INRIA

INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Project-Team Estime

Parameter estimation and modeling in heterogeneous media

Paris - Rocquencourt

Theme : Observation and Modeling for Environmental Sciences

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1. Team

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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 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 : As physical models become more and more sophisticated, we start encountering situations involving different physics. In most situations, the computer codes for the individual components are different (they may even be built by different groups). However, it may be desirable to use a strongly coupled methods, in order to fuly resolve the physics. The Newton–Krylov framework enables to build global methods for the coupled problems, without the need to have a monolithic solver. Again here, reactive transport is a natural application.

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 lagrangian relaxation (including augmented Lagrangian approach and progressive hedging), sequential quadratic programming, interior point methods, nonsmooth methods, 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. Special attention is paid on the so-called Newton-min algorithm, which may be viewed as a semismooth Newton method applied to the following nonsmooth equivalent formulation of the problem: $\min(F(x), G(x)) = 0$.

3. Software

3.1. Modulopt

M1qn3 (version 3.3: October, 2009): 47 downloads in 2010.

SQPlab (version 0.4.4: February 2009): 250 downloads in 2010.

4. New Results

4.1. Coupling transport with Chemistry

We have achieved significant progresses dor the simulation of reactive transport phenomena. B. Gueslin and M. Kern have completed the simulation of a water–gas system, including several aqueous species and minerals, designed by IFP-Energies Nouvelles, In the framework of the SHPCO2 ANR project. A snapshot of the concentrations of some species is shown on figure 1.

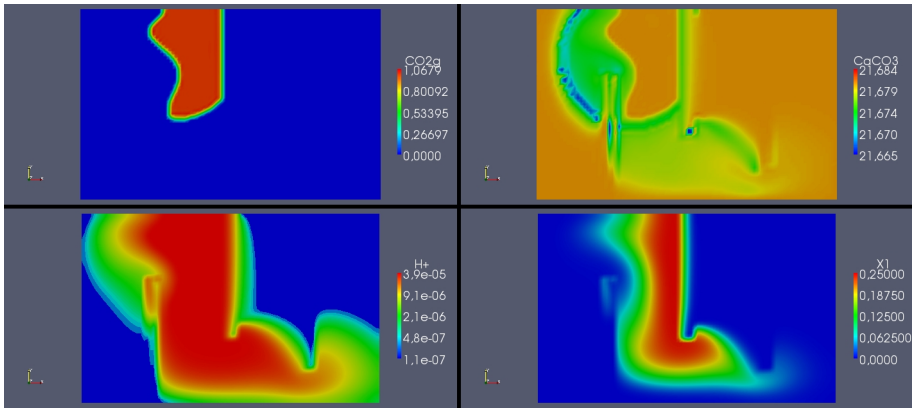

Figure 1. Species concentration for the dissolution of CO2. Upper left: CO2 gas, upper right: calcite, lower left: pH, lower right: chloride (tracer)

The figure shows the initial gas bubble dissolving in water, with a corresponding increase in pH, and calcite dissolution.

5. Contracts and Grants with Industry

5.1. Contracts with Industry

(EdF) A. Chiche is preparing a PhD thesis (Cifre EdF-Inria, direction J. Ch. Gilbert) on decomposition-coordination methods for the middle-term optimization of the electricity production. The case where uncertainties are present is also considered, using scenario trees, which leads to even larger deterministic optimization problems. Improvements have been brought

- on the solution of *infeasible* convex quadratic optimization problems using the augmented Lagrangian approach [10] and
- on the solution of the optimization of the electricity production under uncertainties, using the progressive hedging algorithm.

5.2. Grants with Industry

ANDRA

1. Phuong Hoang Thi Thao's PhD began in October her PhD thesis on subdomain time stepping formulated as a time and space domain decomposition problem. Her thesis is supported by a contract between INRIA and ANDRA.
2. Another contract between INRIA and ANDRA concerns M. Kern's consulting support on high performance computing.

5.3. National Initiatives

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

Agence Nationale de la Recherche ANR Fost (Formal prOofs about Scientific compuTations), with EPI Proval from INRIA Saclay - Île-de-France, Laboratoire de Recherche en Informatique from University of Paris 11, and Laboratoire d'Informatique de l'Université Paris-Nord from University of Paris 13.

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

5.4. International Initiatives

Estime is also associated with Lamsin-ENIT in the DGRSRT(Tunisie)/INRIA STIC project "Identification de paramètres en milieu poreux : analyse mathématiques et étude numérique". From 2008.

Estime is also 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.

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.

