



INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

*Project-Team Estime*

*Parameter Estimation and Modeling in  
Heterogeneous Media*

*Paris - Rocquencourt*

THEME NUM

*Activity*  
*R* *eport*

2007



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# 1. Team

## Head of project-team

Jérôme Jaffré [ DR, Inria, HdR ]

## Vice-Head of project-team

François Clément [ CR ]

## Administrative assistant (shared with project Poems)

Nathalie Bonte

## Research scientists

J. Charles Gilbert [ DR ]

Michel Kern [ CR, part time at the Ministère de la Recherche ]

Jean E. Roberts [ DR, HdR ]

## External collaborators

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

Guy Chavent [ University Paris 9, HdR ]

Ali Saâda [ Lamsin-ENIT, Tunisia ]

## Visiting Scientist

Peter Knabner [ University of Erlangen, Germany, 1 month ]

## Post-doctoral fellows

Amel Sboui [ ANDRA ]

## Ph.D. Students

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

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

Estelle Marchand [ ANDRA fellowship, University of Paris 9 ]

Kamel Mezlini [ ENIT-LAMSIN ]

## Internships

Emmanuelle Martin-Connerardy

# 2. Overall Objectives

## 2.1. Introduction

**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.

**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 microbes which are present in the earth. Another important application is the assessment of long-term nuclear waste storage in the underground. Multi-species reactive flow problems in porous media are described by a set of partial differential equations for the mobile species and ordinary differential 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 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.

## 2.2. Highlights of the year

1. Co-organisation of the conference **SIAM Conference on Mathematical & Computational Issues in the Geosciences, GS07**, Santa Fe, March 2007.
2. Co-organisation of the conference **Mod & Sim 07: Partial Differential Equations in Applied and Engineering Sciences: Modelling and Simulation**, Rocquencourt, December 13-14, 2007. A conference honoring Jim Douglas Jr on the occasion of its 80th birthday.
3. Distribution of OcamlP3L version 2.03 (<http://camlp3l.inria.fr>).

## 3. Contracts and Grants with Industry

### 3.1. ANDRA

ANDRA is the French National Agency for Nuclear Waste Management.

1. Sensitivity analysis for the simulation of the transport of nuclear contaminants around a nuclear waste disposal site. This contract provided financial support for Estelle Marchand's PhD thesis.
2. Numerical methods for simulating the migration, in and around a nuclear waste repository, of hydrogen produced by the corrosion of waste packages.

### 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

CNRS **GDR Momas** (Mathematical Modeling and Numerical Simulation for a 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 Mediterranean program. From 2006.

There is also 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.

- J. Jaffré co-organized the conference **Mod & Sim 07: Partial Differential Equations in Applied and Engineering Sciences: Modelling and Simulation**, Rocquencourt, December 13-14, 2007. A conference honoring Jim Douglas Jr on the occasion of its 80th birthday.
- M. Kern and J. E. Roberts were members of the organizing committee for the **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**.
- J. E. Roberts co-organized the conference **Mod & Sim 07: Partial Differential Equations in Applied and Engineering Sciences: Modelling and Simulation**, Rocquencourt, December 13-14, 2007. A conference honoring Jim Douglas Jr on the occasion of its 80th birthday.
- J. E. Roberts is membre suppléant of the Commission d'Évaluation de l'Inria.
- J. E. Roberts is Vice chair of the SIAM Activity Group on Geosciences.

## 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
- F. Clément École des Mines de Paris. 1st year: *Differential Calculus*, 22 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 I, M2 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.
- 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,
- 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

- F. Clément *Programmation fonctionnelle, couplage de code et parallélisation*, Journée MODESS, Tunis, Tunisia, May 22.
- N. Frih *Flow in Porous media with fractures: Modeling Forchheimer fractures as interfaces*, SIAM International Conference on Mathematical & Computational Issues in the Geosciences, Santa Fe, USA, March 19–22.
- Un modèle Darcy-Forchheimer dans un milieu poreux fracturé : Maillage non conforme et fractures qui s'intersectent*, Trends in Applied Mathematics in Tunisia, Algeria, Marocco (TAM-TAM'07), Tipasa, Algeria, 14-18 Avril 2007.
- Modeling Intersecting Forchheimer fractures as interfaces with nonconforming grids*, MAMERN 07, July 11-13, 2007, Grenada, Spain.
- Modélisation numérique d'un écoulement dans un domaine fracturé : couplage Darcy-Forchheimer*, MEMO 07, December 13-15, 2007, Tunis, Tunisia.



