Activity Report 2011

Project-Team ESTIME

Parameter estimation and modeling in heterogeneous media

RESEARCH CENTER
Paris - Rocquencourt

THEME
Observation and Modeling for Environmental Sciences

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Project-Team ESTIME

Keywords: Environment, Fluid Dynamics, Scientific Computation, Model Coupling, Porous Media

1. Members

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Michel Kern [CR]
Jean E. Roberts [DR, HdR]
Pierre Weis [DR]

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PhD Students

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Other

Quentin Carbonneaux [Internship, École des Ponts ParisTech]

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 $F(x)^\top G(x) = 0$, $F(x) \geq 0$, and $G(x) \geq 0$, 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 to 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. M1cg1

– Participant: J. Ch. Gilbert.
– Version: 1.2.
– Programming language: Fortran 77.
– Solves a convex quadratic optimization problem and builds a preconditioning matrix, 1 download in 2011.
– See also the web page http://www-roc.inria.fr/~gilbert/modulopt/optimization-routines/m1cg1/m1cg1.html.

3.2. M1qn3

– Participants: J. Ch. Gilbert, Cl. Lemaréchal.
– Version: 3.3.
– Programming language: Fortran 77.
– Solves a very large scale differentiable optimization problem, 45 downloads in 2011.
– See also the web page http://www-roc.inria.fr/~gilbert/modulopt/optimization-routines/m1qn3/m1qn3.html.

3.3. PHlab

– Participant: J. Ch. Gilbert.
– Version: 0.1.
– Programming language: Matlab.
– Solves a stochastic linear optimization problem defined on a scenario tree by the Progressive Hedging algorithm [12].

3.4. Sklml

Participants: Quentin Carbonneaux, François Clément, Pierre Weis.

Easy coarse grain parallelization.

See also the web page http://sklml.inria.fr/.

- Version: 1.0+pl1
- Programming language: OCaml

3.5. SQPlab

– Participant: J. Ch. Gilbert.
– Version: 0.4.5.
– Programming language: Matlab.
– Solves a constrained differentiable optimization problem, 232 downloads in 2011.

– See also the web page http://www-roc.inria.fr/~gilbert/modulopt/optimization-routines/sqplab/sqplab.html.

3.6. LifeV

Participant: Michel Kern.

Finite element library with emphasis on life and environemntal sciences. LifeV is the joint collaboration between École Polytechnique Fédérale de Lausanne (Switzerland), Politecnico di Milano (Italy), Inria (France) and Emory University (U.S.A.).

- Version 2.0
- Programming language: C++

3.7. SOPRANO_scenarios

– Participant: A. Chiche, J. Ch. Gilbert, M. Porcheron
– Version: 0.1.
– Programming language: C++.
– Solves the medium-term electricity planning problem defined on a scenario tree by the Progressive Hedging algorithm.

4. Contracts and Grants with Industry

4.1. 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 to *infeasible* convex quadratic optimization problems using the augmented Lagrangian approach [8] and
- on the solution to the optimization of the electricity production under uncertainties, using the progressive hedging algorithm.

(Andra) Estime takes part in 2 projects in the framework of the Andra–Inria research agreement;

- Ph. Hoang–Thi–THao is preparing a PhD (surpervised by J. E. Roberts, C. Japhet and M. Kern) on space–time domain decomposition methods for modeling transport in porous media. At the end of the first year, a Matlab prototype has been developed, that enables comparing different domain decomposition methods.
- M. Kern is advising Andra in the choice of high performance linear algebra solvers for the heterogeneous problems encountered in flow simulations. The numerical properties and expected parallel performance have been analyzed.

5. Partnerships and Cooperations

5.1. 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, École des Mines de St Etienne and BRGM.

5.2. International Initiatives

5.2.1. Visits of International Scientists

5.2.1.1. Invited scientists

Luca Formaggia (June 16-17), Politecnico di Milano (Italy)

5.2.1.2. Internships

Mohamed El Hedi Riahi (1/11 – 31/12 2011)

Subject: Estimation de paramètres hydrogéologiques

Institution: Ecole Nationale d'Ingénieurs de Tunis (Tunisia)

Fatma Cheikh (1/11 – 31/12 2011)

Subject: Détermination de fractures dans un milieu poreux par la méthode du zoning

Institution: Ecole Nationale d'Ingénieurs de Tunis (Tunisia)

Alessio Fumagalli (from jan 22 to Feb 23)

Subject: Numerical methods for flow and transport in porous media

Institution: Politecnico di Milano (Italy)

5.2.2. Participation In International Programs

Estime is 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.

6. Dissemination

6.1. Animation of the scientific community

J. E. Roberts:

Member of the External Advisory Board for CFSES (Center for Frontiers of Subsurface Energy Security).

Member of the International Scientific Committee for the conference Interpore 2011, Bordeaux, March 2011, and organization (with R. Helmig) of the minisymposium "Advanced Numerical Modeling".

Chair of the prize commitee for the SIAM conference on Geosciences, Long Beach, March 2011, and organization of the minisymposium.

