



INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

*Project-Team Estime*

*Parameter Estimation and Modeling in  
Heterogeneous Media*

*Rocquencourt*

THEME NUM

*Activity*  
*R* *eport*

2005



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# 1. Team

## Head

Jérôme Jaffré [DR, Inria]

## Deputy Head

Michel Kern [CR]

## Administrative Assistants (shared with project Ondes)

Hélène Kutniak [until 30/09]

Nicole Loza [since 1/08]

## INRIA Researchers

François Clément [CR]

Jean Charles Gilbert [DR]

Jean E. Roberts [DR]

## Scientific Advisor

Guy Chavent [University Paris 9]

## External Collaborator

Hassan Kaddouri [Université du Littoral]

## Visiting Scientists

Hend Ben Ameer [University of Bizerte and Lamsin-ENIT, Tunisia, 4 months]

Hedia Chaker [Lamsin-ENIT, Tunisia, 3 weeks]

## postdoc

Shalini Gupta [ERCIM fellowship]

## Ph.D. Students

Laila Amir [Cifre Itasca fellowship, University of Paris 9]

Philippe Al Khoury [Cifre Auxitrol fellowship, Universities of Paris 9 and Paris 10]

Najla Frih [ENIT-LAMSIN and University of Paris 9]

Estelle Marchand [ANDRA fellowship, University of Paris 9]

Amel Sboui [Inria fellowship, University of Paris 9]

Berre Inga [University of Bergen, 2 months]

## Internships

Souaid Mezouar [Master de Sciences et Technologie, Mathématiques de la Modélisation, Parcours OJME, 1/6–30/9]

Émilie Pertuiset [Master Modélisation et Simulation, INSTN, 1/4–30/8]

# 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 computing. 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.

**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 OCamlP31, 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 developed to estimate at the same time the zonation and the values of the hydraulic transmissivities in groundwater 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 Moproco** (Functional Programming for Scientific Computation), with Cristal group, Laboratoire PPS from University of Paris 7 and 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, ACI "Globalization of Computer Resources and Data", **Project Hydrogrid**, with projects Aladin and Paris at Inria-Rennes, with IMFS at Louis Pasteur University in Strasbourg, and with the "Transferts physiques et chimiques" group at UMR Geosciences, Rennes.

### 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 **E-Didon** and is supported by INRIA. From 2002.

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

## 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**
- M. Kern and J. E. Roberts organized the **SIAM Conference on Mathematical & Computational Issues in the Geosciences**, Avignon, June 7-10, 2005.
- M. Kern (with A. Bourgeat from Université Lyon 1) was the organizer of the CEA-EDF-INRIA school on "Flow in unsaturated porous media: mathematical and numerical aspects", on September 12-15 at INRIA.
- M. Kern is Scientific Secretary 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

- F. Clément École des Mines de Paris. 1st year: *Differential Calculus*, 22 h
- J. Ch. Gilbert University Paris I, DEA Modélisation et Méthodes Mathématiques en Économie, *Méthodes newtoniennes en optimisation avec contraintes*, 21 h. 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.
- J. Jaffré Université Paris-Dauphine, DESS Mathématiques de la décision (Master level), *Numerical Analysis: Numerical Solution of Large Systems*, 18 hours  
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).  
Saint-Joseph University, Beirut, Lebanon, DEA PDE's and Numerical Analysis, *Finite elements*, 25 h with J. E. Roberts.
- 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.
- 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.  
Saint-Joseph University, Beirut, Lebanon, DEA PDE's and Numerical Analysis, *Finite elements*, 25 h with J. Jaffré.

## 5.3. Conferences, Seminars, Invitations

- L. Amir *Décomposition de domaine pour un milieu poreux fracturé*, 2ème colloque sur les Tendances dans les Applications Mathématiques en Tunisie, Algérie, Maroc, Tunis, April 26–28, 2005.  
*Domain decomposition for a fractured porous medium*, 8th SIAM Conference on Mathematical and Computational Issues in the Geosciences, Avignon (France), June 7–10, 2005.  
*Décomposition de domaine et préconditionnement pour un modèle 3D en milieu poreux fracturé*, 8èmes Journées d'Analyse Numérique et Optimisation, Rabat (Maroc), December 14–16, 2005.
- F. Clément *Domain Decomposition and Functional Programming with OCamlP3l*, International Conference on Computational Methods for Coupled Problems in Science and Engineering, Santorini Island, May 25–28.  
*Automatic Parallelism and Domain Decomposition with OCamlP3l*, 8th SIAM Conference on Mathematical and Computational Issues in the Geosciences, Avignon (France), June 7–10.  
*Domain Decomposition and Skeleton Programming with OCamlP3l*, International Conference on Parallel Computing, Malaga (Espagne), September 13–16.  
*Scientific Computation and Functional Programming with OCaml*, Dept. of Mathematics, University of Bergen, November 21.  
*Inverse Problem, Sensitivity Analysis and Functional Programming with OCaml*, Journées MOMAS, CIRM, Luminy, November 28–30.



