INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

# *Project-Team Estime*

# *Parameter Estimation and Modeling in Heterogeneous Media*

*Paris - Rocquencourt*

THEME NUM

Activity Report

2008

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# 1. Team

**Research Scientist**
François Clément [ CR ]
Jean Charles Gilbert [ DR ]
Jérôme Jaffré [ DR, Inria, HdR ]
Michel Kern [ CR, part time at the Ministère de l'Enseignement Supérieur et de la Recherche ]
Jean E. Roberts [ DR, HdR ]
Pierre Weis [ DR ]

**Faculty Member**
Hend Ben Ameur [ University of Bizerte and Lamsin-ENIT, Tunisia, HdR ]
Guy Chavent [ University Paris 9, HdR ]
Ali Saâda [ Lamsin-ENIT, Tunisia ]

**PhD Student**
Laila Amir [ Cifre Itasca fellowship, University of Paris 9 ]
Ibtihel Ben Gharbia [ University of Paris 9 ]
Alice Chiche [ Cifre EdF, University of Paris 6 ]
Najla Frih [ ENIT-LAMSIN and University of Paris 9 ]
Ouacil Saouli [ University of Constantine, Algeria ]

**Post-Doctoral Fellow**
Suresh Kumar Nadupuri [ CEFIPRA fellowship ]
Amel Sboui [ ANDRA ]

**Visiting Scientist**
Peter Knabner [ University of Erlangen, Germany, 1 month ]

**Administrative Assistant**
Nathalie Bonte

**Other**
Alexandra Keller [ Stagiaire, Université Paris 11 ]
Aodren Perrin [ Stagiaire, Université de Pau ]

# 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 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 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 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 theories 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, algebraic optimization, optimization without derivative, decomposition methods for large scale problems, bilevel optimization, *etc*. There are many applications: seismic tomography data inversion, shape optimization (aeronautic and tyre industry), mathematical modelling in medicine and biology (cancer chronotherapy), optimization of the electricity production, to mention a few of those that have been considered by the team. Outcomes of this activity are also the *Modulopt library*, which gathers optimization pieces of software produced by the team, and the *Libopt environment*, which is a platform for testing and profiling solvers on heterogeneous collections of problems.

**Complementarity problems:** Extending optimization, *complementarity problems* occur when two systems of equations are in competition, the one that is active being determined by variables reaching threshold values. Mathematically, these conditions can be expressed by $F(x)^{\top}G(x) = 0$, $F(x) \geqslant 0$, and $G(x) \geqslant 0$, where $F$ and $G : \mathbb{R}^n \to \mathbb{R}^n$ are two functions. Usually, a model will include other equations and inequations. The full system can be viewed as a special case of *variational inequalities*. The numerical techniques to solve such a problem have known a spectacular development during these recent years and have a vast domain of applications. Complementarity can indeed be used to model contact problems, chemical or economical equilibria, precipitation-dissolution phenomena, *etc*. We have started in 2008, with the PhD thesis of Ibtihel Ben Gharbia, to apply nonlinear complementarity techniques to the solution of a diphasic (water and hydrogen) flow with phase exchange in a porous medium. The appearance/disappearance of the hydrogen gas phase can indeed be modeled by nonlinear complementarity conditions. We plan, in the framework of this PhD thesis, to contribute to the development of the numerical methods in nonlinear complementarity.

## 2.2. Highlights of the year

P. Weis joined the Estime project team.

# 3. Software

## 3.1. Modulopt

`M1qn3` [19] is a Fortran-77 piece of software that can solve a large scale unconstrained minimization problem. This solver, whose first version dates back to 1988, implements a limited memory quasi-Newton approximation technique and has been used to solve problems with as many as $10^8$ variables. It is widely used in meteorology and oceanography. Since December 2008, the code (version 3.2) is distributed under the GNU General Public License