6.2. Conferences, Seminars, Invitations

I. Ben Gharbia:

Benchmark 3D : a Composite Hexahedral Mixed Finite Element, International Symposium on Finite Volumes for Complex Applications 6, Prague, Czech Republic, June 6–10, 2011.

Modeling hydrogen-water flow with hydrogen dissolution as a problem with complementarity constraints, SIAM Conference on Geosciences, Long Beach, California, March 21–24, 2011, in minisymposium "Numerical Methods for Compositional Liquid-Gas Flow in Porous Media".

Gas Phase Appearance and Disappearance as a Problem with Complementarity Constraints, 4th International Conference on Approximation Methods and numerical Modeling in Environment and Natural Resources (MAMERN'11), Morocco, May 23 –26, 2011.

Nonlinear complementarity constraints for two-phase flow in porous media with gas phase appearance and disappearance, TAM–TAM'11, Tunis, Tunisia, April 23–26, 2011.

Complementarity problem for hydrogen-water flow with hydrogen dissolution (Poster), Journées scientifiques du GNR MOMAS, CIRM, Marseille, France, 02–04 novembre, 2011.

Q. Carbonneaux:

Parallel programming with Sklml, MaGiX@LiX 2011, École Polytechnique, Palaiseau (France), September 19–23, 2011 (with F. Clément and P. Weis).

A. Chiche:

Convergence of the progressive hedging algorithm applied to the medium-term electricity planning problem, Conference on Optimization and Practices in Industry (COPI) 2011, Paris, France, 23-25 november 2011.

F. Clément:

Formalisation de la preuve de convergence d'un schéma numérique pour la résolution de l'équation des ondes mono-dimensionnelle, 4es Rencontres Arithmétique de l'Informatique Mathématique (RAIM'11), Perpignan (France), February 7–10, 2011

J. Jaffré:

A discrete fracture model for two-phase flow with different rock types, Interpore 2011, Bordeaux, March 2011, in minisymposium "Advanced Numerical Modeling", (with M. Mnejja and J. E. Roberts).

Two-phase Flow in Porous Media with Discrete Fractures, SIAM conference on Geosciences, Long Beach, USA, March 2011, in minisymposium "Modeling Flow in Porous Media with Fractures", (with M. Mnejja and J. E. Roberts).

Mathematics to validate numerical methods for simulation, HLRS German-French Workshop, Fellbach, Germany, April 2011.

M. Kern:

Iterative methods and preconditioning for a model of transport with sorption, SIAM Conference on Geosciences, March 2011 (with A. Taakili).

Reactive transport in Porous Media — Applications to CO2 storage, Université de Pau, October 2011 (with L. Amir, B. Gueslin, A. Taakili).

Des mathématiques pour modéliser les eaux souterraines, Lycée Talma (Brunoy), March 2011.

J. E. Roberts:

Flow in porous media with fractures: modeling fractures as interfaces, seminar, university of Zaghreb, Croatia, February 2011.

Mathematics and simulation of subsurface flow, HLRS German-French Workshop, Fellbach, Germany, April 2011.

A discrete fracture model for two-phase flow with matrix-fracture interaction, ICCS 2011 (International Conference on Computer Science), Singapore, June 2011, (with J. Jaffré and M. Mnejja).

6.3. Teaching

I. Ben Gharbia:

Université Paris–Dauphine, *Algèbre linéaire*, License 1 TD, 39 h.

A. Chiche:

ENSTA ParisTech, *Optimisation différentiable – théorie et algorithmes*, Master 1 TD, 26 h.

F. Clément:

Mines ParisTech, *Calcul différentiel*, Licence 3, 17 h.

J. Ch. Gilbert:

ENSTA ParisTech, *Optimisation différentiable – théorie et algorithmes*, Master 1, 42 h.

J. Jaffré:

École Nationale d'Ingénieurs de Tunis (ENIT), Tunisia, *Volumes finis et éléments finis mixtes*, Mastère 2, 20 h (with J. E. Roberts).

M. Kern:

Mines ParisTech, *Éléments finis*, Master 1, 30 h.

Mines ParisTech, *Problèmes inverses*, Master 1, 26 h.

J. E. Roberts:

École Supérieure d'Ingénieurs Léonard de Vinci, *Approximation methods*, Master 1, 20 h.

École Nationale d'Ingénieurs de Tunis (ENIT), Tunisia, *Volumes finis et éléments finis mixtes*, Mastère 2, 20 h (with J. Jaffré).

PhD: O. Saouli, *Simulation du transport de solutés réactifs en milieux poreux hétérogènes*, université Mentouri, Constantine, Algérie, July 2011 (Advisers: J. Jaffré, M. Kern, M. Bencheikh Leocine).

PhD in progress: I. Ben Gharbia, *Résolution numérique de problèmes non-linéaires singuliers – Application aux écoulements diphasiques*, October 2008 (Advisers: J. Ch. Gilbert and J. Jaffré).