- N. Frih *Écoulement Darcy-Forchheimer dans un milieu poreux fracturé* 2ème Colloque sur les Tendances dans les Applications Mathématiques en Tunisie, Algérie, Maroc, Tunis, April 26–28, 2005.  
*Modèle d'un écoulement dans un milieu poreux fracturé en présence de termes d'inertie*, Atelier de Modélisation des Ecosystèmes Marin, Tunis, Tunisia, September 18–21, 2005.
- J. Jaffré On numerical methods for two-phase flow in porous media, *International Conference on Approximation Methods and Numerical Modeling in Environment and Natural Resources, MAMERN 2005*, Oujda, Morocco, May 9-11. Invited lecture  
Numerical Challenges in Simulation and Performance Assessment of Contaminant Transport Around a Nuclear Waste Repository, *SIAM Conference on Mathematical and Computational Issues in the Geosciences*, Avignon, France, June 5-7, 2005. Invited lecture.  
On numerical methods for two-phase flow in porous media, *9th International Conference Zaragoza-Pau on Applied Mathematics and Statistics*, Jaca, Spain, September 19-21, 2005. Invited lecture.  
Eléments finis mixtes pour les problèmes du 2nd ordre, *Journée Méthodes numériques pour les fluides, GDR-Momas et Gamni*, CNAM, Paris, December 19, 2005.  
Méthodes de Godounov et du décentrage des mobilités dans les écoulements diphasiques en milieu poreux, *Séminaire du groupe de travail "Méthodes Numériques"*, Laboratoire J.-L. Lions, Université Pierre et Marie Curie, Paris, December 19, 2005.
- M. Kern *A Schwarz Waveform Relaxation Method for Advection–Diffusion–Reaction Problems with Discontinuous Coefficients and Non-matching Grids*, 16th International Conference on Domain Decomposition Methods, New-York, NY, January 10–16.  
*Solving Chemical Precipitation–Dissolution Problems with an Interior Point Methods*, 8th SIAM Conference on Mathematical and Computational Issues in the Geosciences, Avignon (France), June 7–10.  
*Models and methods in geochemistry*, lecture at the CEA–EDF–INRIA school on “Flow in unsaturated porous media: mathematical and numerical aspects”, INRIA, Rocquencourt, September 12–15.  
*A Schwarz Waveform Relaxation Method for Advection–Diffusion–Reaction Problems with Discontinuous Coefficients and Non-matching Grids*, séminaire Analyse Numérique et Équations aux Dérivées Partielles, université Paris Sud, Orsay, October 20.  
*Numerical Methods for Chemistry and for Coupling Transport with Chemistry in Porous Media*, Oberwolfach Workshop on “Reactive Flows through Complex Media”, Oberwolfach, October 30–November 5.  
*An interior points method for solving chemical precipitation–dissolution problems*, Journées MO-MAS, CIRM, Luminy, November 28–30.
- E. Marchand *La pression dans les écoulements eau/air*, 2ème colloque sur les Tendances dans les Applications Mathématiques en Tunisie, Algérie, Maroc, Tunis, April 26–28, 2005.
- J. E. Roberts *Multidomain modeling for the simulation of flow and transport in a neighborhood of an underground nuclear waste repository*, International Topical Meeting on Mathematics and Computational Supercomputing, Reactor Physics and Nuclear and Biological Applications, Avignon, France, September 12–15, 2005, Invited lecture.  
Invitation from Professor R. E. Ewing to visit Institution for Scientific Computation, Texas A&M University, College Station, Texas, July 20–22, 2005, seminar, *Flow in porous media with fractures*.
- A. Sboui *Raffinement en temps par sous-domaine pour un problème de convection en milieu poreux*, 2ème colloque sur les Tendances dans les Applications Mathématiques en Tunisie, Algérie, Maroc, Tunis, April 26-28, 2005.  
*Subdomain Time Stepping For Advection*, 8th SIAM Conference on Mathematical and Computational Issues in the Geosciences, Avignon (France), June 7–10.  
*A Mixed Finite Macroelement for distorted Hehahedral Grids*, 8th US National Congress on Computational Mechanics , Austin, Texas, July 25-27, 2005.