- J. Jaffré SIAM Geosciences GS07, 19-22 mars 2007 Santa Fe, New Mexico. J. Jaffré organized the minisymposium *3-D Numerical Modeling of Flow and Transport around a Nuclear Waste Repository*.  
 In this minisymposium presentation of *Kuznetsov-Repin hexahedral mixed finite elements and their application to the 3-D Andra benchmark* (with A. Sboui and J. E. Roberts).  
*Subdomain time stepping for contaminant transport in the subsurface*, MAMERN 07, July 11-13, 2007, Grenada, Spain.  
*Multiscale Time Stepping For Contaminant Transport in a Heterogeneous Medium*, a seminar given during a 10 day stay at the TIFR-CAM, Bangalore, India.
- M. Kern *Analytical Study of a Preconditioner for Fractured Porous Media*, SIAM International Conference on Mathematical & Computational Issues in the Geosciences, Santa Fe, USA, March 19–22.  
*A Schwarz-Waveform Relaxation Method for Advection-Diffusion-Reaction Problems with Discontinuous Coefficients and Non-matching Grids*, Erlangen University, Germany, June 27.  
*A Newton-Krylov Method for coupling Transport with Chemistry in Porous Media*, Journées Scientifiques du GDR MoMaS, Fréjus, November 14–16.  
*Des mathématiques pour modéliser les eaux souterraines*, exposé au Lycée van Gogh, Ermont, 13 décembre 2006, et au Lycée Albert Camus, Bois-Colombes, 12 juin 2007.
- E. Marchand *Deterministic Sensitivity Analysis for a Model for Flow in Porous Media*, SIAM International Conference on Mathematical & Computational Issues in the Geosciences, Santa Fe, United States of America, March 19–22.  
*Deterministic Sensitivity Analysis for a Model for Flow and Transport in Porous Media*, 5th International Conference on Sensitivity Analysis of Model Output, Budapest, Hungary, June 18–22.  
*Deterministic Sensitivity Analysis for a Model for Flow and Transport in Porous Media*, 6th International Congress on Industrial and Applied Mathematics, Zurich, Switzerland, July 16–20.  
*Deterministic Sensitivity Analysis for a Model for Flow and Transport in Porous Media*, 9th US National Congress on Computational Mechanics, San Francisco, United States of America, July 23–26.
- J. E. Roberts SIAM Geosciences GS07, 19-22 mars 2007 Santa Fe, New Mexico. J. E. Roberts organized with Jocelyne Erhel the minisymposium *Modeling Fractures and Fractures Systems, (Parts I and II)*.  
*Numerical simulation of flow and contaminant transport around an underground nuclear waste storage site*, MAMERN 07, July 11-13, 2007, Grenada, Spain, Invited plenary talk.  
*Multiscale time stepping for contaminant transport in a heterogeneous medium*, ICIAM-2007, July 16-20, Zurich, Invited minisymposium talk.  
*Composite mixed finite elements on hexahedral grids for flow around a contaminant repository*, a seminar given during a 10 day stay at the TIFR-CAM, Bangalore, India.

## 5.4. Consulting

J.Ch. Gilbert is a consultant for the Institut Français du Pétrole.

## 6. Bibliography

### Year Publications

#### Doctoral dissertations and Habilitation theses

- [1] E. MARCHAND. *Analyse de sensibilité déterministe pour la simulation numérique du transfert de contaminants*, Ph. D. Thesis, Université de Paris 9, 2007.

- [2] A. SBOUI. *Quelques méthodes numériques robustes pour l'écoulement et le transport en milieu poreux*, Ph. D. Thesis, Université Paris-Dauphine, 2007.

### Articles in refereed journals and book chapters

- [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", To appear, 2007.
- [4] I. BERRE, F. CLÉMENT, M. LIEN, T. MANNSETH. *Data driven reparameterization structure for estimation of fluid conductivity*, in "IAHS RedBook of ModelCARE2007, Calibration and Reliability in Groundwater Modelling: Credibility of Modelling", K. KOVAR (editor), 2007.
- [5] A. CARTALADE, P. MONTARNAL, M. FILIPPI, C. MUGLER, M. LAMOUREUX, J.-M. MARTINEZ, F. CLÉMENT, Y. WILEVEAU, D. COELHO, E. TEVISSSEN. *Application of Inverse Modeling Methods to Thermal and Diffusion Experiments at Mont Terri Rock Laboratory*, in "Physics and Chemistry of the Earth, Parts A/B/C", vol. 32, 2007, p. 491–506.
- [6] N. FRIH, J. E. ROBERTS, A. SAÂDA. *Modeling fractures as interfaces: a model for Forchheimer fractures*, in "Computational Geosciences", To appear.
- [7] J. GILBERT. *Optimisation Différentiable*, in "Techniques de l'Ingénieur", 2007.
- [8] J. GILBERT, X. JONSSON. *LIBOPT – An environment for testing solvers on heterogeneous collections of problems*, in "ACM Transactions on Mathematical Software", submitted.
- [9] E. MARCHAND, F. CLÉMENT, J. E. ROBERTS, G. PÉPIN. *Deterministic Sensitivity Analysis for a Model for Flow in Porous Media*, in "Advances in Water Resources", Submitted, 2007.

### Publications in Conferences and Workshops

- [10] 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 XVI", D. KEYES, O. WINDLUND (editors), Lecture Notes in Computational Sciences and Engineering, n<sup>o</sup> 55, Springer, January 2007.

### Internal Reports

- [11] J. GILBERT. *Organization of the Modulopt collection of optimization problems in the Libopt environment – Version 2.0*, rapport-technique, n<sup>o</sup> 329 (revised), INRIA, BP 105, 78153 Le Chesnay, France, 2007, <http://hal.inria.fr/inria-00132468>.
- [12] J. GILBERT, X. JONSSON. *LIBOPT – An environment for testing solvers on heterogeneous collections of problems – The manual, version 2.0*, rapport-technique, n<sup>o</sup> 331 (revised), INRIA, BP 105, 78153 Le Chesnay, France, 2007, <http://hal.inria.fr/inria-00135013>.
- [13] A. SBOUI, J. JAFFRÉ, J. E. ROBERTS. *A Composite Mixed Finite element for general hexahedral grids for Darcy flow calculations*, submitted, Technical report, n<sup>o</sup> 6300, INRIA, 2007, <http://hal.inria.fr/inria-00173453/fr/>.

**Miscellaneous**

- [14] J. GILBERT. *SQPlab – A Matlab software for solving nonlinear optimization problems and optimal control problems – Version 0.4*, Online Paper, 2007.
- [15] J. GILBERT. *SQPpro – A software for solving nonlinear optimization problems – Version 0.1*, Online Paper, 2007.
- [16] M. KERN. *Des mathématiques pour modéliser les eaux souterraines*, 2007, <http://interstices.info/expose-eaux-souterraines>, Video sur le site Interstices.