`Qpal` [17] is a Fortran-2003 implementation of an augmented Lagrangian approach for solving a convex quadratic optimization problem (QP). The version 0.5 (October 2008) of the solver has the possibility to have an $\ell$-BFGS matrix as Hessian, which is useful when the solver is used in an SQP solver like `SQPpro`,

`SQPpro` [18] is a Fortran-2003 implementation of the SQP algorithm for solving constrained optimization problems. The functions defining the problem can be nonlinear and nonconvex, but must be differentiable. The version 0.3 (October 2008) of the solver implements the following new features:

- the solver variables have been redesigned so that `SQPpro` can now be used more than once in the same program;
- the Hessian of the Lagrangian can now be approximated by the direct (for constrained problems) or indirect (for unconstrained problems) $\ell$-BFGS formula, which is useful for very large problems; the performance of `SQPpro` is now similar to those of `Lbfgs` or `M1qn3` (for unconstrained optimization, see figure 1) and close to the one of the bound constrained solver `Lbfgsb` (for bound constrained optimization, see figure 2).

The improvement of the solver `SQPpro` from its version 0.1 (end of 2007) to its version 0.3 (October 2008) is illustrated by the performance profiles given in figure 3. There is one curve per solver and the higher is the curve the better is the solver.

# 4. Contracts and Grants with Industry

## 4.1. ANDRA

ANDRA is the French National Agency for Nuclear Waste Management.

Numerical methods for simulating the migration, in and around a nuclear waste repository, of hydrogen produced by the corrosion of waste packages. Andra supported Amel Sboui's postdoc.

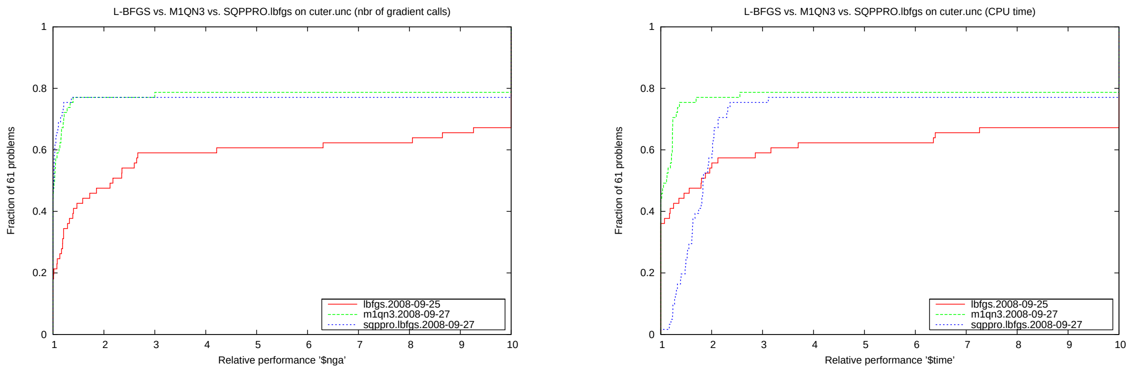


*Figure 1. Performance profiles of the solvers* `Lbfgs` *(plain red curve),* `M1qn3` *(dashed green curve) and* `SQPpro` *(dotted blue curve) on large scale unconstrained problems of the CUTEr collection, using the number of derivative evaluations (left) and CPU time (right)*

