INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Project-Team Estime

Parameter Estimation and Modeling in Heterogeneous Media

Rocquencourt

THEME NUM

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1. Team

Head
Jérôme Jaffré [DR, Inria, HdR]

Deputy Head
Michel Kern [CR, since 1/09 part time at the Ministère de la Recherche]

Administrative Assistants (shared with project Poems)
Irena Winkler [until 31/08]
Nathalie Bonte [from 1/09]

INRIA Researchers
François Clément [CR]
J. Charles Gilbert [DR]
Jean E. Roberts [DR, HdR]

Scientific Advisor
Guy Chavent [University Paris 9, HdR]

Visiting Scientists
Peter Bastian [University of Stuttgart, Germany, 3 weeks]
Hend Ben Ameur [University of Bizerte and Lamsin-ENIT, Tunisia, 4 months]

Postdoc
Shalini Gupta [ERCIM fellowship, until 31/03]
Guillaume Rousse [INRIA fellowship, until 30/11]
Jalila Sabil [INRIA fellowship, until 31/08]

Ph.D. Students
Laila Amir [Cifre Itasca fellowship, University of Paris 9]
Doublet Daniel [University of Bergen, 3 months]
Najla Frih [ENIT-LAMSIN and University of Paris 9]
Zheng Li [Inria fellowship, University of Paris 7, 3 months]
Estelle Marchand [ANDRA fellowship, University of Paris 9]
Amel Sboui [Inria fellowship, University of Paris 9]

Internships
Alice Chiche [ENSTA, second year (PPL), 1/5–31/7]
Jan Stuchly [University of Paris 6, Master de Sciences et Technologie, Mathématiques de la Modélisation, Parcours OJME, 1/2–30/6]

2. Overall Objectives

2.1. Overall Objectives

Multidomain simulation: When simulating phenomena on a large scale, it is natural to try to divide the domain of calculation into subdomains with different physical properties. According to these properties one may think of using in the subdomains different discretizations in space and time, different numerical schemes and even different mathematical models. Research toward this goal includes the study of interface problems, subdomain time discretization, implementation using high level programming languages and parallel computating. Applications are mostly drawn from environmental problems from hydrology and hydrogeology, such as studies for a deep underground nuclear waste disposal and for the coupling of water tables with surface flow.

Flow and transport in porous media with fractures: Looking at a scale where the fractures can be represented individually and considering the coupling of these fractures with the surrounding matrix rock, various numerical models where the fracture is represented as an interface between subdomains are proposed and analyzed. Transmission conditions are then nonlocal. One phase and twophase flow are studied.

Interphase problems for twophase flow in porous media: Twophase flow is modeled by a system of nonlinear equations which is either of parabolic type or of hyperbolic type depending on whether capillary pressure is taken into account or not. Interface problems occur when the physical parameters change from one rock type to the other, including the nonlinear coefficients (relative permeabilities and capillary pressure). The study of these interface problems leads to the modeling of twophase flow in a porous medium with fractures.

Reactive transport Efficient and accurate numerical simulation is important in several situations: the need to predict the fate of contaminated sites is the primary applications. Numerical simulation tools help to design remediation strategies, for example by natural degradation processes catalyzed by microbia which are present in the earth. Another important application is the assessment of long-term nuclear waste storage in the underground. Multi-species reactive ow problems in porous media are described by a set of partial dierential equations for the mobile species and ordinary dierential equations for the immobile species (which may be viewed as attached to the interior surfaces of the soil matrix) altogether coupled through nonlinear reaction terms. The large variety of time scales (e.g., fast aqueous complexation in the ground water and relatively slow biodegradation reactions and transport processes) makes it desirable to describe fast reactions by equilibrium conditions, i.e., by nonlinear algebraic equations.

Code Coupling and Grid Computing: As physical models become more and more sophisticated, we start encountering situations involving different physics. This leads naturally to a computer code built from individual components, where each component simulates one of the physical models. A natural extension is to have the individual components running on different computers (each one possibly being parallel). Applications include density–driven flow, modelling seawater intrusion in aquifers and reactive transport in porous media.

Functional Programming and scientific computation: Implementing subdomain coupling requires complex programming. This can be done efficiently using OCamlP3l, a recent development of the language OCaml which allows for parallel computing. This provides an alternative to Corba and MPI. Another example of implementation with OCaml is the programming of a parameterization method developped to estimate at the same time the zonation and the values of the hydraulic transmissivities in groudwater flow.