5.5. Exterior research visitors

A. Taakili, Univ. of Errachidia (Marrocco), 09/09/2010 to 30/07/2010.

A. Fumagalli, PhD student, MOX, Politecnico di MIlano (Itlay), 06/09/2010 to 24/09/2010.

6. Dissemination

6.1. Animation of the scientific community

M. Kern is a member of the Scientific Board of Groupement MoMaS.

M. Kern is a member of the Scientific Board of UNIT, l'Université Numérique Ingénierie et Technologie.

6.2. Teaching

I. Ben Gharbia:

- Université Paris Dauphine, License 2nd year, *Calcul matriciel*, 54 h.
- Université Paris Dauphine, License 1st year, *Linear algebra* , 39 h.

A. Chiche: ENSTA, 2nd year, *Optimisation différentiable – théorie et algorithmes*, 26 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, Mastère Mathématiques Appliquées, *Volumes finis et éléments finis mixtes*, 20 h with J. E. Roberts.

M. Kern: Mines-ParisTech, *Introduction au calcul scientifique*, 2nd year students, 10 h, *Eléments finis*, 2nd year students, 30 h, *Approximation et évolution : aspects numériques*, 2nd year students, 20 h.

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, Mastère Mathématiques Appliquées, *Volumes finis et éléments finis mixtes*, 20 h with J. Jaffré.

6.3. Conferences, Seminars, Invitations

I. Ben Gharbia

- (with J. Ch. Gilbert and J. Jaffré) *Henry's law and gas phase appearance and disappearance modeled as a complementarity problem*, European Geosciences Union General Assembly 2010 (EGU), Vienna, Austria, May 02-07, 2010.
- (with J. Ch. Gilbert and J. Jaffré) *Formulation avec contraintes de complémentarité pour un modèle diphasique en milieux poreux avec échange entre les phases*, Journée scientifique du GNR MOMAS, Paris, 3 décembe 2010.

A. Chiche *How the augmented Lagrangian algorithm deals with an infeasible convex quadratic optimization problem*, The International Conference on Continuous Optimization (ICCOPT) 2010, Santiago, Chili, 26-29 juillet 2010.

Comportement et usage de l'algorithme de Lagrangien augmenté dans le cas d'un problème quadratique convexe non-réalisable, Groupe de travail de l'équipe Commands (Inria-Ensta-Cmap-Cnrs), Journée des doctorants, Paris, France, 18 juin 2010.

B. Gueslin (with M. Kern) *Simulation numérique du stockage du CO2*, 10èmes Journées d'Étude sur les Milieux Poreux, Nancy (France), October 20-21, 2010.

J. Ch. Gilbert *How the augmented Lagrangian algorithm can deal with an infeasible convex quadratic optimization problem*, Erice, Sicile, Italy, July 2-10, 2010.

J. Jaffré

- *Flow in porous media with fractures: a discrete fracture model using cell-centered discretization methods*, Premières Journées Scientifiques du Laboratoire Euro-Maghrébin de Mathématiques et de leurs interaction (LEM2I), Tipaza, Algérie, 13-22 juin 2010.

- *Henry's law and gas phase disappearance solved as a complementarity problem* (with I. Ben Gharbia and J.-C. Gilbert), 2ième Congrès de la Société Marocaine de Mathématiques Appliquées (SM2A), Rabat, Maroc, 28-30 juin 2010.
- *Mixed finite elements on hexahedral meshes* (with J. E. Roberts). Workshop on Advanced methods for the diffusion equation on general meshes, 5,6 juillet, 2010, Paris, France.
- *Composite mixed finite elements for deformed cubes*. 2010 Full SIAM meeting, Pittsburg, USA, July 12-16, 2010.
- *On the upstream mobility finite difference scheme*. 12th European Conference on Mathematics for Oil Recovery (ECMOR XII), Oxford, England, 6-9 septembre 2010.
- One week visit to Prof. Zoubida Mghazli, université Ibn Tofaïl, Kenitra, Maroc (PHC Volubilis).

M. Kern

- (with L. Amir, A. Taakili) *Reactive transport in porous media*, visit to MOX, Politecnico di Milano (Italy), April 14 2010.
- (with A. Taakili) *Linear and nonlinear preconditioning for a model of transport with sorption*, XVIII Conference on Computational Methods in Water Resources, Barcelona (Spain), June 21-24, 2010.
- (with A. Michel) organized the SHPCO2 workshop, St Lambert des Bois (France), June 14-15 2010 (30 participants, 15 invited talks).
- (with L. Amir, B. Gueslin, A. Taakili), *Reactive transport in porous media: formulations, non-linear solvers and preconditioners* , High Performance Computing for CO2 Geological Storage, St Lambert des Bois (France), June 14-16, 2010,
- (with L. Amir, B. Gueslin, A. Taakili) *Coupled transport and chemistry*, thematic day "Groupement MoMaS, Numerical Methods", Paris (Fance), October 6, 2010.
- (with L. Amir, B. Gueslin) *Coupled formulations and coupling algorithms for reactive transport in porous media*, DyCap Workshop "Microbiology and Reactive Transport in the Capillary Fringe", University of Heidelberg, (Germany), October 7-8, 2010, invited lecture.
- (with B. Gueslin) *Coupled formulations and coupling algorithms for reactive transport in porous media* , seminar at LMA, Université Technologique de Compiègne (France), November 16, 2010.
- *Comment calcule un ordinateur ?*, pedagogical presentation to first year university students, Université René Descartes, Paris (France), September 17, 2010.