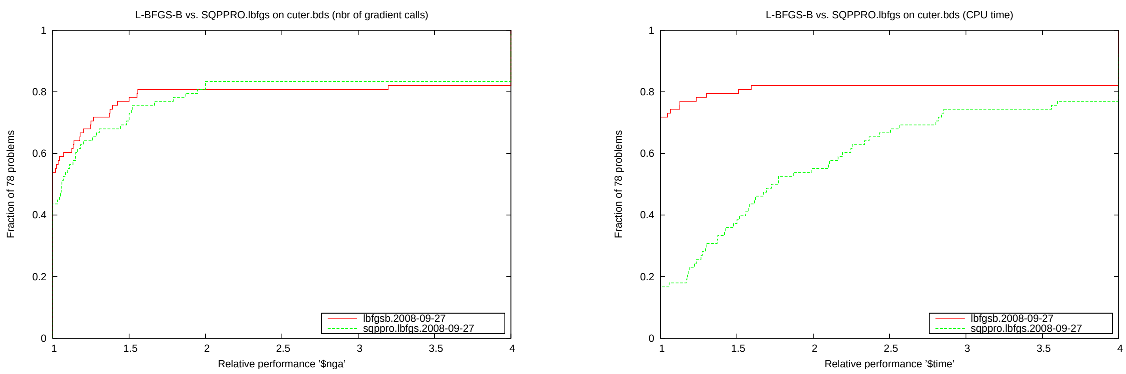


*Figure 2. Performance profiles of the solvers* `Lbfgsb` *(plain red curve) and* `SQPpro` *(dashed green curve) on large scale bound constrained problems of the CUTEr collection, using the number of derivative evaluations (left) and CPU time (right)*

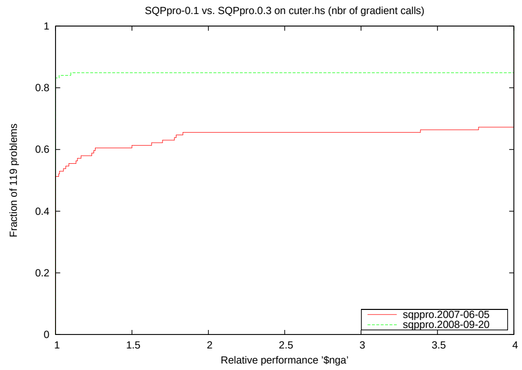


*Figure 3. Performance profiles of the version 0.1 of the solver SQPpro (plain red curve) and its version 0.3 (dashed green curve) on the 119 Hock and Schittkowski problems (a subcollection of the CUTEr collection), using the number of derivative evaluations*

## 4.2. EdF

Alice Chiche has started a PhD thesis (Cifre EdF-Inria) on decomposition-coordination methods for the middle-term optimization of the electricity production. The case where uncertainties are present will also be considered, using scenario trees, which leads to even larger deterministic optimization problems. We intend to bring improvements on augmented Lagrangian like approaches and on nondifferentiable techniques.

## 4.3. 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. Itasca provided financial support for Laila Amir's PhD thesis, through a CIFRE fellowship. The fellowship ended on July 31st, and Laila Amir successfully defended her thesis on December 18th.

# 5. Other Grants and Activities

## 5.1. National Cooperations

CNRS Groupement 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.

Agence Nationale de la Recherche ANR SHPCO2 (Simulation Haute Performance du Stockage Géologique de CO2) with IFP, LAGA laboratory from University Paris 13, École des Mines de St Etienne and BRGM.

INRIA ARC Quotient (certified usage of non-free concrete data types) with Protheo and Gallium groups, with CNAM, with LIP6 from University of Paris 6.