PhD in progress: A. Chiche, *Résolution Numérique de Grands Problèmes d'Optimisation – Application à la Gestion de Production d'Électricité*, Université Paris VI, November 2008 (Adviser: J. Ch. Gilbert).

PhD in progress: Ph. Hoang-Thi-Thao, *Space–time domain decomposition methods for transport in porous media*, October 2010 (Advisers: J. E. Roberts, C. Japhet, M. Kern).

7. Bibliography

Publications of the year

Doctoral Dissertations and Habilitation Theses

[1] O. SAOULI. *Simulation du transport de solutés réactifs en milieux poreux hétérogènes*, université Mentouri, Constantine, Algérie, 2011.

Articles in International Peer-Reviewed Journal

[2] H. BEN AMEUR, G. CHAVENT, F. CLÉMENT, P. WEIS. *Image Segmentation with Multidimensional Refinement Indicators*, in "Inverse Problems in Science and Engineering", 2011, vol. 19, n° 5, p. 577–597, Special Issue: Proceedings of the 5th Internat. Conf. on Inverse Problems: Modeling and Simulation, May 24th–29th, 2010, held in Antalya, Turkey, http://dx.doi.org/10.1080/17415977.2011.579609.

[3] S. BOLDO, F. CLÉMENT, J.-C. FILLIÂTRE, M. MAYERO, G. MELQUIOND, P. WEIS. *Wave Equation Numerical Resolution: Mathematics and Program*, in "J. of Automated Reasoning", 2011, submitted to.

[4] J. JAFFRÉ, M. MNEJJA, J. E. ROBERTS. *A discrete fracture model for two-phase flow with matrix-fracture interaction*, in "Procedia Computer Science", 2011, vol. 4, p. 967–973, Proceedings of the ICCS 2011 conference, Singapore.

International Conferences with Proceedings

[5] I. BEN GHARBIA, J. JAFFRÉ, N. S. KUMAR, J. E. ROBERTS. *Benchmark 3D : a Composite Hexahedral Mixed Finite Element*, in "Finite Volumes for Complex Applications VI Problems & Perspectives", Springer Proceedings in Mathematics, 2011, vol. 4, p. 969–976, http://dx.doi.org/10.1007/978-3-642-20671-9_94.

Research Reports

[6] I. BEN GHARBIA, J. JAFFRÉ. *Gas phase appearance and disappearance as a problem with complementarity constraints*, Inria, Rocquencourt, France, 2011, n° 7803, submitted, http://hal.inria.fr/hal-00641621/.

[7] S. BOLDO, F. CLÉMENT, J.-C. FILLIÂTRE, M. MAYERO, G. MELQUIOND, P. WEIS. *Wave Equation Numerical Resolution: Mathematics and Program*, Inria, Saclay, France, 2011, n° 7826, http://hal.inria.fr/hal-00649240/en/.

[8] A. CHICHE, J. CH. GILBERT. *How the augmented Lagrangian algorithm deals with an infeasible convex quadratic optimization problems*, INRIA, BP 105, 78153 Le Chesnay, France, 2011, To appear.

[9] N. FRIH, V. MARTIN, J. E. ROBERTS, A. SAADA. *Modeling fractures as interfaces with nonmatching grids*, INRIA, February 2011, n° RR-7517, http://hal.inria.fr/inria-00561601/en.

Other Publications

[10] A. CHICHE, J. CH. GILBERT, M. PORCHERON. *On the convergence of the constraint multipliers in the progressive hedging algorithm for solving a stochastic optimization problem on a scenario tree*, 2011, To appear.

[11] J. CH. GILBERT. *Creation of articles on Wikipedia.fr (the number of views in 2011 is sometimes given in parentheses): Algorithme proximal, Algorithme proximal (optimisation), Application non expansive, Complémentarité linéaire, Conditions d'optimalité (dimension finie) (7281), Cône (analyse convexe) (1614), Cône asymptotique (888), Domaine effectif, Enveloppe supérieure, Espace strictement convexe, Fonction asymptotique (1670), Fonction B-différentiable (1198), Fonction conjuguée (1894), Fonction convexe-concave (704), Fonction d'appui (913), Fonction fermée, Fonction indicatrice (analyse convexe) (1722), Fonction marginale, Fonction propre (analyse convexe), Georges Bouligand, Ky Fan, M-matrice (832), Matrice suffisante, Opérateur accrétif, Opérateur monotone (1285), Optimisation linéaire (33972), Pénalisation (optimisation), Préconditionnement, Q0-matrice, R0-matrice, S-matrice, Sous-différentiel (1470), Z-matrice*, 2011.

[12] J. CH. GILBERT. *PHlab – A Matlab software for solving a stochastic optimization problem defined on a scenario tree, using the progressive hedging algorithm*, 2011, To appear.

[13] M. KERN, A. TAAKILI. *Block Preconditioning for a Coupled Model of Transport with Sorption in Porous Media*, May 2011, International Conference on Preconditioning Techniques for Scientific and Industrial Applications, Preconditioning 2011, http://hal.inria.fr/inria-00581566/en.