J. E. Roberts

- (with N. Frih, V. Martin and A. Saada) *Some numerical results for modeling fractures as interfaces with nonconforming grids* (poster presentation), 2010 InterPore Conference and Annual, College Station,Texas, USA, March 15-17, 2010.
- *Flow in heterogeneous porous media: a discrete fracture model with cell centered elements*. International congress in Mathematical Fluid Dynamics and its applications (MFD 2010), Rennes, June 21-24, 2010.
- *Single phase flow in porous media with fractures modeling Forchheimer fractures as interfaces* (with Peter Knabner) and organized with Z. Mghazli the minisymposium *Méthodes et Outils pour les Milieux Poreux*, 2ième Congrès de la Société Marocaine de Mathématiques Appliquées (SM2A), Rabat, Maroc, 28-30 juin 2010.
- One week visit to Prof. Zoubida Mghazli, université Ibn Tofaïl, Kenitra, Maroc (PHC Volubilis).

7. Bibliography

Publications of the year

Articles in International Peer-Reviewed Journal

[1] L. AMIR, M. KERN. *A Newton-Krylov method for coupling transport with chemistry in heterogeneous porous media*, in "Computational Geosciences", 2010, vol. 14, n^{o} 3, p. 465-481, http://dx.doi.org/10.1007/s10596-009-9162-x.

[2] I. BEN GHARBIA, J. GILBERT. *Nonconvergence of the plain Newton-min algorithm for linear complementarity problems with a P-matrix*, in "Mathematical Programming", 2010, To appear, http://www.springerlink.com/content/103081/.

[3] J. CARRAYROU, M. KERN, P. KNABNER. *Reactive Transport Benchmark of MoMaS*, in "Computational Geosciences", 2010, vol. 14, n^{o} 3, p. 385-392, http://dx.doi.org/10.1007/s10596-009-9157-7.

[4] J. JAFFRÉ, A. SBOUI. *Henry's law and gas phase disappearance*, in "Transport in Porous Media", 2010, vol. 82, p. 521-526.

[5] S. MISHRA, J. JAFFRÉ. *On the upstream mobility scheme for two-phase flow in porous media*, in "Computational Geosciences", 2010, vol. 14, p. 105-124.

International Peer-Reviewed Conference/Proceedings

[6] S. BOLDO, F. CLÉMENT, J.-C. FILLIÂTRE, M. MAYERO, G. MELQUIOND, P. WEIS. *Formal Proof of a Wave Equation Resolution Scheme: the Method Error*, in "Proc. of the first Internat. Conf. on Interactive Theorem Proving (ITP 2010)", M. KAUFMANN, L. C. PAULSON (editors), LNCS, Springer, 2010, vol. 6172, p. 147–162, http://dx.doi.org/10.1007/978-3-642-14052-5_12.

Scientific Books (or Scientific Book chapters)

[7] M. KERN. *Problèmes inverses*, in "Techniques de l'Ingénieur", TSI, 2010, n^{o} AF1380.

Research Reports

[8] H. BEN AMEUR, G. CHAVENT, F. CLÉMENT, P. WEIS. *Image Segmentation with Optimal Control Techniques*, Inria, Rocquencourt, France, 2010, n^{o} 7446, http://hal.inria.fr/inria-00533799/.

[9] S. BOLDO, F. CLÉMENT, J.-C. FILLIÂTRE, M. MAYERO, G. MELQUIOND, P. WEIS. *Formal Proof of a Wave Equation Resolution Scheme: the Method Error*, INRIA, Jan 2010, n^{o} 7181, RR-7181, http://hal.inria.fr/inria-00450789/.

[10] A. CHICHE, J. GILBERT. *How the augmented Lagrangian algorithm deals with an infeasible convex quadratic optimization problems*, INRIA, BP 105, 78153 Le Chesnay, France, 2010, To appear.

Other Publications

[11] J. GILBERT. *Contributions to Wikipedia.fr: analyse convexe, intérieur relatif, P-matrice, P_0-matrice, cône tangent, direction de descente, qualification de contraintes, vitesse de convergence des suites, conditions d'optimalité (dimension finie)*, 2010.