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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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 sequential quadratic programming, interior point methods, the augmented Lagrangian approach [19], nonsmooth methods [11], [21], algebraic optimization [20], optimization without derivative [20], 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 (see [11] for a first contribution).

3. Software

3.1. Modulopt

`M1qn3` (version 3.3: October, 2009), unonstrained optimization for huge-scale problems using the ℓ-BFGS technique; written in Fortran-77. The reverse communication mode has been improved. The code is under the GPL license and has been downloaded 46 times in 2009 (mainly for data assimilation and/or by researchers in meteorology and oceanography).

`Qpal` (version 0.6.1: May, 2009), solver of convex quadratic optimization problems using an augmented Lagrangian; written in Fortran-2003. Introduction of the sparse version, see [12].

`SQPlab` (version 0.4.4: February 2009), solver of nonlinear optimization problems using an SQP approach; written in Matlab. The code is under the QPL license and has been downloaded 196 times in 2009 (very diverse users, including teachers).

`SQPpro` (version 0.5: May, 2009), solver of nonlinear optimization problems using an SQP approach; written in Fortran-2003. Introduction of the sparse version, see [13].

3.2. Focalize

The `FoCaLiZe` system provides means for the developers to formally express their specifications and to go step by step (in an incremental approach) to design and implementation while proving that this implementation meets its specification. The `FoCaLiZe` language offers high level mechanisms: multiple inheritance, late binding, redefinition, parametrization, etc. Confidence in proofs submitted by developers or automatically done relies on formal proof verification. `FoCaLiZe` also provides some automation of documentation production and management. A formal specification can be built by declaring names of functions and values and introducing properties. Then, design and implementation can incrementally be done by adding definitions of functions and proving that the implementation meets the specification. Thus, developing in `FoCaLiZe` is a kind of refinement process from formal model to design and code, completely done within `FoCaLiZe` . Taking the global development in consideration within the same environment brings some conciseness, helps documentation and reviewing.

`FoCaLiZe` is free software, distributed under the BSD licence.

`FoCaLiZe` version 0.1.0 has been released in January 2009.

3.3. Htmlc

`Htmlc` a general purpose text file generator with a programmatic approach in the spirit of functional programming.

`Htmlc` is free software, distributed under the artistic licence found in the LICENSE file in the root directory of the distribution.

`Htmlc` version 2.21 has been released in September 2009.

3.4. CamlImages

`CamlImages` is an image processing library for the Objective Caml language.

`CamlImages` is free software, distributed under the licence of Objective Caml libraries.

`CamlImages` version 3.0.2 has been released in October 2009. This is a bug fix release.

4. Contracts and Grants with Industry

4.1. 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. We intend to bring improvements on augmented Lagrangian like approaches and on nondifferentiable techniques.

4.2. IFP

J. Ch. Gilbert is a consultant for the Institut Français du Pétrole (IFP). A new PhD thesis has started in October on derivative free optimization using high degree polynomial models (student E. Echagüe, direction J. Ch. Gilbert, with the supervision by F. Delbos, see [20]) and a study of a nonsmooth method globalized by trust regions in nonlinear optimization is under investigation with a post-doctoral student (N. Metla, direction J. Ch. Gilbert, supervision by F. Delbos and D. Sinoquet, see [21]).

4.3. Total

Estime is discussing with Total the pros and cons of the mixed finite element method for reservoir simulation.

5. Other Grants and Activities

5.1. National Cooperations

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. From 01/01/2009.

Agence Nationale de la Recherche ANR CerPAN (Certification de Programmes d'Analyse Numérique), with Laboratoire d'Informatique de l'Université Paris-Nord from University of Paris 13, Centre d'Étude et de Recherche en Informatique du CNAM, and Laboratoire de Recherche en Informatique from University of Paris 11. Until 19/06/2009.

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 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 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.

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.

6. Dissemination

6.1. Service to the scientific community

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

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

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

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

I. Ben Gharbia: Université Paris Dauphine, License 2nd year, *Calcul matriciel*, 54 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, *Éléments 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. PhD Theses

I. Ben Gharbia (direction J. Jaffré and J. Ch. Gilbert): linear and nonlinear complementarity problems [11], with application to the simulation of a diphasic flow in a porous medium.