Parameter Estimation and sensitivity analysis: When parameters appearing in a Partial Derivative Equation (PDE) are not precisely known, they can be estimated from measures of the solution. The parameter estimation problem is usually formulated as a minimization problem for an Output Least-Squares (OLS) function. The adjoint state technique is an efficient tool to compute the analytical gradient of this OLS function which can be plugged into various local optimization codes. The Singular Value Decomposition is a powerful tool for deterministic sensitivity analysis. It quantifies the number of parameters which can be estimated from the field measures. This can help in choosing a parameterization of the searched coefficients, or even in designing the experiments. Current applications under study are in optometry, in hydrogeology and in reservoir simulation.

Optimization: An important facet of the project deals with the development optimization concepts and algorithms. This activity is in part motivated by the fact that parameter estimation leads to minimization problems. Special focus is on large scale problems, such as those encountered in engineering applications. The developed techniques and domains of interest include sequential quadratic programming, interior point methods, the augmented Lagrangian approach, bilevel optimization, nonlinear complementarity problems, *etc*. There are many applications: seismic tomography data inversion, shape optimization (aeronautic and tyre industry), mathematical modelling in medicine and biology (chronotherapy of cancer), to name a few. An outcome of this activity is also the *Modulopt library*, which gathers optimization softwares produced by the team.

3. Contracts and Grants with Industry

3.1. ANDRA

Sensitivity analysis for the simulation of the transport of nuclear contaminants around a nuclear waste disposal site. ANDRA is the French National Agency for Nuclear Waste Management. It is providing financial support for E. Marchand's PhD thesis.

3.2. Itasca

Numerical methods for coupling transport with chemistry in porous media. Itasca Consultant is part of the HC Itasca group, an independent, international engineering consulting and software development firm that solves hydrogeological- and geomechanics-related problems in the mining, civil, petroleum, waste isolation, and environmental industries. It is providing financial support for Laila Amir's PhD thesis, through a CIFRE fellowship.

4. Other Grants and Activities

4.1. National Cooperations

INRIA ARC Moprosco (Functional Programming for Scientific Computation), with Cristal group, with Laboratoire PPS from University of Paris 7, and with Dept. of Informatics from University of Pisa (Italy).

CNRS GDR Momas (Mathematical Modeling and Numerical Simulation for Deep Underground Disposal of Nuclear Waste).

Ministry of Research, ANR CerPAN (Certification de Programmes d'Analyse Numérique), with Laboratoire d'Informatique de l'Université Paris-Nord from University of Paris 13, with Centre d'Étude et de Recherche en Informatique du Cnam, with Laboratoire de Recherche en Informatique from University of Paris 11.

4.2. International Cooperations

Estime is associated with Lamsin-ENIT (LAboratoire de Mathématiques et de SImulation Numérique, École Nationale d'Ingénieurs de Tunis). This association is called Modess and is supported by INRIA. From 2006.

Estime is collaborating with Lamsin-ENIT through the Comité Mixte Franco-Tunisien pour la Coopération Universitaire (CMCU), Méthodes numériques en Hydrogéologie project. From 2005.

Estime is also participating in the project "Méthodes numériques en hydrogéologie" of the 3+3 Mediteranean program. From 2006.

Finally there is a cooperation with the Tata Institute of Fundamental Research (TIFR) in Bangalore through the CEFIPRA project "Conservation Laws and Hamilton Jacobi equations". From 1/09/2006.

5. Dissemination

5.1. Service to the scientific community

- J. Jaffré is co-editor-in-chief (with M.F. Wheeler) of the journal Computational Geosciences
- J. Jaffré organized the Journée GDR Momas Couplages pour la simulation des écoulements et du transport en milieu poreux, Inria-Rocquencourt, November 14.
- M. Kern and J. E. Roberts are members of the organizing committee for the next SIAM Conference on Mathematical & Computational Issues in the Geosciences, Santa Fe, March 2007.
- M. Kern is Vice Director of CNRS GDR MoMaS.

- J. E. Roberts is a member of the Editorial Board of the International Journal of Numerical Analysis and Modeling.

5.2. Teaching

L. Amir École d'ingénieurs des technologies de l'information et du management. *C Programming Language*, 1st year students, 42 h
École des Mines de Paris. *Finite elements*, 2nd and 3th year students, 9 h

J. Jaffré ENSTA (Master level), *Inverse Problems*, 18 hours
École Nationale d'Ingénieurs de Tunis (ENIT), Tunisia, DEA Mathématiques Appliquées, *Volumes finis et éléments finis mixtes*, 20 h with J. E. Roberts (since 2000).

J.Ch. Gilbert • University Paris VI, Master de Sciences et Technologie (M2), Mathématiques de la Modélisation, Parcours Optimisation & Théorie des Jeux - Modélisation en Économie, *Introduction aux méthodes de points intérieurs*, 18 h.
• ENSTA, 2nd year, *Optimisation différentiable – théorie et algorithmes*, 42 h.