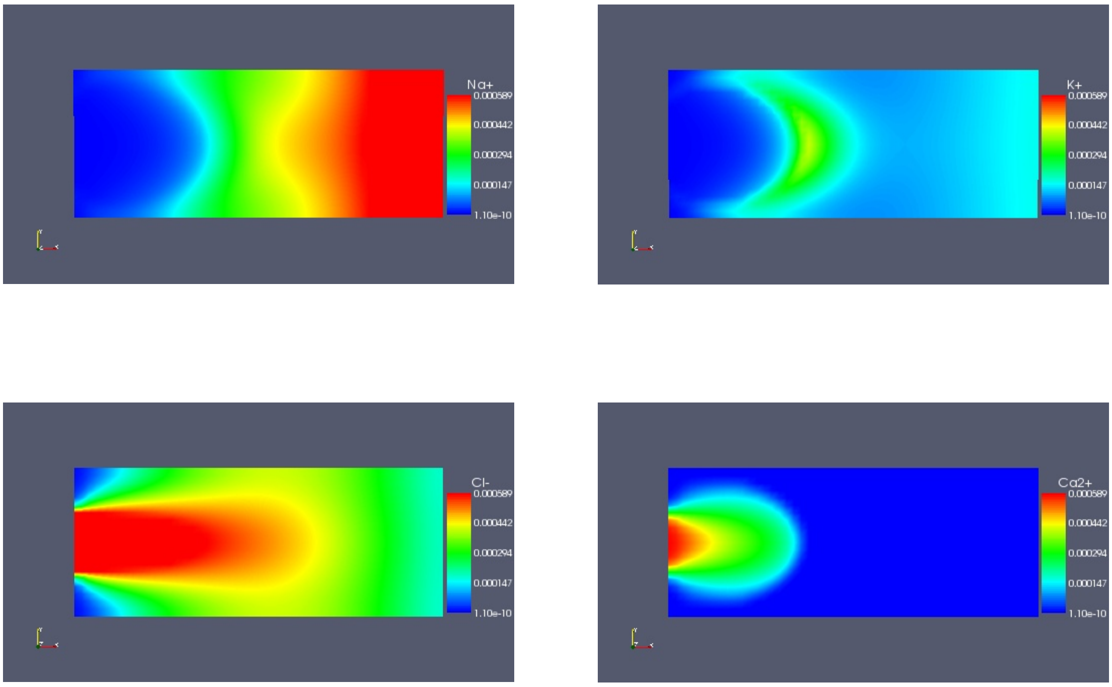


*Figure 4. Reactive transport in a porous medium. These images show the concentrations of different species, subject to advetive and dispersive transport, and chemical reactions. A solution with sodium (top left) and potassium (top right) reacts with chlorine (bottom left) and calcium (bottom right).*

## 5.2. 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". It provides the financial support for Suresh Kumar Nadupuri's postdoc. From 1/09/2006.

# 6. Dissemination

## 6.1. Service to the scientific community

J. Jaffré is co-editor-in-chief (with M.F. Wheeler and C. Dawson) of the journal Computational Geosciences

M. Kern is Vice Director of CNRS Groupement MoMaS.

M. Kern is chargé de mission for high end computing at the Ministère de l'Enseignement Supérieur et de la Recherche.

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

J. E. Roberts was membre suppléant of the Commission d'Evaluation de l'Inria.

J. E. Roberts is Vice chair of the SIAM Activity Group on Geosciences.

P. Weis is President of the Advisory Board of the Conference JFLA (Journées Francophones des Langages Applicatifs).

## 6.2. 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*, 20 h.

J. Ch. Gilbert: ENSTA, 2nd year, *Optimisation différentiable – théorie et algorithmes*, 42 h.

J. Jaffré: École Nationale d'Ingénieurs de Tunis (ENIT), Tunisia, DEA Mathématiques Appliquées, *Volumes finis et éléments finis mixtes*, 20 h with J. E. Roberts.
École CIMPA-INRIA-UNESCO, Mathématiques pour l'écoulement et l'épuration de l'eau, Abou Bekt Belkaid university, Tlemcen, Algeria, May 2008, *Two-phase flow in porous media*, (1h30).

M. Kern: École des Mines de Paris, 2nd year: *Scientific Computing* (30 h) and *Finite elements* (with D. Ryckelinck and V. Chiaruttini, 30 hours).

J. E. Roberts: École Supérieure d'Ingénieurs Léonard de Vinci, *Approximation methods*, 4th year students, 20 h.
École Nationale d'Ingénieurs de Tunis (ENIT), Tunisia, DEA Mathématiques Appliquées, *Volumes finis et éléments finis mixtes*, 20 h with J. Jaffré.
École CIMPA-INRIA-UNESCO, Mathématiques pour l'écoulement et l'épuration de l'eau, Abou Bekt Belkaid university, Tlemcen, Algeria, May 2008, *Two-phase flow in porous mediaMixed finite element methods and finite volume methods for Darcy flow calculations*, (3h).