A. Chiche (direction J. Ch. Gilbert): decomposition-coordination methods for the middle-term optimization of the electricity production. A warm-up study on the behavior of the augmented Lagrangian on infeasible convex quadratic optimization problems has made good progress [19].

E. Echagüe at IFP (direction J. Ch. Gilbert): derivative free optimization using SOS (sums of squares) polynomial models ([20] in progress).

6.4. Conferences, Seminars, Invitations

H. Ben Ameur

(with F. Clément and P. Weis) *The multidimensional refinement indicator*,TAMTAM'09, Kenitra (Maroc), May 6-8.

(with F. Clément and P. Weis) *Multidimensional refinement indicators for adaptive parameterization*, MAMERN'09, Pau (France), June 8-11.

I. Ben Gharbia

(with J. Ch. Gilbert and J. Jaffré) *A liquid-gas system with hydrogen dissolution formulated as a complementary problem*, poster presentation, Journées scientifiques du GNR MOMAS, CIRM, Marseille, 23-25 novembre 2009.

G. Chavent

(with R. Di Chiara and G. Schafer): *Equivalent Global pressure formulation for compressible flows: construction of a global capillary function*, 3rd International Conference on Approximation Methods and numerical Modeling in Environment and Natural Resources, MAMERN'09, Pau (France), June 8-11.

A. Chiche

Comparaison d'algorithmes de décomposition. Application à la gestion de production., ROADEF'09, Nancy (France), February 10-12, 2009.

N. Frih

(with J. E. Roberts and A. Saâda) *Theoretical analysis for modeling fractures as interfaces with nonconforming grids*, MAMERN'09, Pau (France), June 8-11.

J. Jaffré

3 week visit to the TIFR-CAM, Bangalore, India (February 15 - March 2).

Discontinuous flux calculation for two-phase flow (poster presentation), 1st International Conference on Challenges of Porous Media (Interpore), Kaiserslautern, Germany March 11-14.

(with I. Ben Gharbia, J. Ch. Gilbert and A. Sboui):*Phase Exchange in Two-phase Flow in Porous Media and Complementary Problems*, 2009 SIAM Conference on Mathematical & Computational Issues in the Geosciences, Leipzig (Germany), June 15-18.

(with C. Japhet, M. Kern, J. E. Roberts): *Subdomain Time Stepping for Transport in Porous Media*, 2009 SIAM Conference on Mathematical & Computational Issues in the Geosciences, Leipzig (Germany), June 15-18.

(with P. Knabner) Organization of the minisymposium *Liquid and Gas Flow in Porous Media: Modelling, Analysis, Simulation*,2009 SIAM Conference on Mathematical & Computational Issues in the Geosciences, Leipzig (Germany), June 15-18.

(with C. Japhet, M. Kern, J. E. Roberts): *Subdomain time stepping and space time domain decomposition*, 13th Conference on the Mathematics of Finite Elements and Applications (MAFELAP), Uxbridge (UK), 9-12 June 2009.

3 week visit to Center of Subsurface Modeling,ICES, University of Texas at Austin, USA (September 20 - November 10).

M. Kern

Flow, transport and chemistry in porous media : numerical methods for coupled problems, Visit to EPFL, Lausanne, Switzerland.

(with A. Amir, A. Taakili), *A Newton–Krylov method for reactive transport in porous media*, 2009 SIAM Conference on Mathematical & Computational Issues in the Geosciences, Leipzig (Germany), June 15-18.

(with A. Michel) Organization of the minisymposium *Challenges in Numerical Modelling of CO2 Geological Storage*, 2009 SIAM Conference on Mathematical & Computational Issues in the Geosciences, Leipzig (Germany), June 15-18.