M. Kern École des Mines de Paris, *Introduction to Scientific Computing*, 2nd year students, 24 hours
École des Mines de Paris, *Finite elements*, 2nd year students, 30 hours,
École Polytechnique, teaching assistant for *Modeling and Simulation Projects*, applied mathematics section, 4th year students, 20 hours.

E. Marchand Université Paris 2. 2nd year: *Mathematics and Statistics*, 21 h
École des Mines de Paris. 1st year: *Differential Calculus*, 22 h.

J. E. Roberts École Supérieure d'Ingénieurs Léonard de Vinci, *Approximation methods*, 4th year students, 20 hours,
École Nationale d'Ingénieurs de Tunis (ENIT), Tunisia, DEA Mathématiques Appliquées, *Volumes finis et éléments finis mixtes*, 20 h with J. Jaffré.

5.3. Conferences, Seminars, Invitations

L. Amir *Les méthodes de Newton-Krylov pour le couplage transport chimie* Congrès CANUM (38ème Congrès National d'Analyse Numérique), Beg er Lenn Guidel Morbihan, France, May 29-June 2.

Newton-Krylov methods for coupling transport with chemistry in porous media, 16th International Conference on Computational Methods in Water Resources(CMWR XVI), Copenhagen, Denmark, June 19-22.

Full coupling in transport of solutes in porous media with chemistry Workshop3+3, Numerical computing for groundwater flows, Mohammadia school engineering, Rabat, Morocco, September 20-22.

F. Clément *Inverse Problem, Image Processing and Functional Programming*, 1ères Rencontres MIP-LAMSIN en Imagerie Mathématique, RIMA'06, Tunis, May 4-5.
Moprosco : programmation fonctionnelle et calcul scientifique, Journées Nationales des ARC 2006, Grenoble, October 17-18.

N. Frih *Modeling Forchheimer Fractures as Interfaces*, 16th International Conference on Computational Methods in Water Resources(CMWR XVI), Copenhagen, Denmark, June 19-22.

J. Jaffré *Numerical Challenges in the Simulation of Contaminant Transport Around a Waste Repository*, Porous Media Day, Center for Analysis, Scientific Computing and Applications, Technische Universiteit Eindhoven, The Nederlands, April 26, an invited lecture in the honor of Mary F. Wheeler.
Darcy Flow Calculation with the Kuznetsov-Repin hexahedral mixed finite elements, Institute for Computational and Engineering Science, University of Texas at Austin, May 18.
Flux calculation at the interface between two rock types, Conference "The Mathematics of Finite Elements and Applications" (MAFELAP), Brunel university, Uxbridge, UK, June 13-16.
Darcy Flow Calculation with the Kuznetsov-Repin hexahedral mixed finite elements, Conference "The Mathematics of Finite Elements and Applications" (MAFELAP), Brunel university, Uxbridge, UK, June 13-16.
Mixed finite element and local time stepping for the transport of contaminant, Workshop3+3, Numerical computing for groundwater flows, Mohammadia school engineering, Rabat, Morocco, September 20-22.
L'analyse numérique au service du stockage des déchets radioactifs, Série d'exposés TPE à l'intention des professeurs de mathématiques des lycées, Inria-Rocquencourt, October 11. *Le benchmark 3-D champ lointain et ses difficultés*, Journée GDR Momas Couplages pour la simulation des écoulements et du transport en milieu poreux, Inria-Rocquencourt, November 14.
Simulation 3-D d'un problème de transport de contaminant en vue d'un stockage profond, Unesco High Performance Computing Workshop, Enit-Lamsin, Tunis, November 27- December 1.

M. Kern *Newton-Krylov methods for coupling transport with chemistry in porous media*, journée thématique << Transport réactif >> du GDR MoMaS, October 18.
A Newton–Krylov method for coupling transport with chemistry in porous media, Groupe de travail << Méthodes Numériques >>, Laboratoire Jacques-Louis Lions, Université Paris 6, December 4.

E. Marchand *Deterministic Sensitivity Analysis for the Numerical Simulation of the Transport of Contaminants*, Journée Andra des Doctorants, Paris, France, June 6.
Deterministic Sensitivity Analysis for the Numerical Simulation of the Transport of Contaminants, 16th International Conference on Computational Methods in Water Resources(CMWR XVI), Copenhagen, Denmark, June 19-22.
Parallel Computation with OcamlP3L, Workshop 3+3, Numerical Computing for Groundwater Flow, Rabat, Maroc, September 20-22.