## 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.
- 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

### Articles in refereed journals and book chapters

- [1] P. AL KHOURY, G. CHAVENT, F. CLÉMENT, P. HERVÉ. *Inversion of spectroscopique data of CO<sub>2</sub> radiation*, in "Inverse Problems in Engineering", vol. 13, 2005, p. 210–240.
- [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*, submitted, 2004.
- [3] F. DELBOS, J. GILBERT, R. GLOWINSKI, D. SINOQUET. *Constrained optimization in seismic reflection tomography: an SQP augmented Lagrangian approach*, in "Geophysical Journal International", to appear, 2005.
- [4] N. FRIH, J. E. ROBERTS, A. SAÂDA. *Coupage Darcy-Forchheimer dans un milieu poreux fracturé*, submitted, 2005.
- [5] V. MARTIN, J. JAFFRÉ, J. E. ROBERTS. *Modeling fractures and barriers as interfaces for flow in porous media*, in "SIAM Journal on Scientific Computing", vol. 26, n° 5, 2005, p. 1667-1691.
- [6] J. NIESSNER, R. HELMIG, H. JAKOBS, J. E. ROBERTS. *Interface condition and linearization schemes in the Newton iterations for two-phase flow in heterogeneous porous media*, in "Advances in Water Resources", vol. 28, 2005, p. 671-687.
- [7] A. SBOUI, J. JAFFRÉ, J. E. ROBERTS. *A Mixed Finite Macroelement for distorted Hehahedral Grids*, in preparation, 2005.
- [8] A. SBOUI, J. JAFFRÉ. *Discrétisation en temps par sous-domaine pour un problème d'advection en milieu poreux*, submitted, 2005.
- [9] SIDDHARTHA, J. JAFFRÉ. *On the upstream mobility scheme for two phase flow in porous media*, submitted, 2005.

### Publications in Conferences and Workshops

- [10] A. CARTALADE, P. MONTARNAL, M. FILIPPI, C. MUGLER, M. LAMOUREUX, J.-M. MARTINEZ, F. CLÉMENT, Y. WILEVEAU, D. COELHO, E. TEVISSSEN. *An Overview of Inverse Modeling Methods Applied to the Thermal and Diffusion Experiments at Mont Terri Rock laboratory*, in "Proc. of the 2nd Internat. Meeting on Clays in Natural and Engineered Barriers for Radioactive Waste Confinement".

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- [11] F. CLÉMENT, V. MARTIN, A. VODICKA, R. DI COSMO, P. WEIS. *Domain Decomposition and Functional Programming with OCaml P3l*, in "Proc. of the Internat. Conf. on Computational Methods for Coupled Problems in Science and Engineering", M. PAPADRAKAKIS, E. ONATE, B. SCHREFLER (editors). , 2005.
- [12] J. ERHEL, M. KERN. *Numerical Methods for Chemistry and for Coupling Transport with Chemistry in Porous Media*, in "Oberwolfach Workshop on Reactive Flows through Complex Media", Oberwolfach reports, European MATHematical Society, 2006.
- [13] M. J. GANDER, L. HALPERN, M. KERN. *A Schwarz Waveform Relaxation Method for Advection–Diffusion–Reaction Problems with Discontinuous Coefficients and non-Matching Grids*, in "Domain Decomposition Methods 10", D. KEYES, O. WINDLUND (editors). , Lecture Notes in Computational Sciences and Engineering, à paraître, Springer, 2006.
- [14] V. MARTIN, F. CLÉMENT, A. DECOENE, J.-F. GERBEAU. *Parameter identification for a one-dimensional blood flow model*, in "Proceedings of CEMRACS 2004 on Mathematics and Applications to Biology and Medicine", E. CANCÈS, J.-F. GERBEAU (editors). , ESAIM Proceedings, vol. 14, EDP Sciences, 2005, p. 174–200.

## Miscellaneous

- [15] J. GILBERT. *QPAL – A code for solving convex quadratic optimization problems using the augmented Lagrangian. Version 1.0*, 2005.
- [16] J. GILBERT, S. MEZOUAR. *SQPAL – A software for nonlinear programming, using an augmented Lagrangian QP solver. Preliminary version*, 2005.
- [17] S. MEZOUAR. *Méthodes de programmation quadratique successive et application à un problème de chronothérapie des cancers*, Internship report, 2005.