## 6.3. PhD Theses

L. Amir, December 18, 2008.

## 6.4. Conferences, Seminars, Invitations

L. Amir *Application of Newton-Krylov methods to the MoMaS benchmark problem*, International Workshop on Modelling Reactive Transport in Porous Media Strasbourg (France), January 21–24, 2008.
*Preconditioning Newton-Krylov methods for reactive transport*, International Conference on Computational Methods in Water Resources (CMWR XVII), San Francisco, Etats-Unis, July 6–10, 2008.

G. Chavent *Global pressure revisited: Three-phase flow*, International Conference Scaling Up and Modeling for Transport and Flow in Porous Media, Dubrovnik, Croatia, 13–16 October 2008.

F. Clément *The Multidimensional Refinement Indicator Algorithm for Adaptive Parameterization*, 8th World Congress on Computational Mechanics (WCCM8), 5th European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2008), Venice, Italy, June 30–July 5, 2008.

J. Jaffré *Méthodes numériques de flux discontinus pour des écoulements diphasiques*, Premier Congrès de la Société Marocaine de Mathématiques Appliquées, Rabat, Maroc, February 6–8.
*Henry's law, phase diagrams and complementary constraints for two-phase flow with dissolution*, Conférence EUROMECH 499 "Nonlinear Mechanics of Multiphase Flow in Porous Media", Nancy, June 9–12, 2008.
*Numerical simulation of the far field for a French deep underground repository of long life radionuclides*, International Conference on Computational Methods in Water Resources (CMWR XVII), San Francisco, Etats-Unis, July 6–10, 2008.
*Phase exchange for flow in porous media and complementary problems*, International Conference Scaling Up and Modeling for Transport and Flow in Porous Media, Dubrovnik, Croatia, 13–16 October 2008.

M. Kern *The MoMaS Reactive Transport Benchmark: Presentation of the Models*, International Workshop on Modelling Reactive Transport in Porous Media Strasbourg (France), January 21–24, 2008.

*Flow and transport of pollutants in the subsurface: coupled models and numerical methods*, Recherche et Innovation Campus Day Stratégies et opportunités pour la Recherche à l'ère du Petaflops, séminaire IBM-INRIA-LIP 6, Paris (France), September 18th, 2008.

*Coupled transport and chemistry*, Scientific meeting for MoMaS "Numerical methods" group, Paris, November 14th, 2008.

*HPC in France: Organisation, computers and software*, Keynote presentation at the 2nd workshop, UK initiative "Developing an HPC/NA Roadmap", Manchester (UK), December 8–9, 2008.

J. E. Roberts *Mixed finite elements for hexahedra*, Premier Congrès de la Société Marocaine de Mathématiques Appliquées, Rabat, Maroc, February 6–8, 2008.
*Modeling fractures as interfaces using domain decomposition techniques*, Workshop "Coupling of Flow and Deformation Processes for Modeling the Movement of Natural Slope", Freudenstadt, Allemagne, March 26–28, invited conference.
*Modeling fractures as interfaces: nonconforming grids and a posteriori error estimates*, SIAM Annual Meeting, San Diego, Etats-Unis, July 7–11, 2008.

P. Weis *Les types à relations.*, JFLA 2008, Étretat, France, January 26–29, 2008 (Invited Conference).

## 6.5. Consulting

F. Clément was a consultant for LASUR (Laboratoire d'Énergétique et d'Économie d'Énergie, University of Paris 10).

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

# 7. Bibliography

## Year Publications

### Doctoral Dissertations and Habilitation Theses

[1] L. AMIR. *Modèles couplés en milieux poreux : transport réactif et fractures*, Ph. D. Thesis, Unviersité Paris IX, 2008.

### Articles in International Peer-Reviewed Journal

[2] L. AMIR, M. KERN. *A Newton-Krylov method for coupling transport with chemistry in heterogeneous porous media*, in "Computational Geosciences", submitted, 2008.

[3] J.-B. APOUNG, P. HAVÉ, J. HOUOT, M. KERN, A. SEMIN. *Reactive Transport in Porous Media*, in "ESIAM Proceedings", submitted, 2008.

