PhD in progress: Paul-Marie Berthe, Méthode de décomposition de domaines espace-temps pour la mécanique des fluides, septembre 2009, Pascal Omnes (CEA, Université Paris 13), Caroline Japhet.

PhD in progress: Hoang PHUONG THI THAO, *Space Time Domain Decomposition Methods for Transport in Porous Media*, University Pierre et Marie Curie, October 2010, supervision: Jean E. Roberts, Caroline Japhet, Michel Kern.

PhD in progress: Mohamed Hedi Riahi, Identification de paramètres hydrogéologiques dans un milieu poreux, Ecole Nationale d'Ingénieurs de Tunis and University Pierre et Marie Curie, October 2011, supervision: Jérôme Jaffré and Hend Ben Ameur.

PhD in progress: Fatma Cheikh, Identification de failles dans un milieu poreux par une méthode d'indicateurs, Ecole Nationale d'Ingénieurs de Tunis and University Pierre et Marie Curie, October 2011, supervision: Jean E. Roberts and Hend Ben Ameur.

PhD in progress: Elyes Ahmed, Méthodes numériques pour la simulation d'écoulements diphasiques dans un milieu poreux fracturé, Ecole Nationale d'Ingénieurs de Tunis, October 2011, supervision: Jean E. Roberts and Amel Ben Abda.

6.2.3. *Juries*

- Martin Vohralík a été rapporteur de la thèse de Florent Pled (Vers une stratégie robuste et efficace pour le contrôle des calculs par éléments finis en ingénierie mécanique, ENS Cachan, directeur de thèse Pierre Ladevèze), soutenue le 13 décembre 2012.

- Jérôme Jaffré a été rapporteur de la thèse de Merline Flore Djouwe Meffeja (Simulation et modélisation de milieux granulaires confinés, université de Rennes I, directeurs de thèse Patrick Richard et Edouart Canot), soutenue le 20 janvier2012.

- Jérôme Jaffré a été aussi rapporteur de la thèse de Alessio Fumagalli (Numerical Modelling of Flows in Fractured Porous Media by the XFEM Method, Politecnico di Milano, directeur de thèse Luca Fromaggia), soutenue le 8 mai 2012.

- Jean E. Roberts a été rapporteur de la thèse de Xavier Tunc (Université de Provence, Marseille, directeur de thèse Thierry Gallouet), soutenue le 15 février 2012.

6.3. Popularization

- Creation of articles on Wikipedia.fr [19].
- Seminar on "Mathématiques pour modéliser les eaux souterraines" at "Faites de la Science" (M. Kern).
- Two seminars at the German-French worksop, October 18-19, Fellbach, Germany: J. Jaffré, "Mathematics for computing on a computer: The computer does not calculate exactly", J. E. Roberts, "Mathematics and simulation of subsurface flow".

7. Bibliography

Publications of the year

Doctoral Dissertations and Habilitation Theses

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[2] A. CHICHE. *Théorie et Algorithmes Pour la Résolution de Problèmes d'Optimisation de Grande Taille – Application à la Gestion de Production d'Électricité*, Université Pierre et Marie Curie, 2012, https://who.rocq.inria.fr/Jean-Charles.Gilbert/publications/theses/06-alice-chiche.pdf.

Articles in International Peer-Reviewed Journals

[3] I. BEN GHARBIA, JEAN CHARLES. GILBERT. *Nonconvergence of the plain Newton-min algorithm for linear complementarity problems with a P-matrix*, in "Mathematical Programming", 2012, vol. 134, p. 349-364, http://dx.doi.org/10.1007/s10107-010-0439-6.

[4] I. BEN GHARBIA, JEAN CHARLES. GILBERT. *An algorithmic characterization of P-matricity*, in "SIAM Journal on Matrix Analysis and Applications", 2013, in revision, http://hal.archives-ouvertes.fr/hal-00713330/en.

[5] I. BEN GHARBIA, J. JAFFRÉ. *Gas phase appearance and disappearance as a problem with complementarity constraints*, in "Mathematics and Computers in Simulation", 2013, to appear, http://hal.inria.fr/hal-00641621/.

[6] S. BOLDO, F. CLÉMENT, J.-C. FILLIÂTRE, M. MAYERO, G. MELQUIOND, P. WEIS. *Wave Equation Numerical Resolution: a Comprehensive Mechanized Proof of a C Program*, in "J. of Automated Reasoning", 2012, http://dx.doi.org/10.1007/s10817-012-9255-4.

[7] N. FRIH, V. MARTIN, J. E. ROBERTS, A. SAÂDA. *Modeling fractures as interfaces with nonmatching grids*, in "Computational Geosciences", 2012, vol. 16, p. 1043-1060, http://dx.doi.org/10.1007/s10596-012-9302-6.

[8] M. J. GANDER, C. JAPHET. *An algorithm for non-matching grid projections in 2d and 3d with linear complexity*, in "ACM Transaction on Mathematical Software", 2012, in revision.

[9] L. HALPERN, C. JAPHET, J. SZEFTEL. *Optimized Schwarz waveform relaxation and discontinuous Galerkin time stepping for heterogeneous problems*, in "SIAM J. Numer. Anal.", 2012, vol. 50(5), p. 2588-2611.

[10] C. JAPHET, Y. MADAY, F. NATAF. *A New Interface Cement Equilibrated Mortar (NICEM) method with Robin interface conditions : the P1 finite element case*, in "M3AS", 2012, to appear.

[11] P. KNABNER, J. E. ROBERTS. *Mathematical analysis of a discrete fracture model coupling Darcy flow in the matrix with Darcy-Forchheimer flow in the fracture*, in "M2AN", 2012, in revision.

International Conferences with Proceedings

[12] P.-M. BERTHE, C. JAPHET, P. OMNES. *Space-time domain decomposition with finite volumes for porous media applications*, in "Proceeding of the 21th International Conference on Domain Decomposition Methods", 2013, to appear.

[13] THI-THAO-PHUONG. HOANG, J. JAFFRÉ, C. JAPHET, M. KERN, J. E. ROBERTS. *Space Time Domain Decomposition for Mixed Formulation of Diffusion Equations*, in "Proceeding of the 21st International Conference on Domain Decomposition Methods", 2013, to appear.

[14] C. JAPHET, Y. MADAY, F. NATAF. *A new interface cement equilibrated mortar method with Ventcel conditions*, in "Proceeding of the 21th International Conference on Domain Decomposition Methods", 2013, to appear.

[15] C. JAPHET, P. OMNES. *Optimized Schwarz waveform relaxation for porous media applications*, in "Proceeding of the 20th International Conference on Domain Decomposition Methods", 2012, to appear.

Research Reports

[16] I. BEN GHARBIA, J. JAFFRÉ, J. E. ROBERTS, KUMAR N. SURESH. *A Composite Hexahedral Mixed Finite Element with Kershaw meshes*, Inria, April 2012, n$^{\mathrm{o}}$ RR-7936, 13, http://hal.inria.fr/hal-00690019.

[17] 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*, Inria, Rocquencourt, France, 2012, n$^{\mathrm{o}}$ 8197, http://hal.inria.fr/hal-00769201/en/.

[18] A. ERN, M. VOHRALÍK. *Adaptive inexact Newton methods with a posteriori stopping criteria for nonlinear diffusion PDEs*, Inria, October 2012, http://hal.inria.fr/hal-00681422.

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