J. E. Roberts *Mixed Finite Macroelements for Hexahedral Grids*, Séminaire Lamsin, ENIT, Tunis, January 20.
Simulating Flow in Porous Media With Fractures by Modeling Fractures as Interfaces, Conference "The Mathematics of Finite Elements and Applications" (MAFELAP), Brunel university, Uxbridge, UK, June 13-16.
Simulating Flow in Porous Media With Fractures by Modeling Fractures as Interfaces, Workshop 3+3, Numerical Computing for Groundwater Flow, Mohammadia school engineering, Rabat, Morocco, September 20-22.
Introduction aux méthodes de décomposition de domaines, Unesco High Performance Computing Workshop, Enit-Lamsin, Tunis, November 27-December 1.

A. Sboui *Mixed Hexahedral Finite Elements For Darcy Flow Calculations*, 16th International Conference on Computational Methods in Water Resources(CMWR XVI), Copenhagen, Denmark, June 19-22.

5.4. Consulting

- J.Ch. Gilbert is a consultant for the Institut Français du Pétrole. He had also consulting activities for Michelin at Clermont-Ferrand and EdF at Clamart.
- J. Jaffré is a member of the Scientific Advisory Board of CIPR, the Center for Integrated Petroleum Research at the university of Bergen.

6. Bibliography

Year Publications

Books and Monographs

[1] J.-F. BONNANS, J.-C. GILBERT, C. LEMARÉCHAL, C. SAGASTIZÁBAL. *Numerical Optimization – Theoretical and Practical Aspects(second edition)*, Universitext, Springer Verlag, Berlin, 2006.

Articles in refereed journals and book chapters

[2] L. AMIR, M. KERN, V. MARTIN, J.-E. ROBERTS. *Décomposition de domaine pour un milieu poreux fracturé : un modèle en 3D avec fractures qui s'intersectent*, in "ARIMA", vol. 5, 2006, p. 11-25, http://www-direction.inria.fr/international/arima/005/00502.htm.

[3] H. BEN AMEUR, F. CLÉMENT, P. WEIS, G. CHAVENT. *The Multidimensional Refinement Indicators Algorithm for Optimal Parameterization*, in "Journal of Inverse and Ill-Posed Problems", Submitted to, 2006.

[4] V. BOUYER, I. DARBORD, P. HERVÉ, G. BAUDIN, C. LE GALLIC, F. CLÉMENT, G. CHAVENT. *Shock-to-detonation transition of nitromethane: Time-resolved emission spectroscopy measurements*, in "Combustion and Flame", vol. 144, n^{o} 1–2, 2006, p. 139–150, http://dx.doi.org/10.1016/j.combustflame.2005.07.004.

[5] F. CLÉMENT, V. MARTIN, A. VODICKA, R. DI COSMO, P. WEIS. *Domain Decomposition and Skeleton Programming with OCamlP3l*, in "Parallel Computing", Special Issue on Algorithmic Skeletons, vol. 32, 2006, p. 539–550, http://dx.doi.org/10.1016/j.parco.2006.04.003.

[6] N. FRIH, J.-E. ROBERTS, A. SAÂDA. *Un modèle darcy-Forchheimer pour un écoulement dans un milieu fracturé*, in "ARIMA", vol. 5, 2006, p. 129-143.

[7] J.-C. GILBERT, P. JOLY. *Higher order time stepping for second order hyperbolic problems and optimal CFL conditions*, in "Computational Modeling with Partial Differential Equations in Science and Engineering", 2006.

[8] A. SBOUI, J. JAFFRÉ, J.-E. ROBERTS. *A Composite Mixed Finite element for general hexahedral grids for Darcy flow calculations*, Submitted, 2006.

[9] A. SBOUI, J. JAFFRÉ. *Discrétisation en temps par sous-domaine pour un probème d'advection en milieu poreux*, in "ARIMA", vol. 5, 2006, p. 330-346.

Publications in Conferences and Workshops

[10] L. AMIR, M. KERN. *Newton-Krylov methods for coupling transport with chemistry in porous media*, in "XVI International Conference on Computational Methods in Water ressources (CMWR XVI), Copenhagen, Denmark", P. BINNING, P. ENGESGAARD, H. DAHLE, G. PINDER, W. G. GRAY (editors). , 2006, http://proceedings.cmwr-xvi.org/getFile.py/access?contribId=315&sessionId=12&resId=0&materialId=paper&confId=a051.

[11] F. CLÉMENT, V. MARTIN, A. VODICKA, R. DI COSMO, P. WEIS. *Domain Decomposition and Skeleton Programming with OCamlP3l*, in "Proc. of the Internat. Conf. on Parallel Computing: Current & Future Issues

of High-End Computing", G. R. JOUBERT, W. E. NAGEL, F. J. PETERS, O. PLATA, P. TIRADO, E. ZAPATA (editors). , J. von Neumann Institute for Computing (NIC), vol. 33, NIC-Directors, 2006, p. 811–818.

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