[4] 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", vol. 16, 2008, p. 107–126.

[5] J. CARRAYROU, P. KNABNER, M. KERN. *Reactive Transport Benchmark of MoMaS*, in "Computational Geosciences", submitted, 2008.

[6] F. DELBOS, T. FENG, J. GILBERT, D. SINOQUET. *SQP methods for reservoir characterization*, submitted to Engineering Optimization, 2008.

[7] N. FRIH, J. E. ROBERTS, A. SAÂDA. *Modeling fractures as interfaces: a model for Forchheimer fractures*, in "Computational Geosciences", vol. 12, 2008, p. 91-104.

[8] 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", vol. 31, 2008, p. 1025–1037, http://dx.doi.org/10.1016/j.advwatres.2008.04.004.

[9] C. DE DIEUVELEULT, J. ERHEL, M. KERN. *A global strategy for solving reactive transport equations*, in "J. Computational Physics", submitted, 2008.

### Scientific Books (or Scientific Book chapters)

[10] I. BERRE, F. CLÉMENT, M. LIEN, T. MANNSETH. *Data driven reparameterization structure for estimation of fluid conductivity*, in "Proc. of the Internat. Conf. ModelCARE2007, Calibration and Reliability in Groundwater Modelling: Credibility of Modelling", J. REFSGAARD, K. KOVAR, E. HAARDER, E. NYGAARD (editors), vol. 320, IAHS, 2008, p. 310–315, http://www.iahs.info/redbooks/a320/iahs_320_0310.htm.

### Research Reports

[11] A. ADI, V. GOWDA, J. JAFFRÉ. *Monotonization of flux, entropy and numerical schemes for conservation laws*, to appear in Journal of Mathematical Analysis and Applications 352 (2009), pp. 427-439, Rapport de Recherche, n$^{o}$ 6787, INRIA, Rocquencourt, France, 2008.

[12] G. CHAVENT. *A Fully Equivalent Global Pressure Formulation for Three-Phase Compressible Flow*, submitted, Rapport de Recherche, n° 6788, INRIA, Rocquencourt, France, 2008.

[13] J. JAFFRÉ, S. MISHRA. *On the upstream mobility scheme for two phase flow in porous media*, to appear in Computational Geosciences, Rapport de Recherche, n° 6789, INRIA, Rocquencourt, France, 2008.

[14] E. MARCHAND, F. CLÉMENT, J. E. ROBERTS, G. PÉPIN. *Deterministic Sensitivity Analysis for a Model for Flow in Porous Media*, Rapport de Recherche, n° 6502, Inria, Rocquencourt, France, 2008, https://hal.inria.fr/inria-00271986/.

[15] A. SBOUI, J. JAFFRÉ, J. E. ROBERTS. *A Composite Mixed Finite element for general hexahedral grids for Darcy flow calculations*, version 2, to appear SIAM J. of Scientific Computing, Rapport de Recherche, n° 6300, INRIA, 2008, http://hal.inria.fr/inria-00173453/fr/.

### Scientific Popularization

[16] M. KERN. *Problèmes inverses*, in "Techniques de l'Ingénieur", to appear, TSI, 2008.

### Other Publications

[17] J. GILBERT. *QPAL – A solver of convex quadratic optimization problems, using an augmented Lagrangian approach – Version 0.5*, 2008, http://www-rocq.inria.fr/estime/modulopt/optimization-routines/qpal/qpal.html.

[18] J. GILBERT. *SQPpro – A solver of nonlinear optimization problems, using an SQP approach – Version 0.3*, 2008, http://www-rocq.inria.fr/estime/modulopt/optimization-routines/sqppro/sqppro.html.

[19] J. GILBERT, C. LEMARÉCHAL. *The module M1QN3 – Version 3.3*, 2008, http://www-rocq.inria.fr/estime/modulopt/optimization-routines/m1qn3/m1qn3.html.