J. E. Roberts

3 week visit to the TIFR-CAM, Bangalore, India (February 15 - March 2).
Flow in porous media with fractures: modelling fractures as interfaces, 1st International Conference on Challenges of Porous Media (Interpore), Kaiserslautern, Germany March 11-14, invited lecture.
(with N. Frih, P. Knabner, A. Saâda): *Some Results Concerning a Model for Fractures with Forchheimer Flow*, 2009 SIAM Conference on Mathematical & Computational Issues in the Geosciences, Leipzig (Germany), June 15-18.
(with J. Erhel) Organization of the minisymposium *Modeling Flow in Porous Media with Fractures*, 2009 SIAM Conference on Mathematical & Computational Issues in the Geosciences, Leipzig (Germany), June 15-18.
3 week visit to Center of Subsurface Modeling,ICES, University of Texas at Austin, USA (September 20 - November 10).

P. Weis

Vingt années de JFLA, JFLA 2009, Saint-Quentin sur Isère, France, January 31–February 3, 2009 (Invited Conference).

6.5. Consulting

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

7. Bibliography

Year Publications

Articles in International Peer-Reviewed Journal

[1] ADIMURTHI, G. VEERAPPA GOWDA, J. JAFFRÉ. *Monotonization of flux, entropy and numerical schemes for conservation laws*, in "Journal of Mathematical Analysis and Applications", vol. 352, 2009, p. 427-439.

[2] L. AMIR, M. KERN. *A Newton-Krylov method for coupling transport with chemistry in heterogeneous porous media*, in "Computational Geosciences", 2009, http://dx.doi.org/10.1007/s10596-009-9162-x.

[3] J.-B. APOUNG, P. HAVÉ, J. HOUOT, M. KERN, A. SEMIN. *Reactive Transport in Porous Media*, in "ESAIM Proceedings", vol. 27, 2009, p. 227-245.

[4] J. CARRAYROU, M. KERN, P. KNABNER. *Reactive Transport Benchmark of MoMaS*, in "Computational Geosciences", 2009, http://dx.doi.org/10.1007/s10596-009-9157-7Germayny.

[5] G. CHAVENT. *A fully equivalent global pressure formulation for three-phase compressible flows*, in "Applicable Analysis", vol. 88, 2009, p. 1527-1541.

[6] F. DELBOS, T. FENG, J. GILBERT, D. SINOQUET. *SQP methods for reservoir characterization*, in "eo", 2009, submitted to.

[7] A. SBOUI, J. JAFFRÉ, J. E. ROBERTS. *A composite mixed finite element for hexahedral grids*, in "SIAM J. Sci. Comput.", 2009, p. 2623-2641.

[8] C. DE DIEUVELEULT, J. ERHEL, M. KERN. *A global strategy for solving reactive transport equations*, in "J. Computational Physics", vol. 228, 2009, p. 6395-6410.

Scientific Books (or Scientific Book chapters)

[9] G. CHAVENT. *Nonlinear least squares for inverse problems*, Springer, 2009.

Research Reports

[10] ADIMURTHI, G. VEERAPPA GOWDA, J. JAFFRÉ. *Applications of the DFLU flux to systems of conservation laws*, n° 7009, INRIA, B.P. 105, 78153 Le Chesnay cedex, France, July 2009, submitted, Technical report.

[11] I. BEN GHARBIA, J. GILBERT. *Nonconvergence of the plain Newton-min algorithm for linear complementarity problems with a P-matrix*, n° 7160, INRIA, BP 105, 78153 Le Chesnay, France, 2009, http://hal.archives-ouvertes.fr/inria-00442293/en, Research Report.

[12] J. GILBERT. *QPAL – A solver of convex quadratic optimization problems, using an augmented Lagrangian approach – Version 0.6.1*, n° 0377, INRIA, BP 105, 78153 Le Chesnay, France, 2009, Technical Report.

[13] J. GILBERT. *SQPpro – A solver of nonlinear optimization problems, using an SQP approach – Version 0.5.1*, n° 0378, INRIA, BP 105, 78153 Le Chesnay, France, 2009, Technical Report.

[14] J. JAFFRÉ, A. SBOUI. *Henry's law and gas phase disappearance*, n° 6891, INRIA, B.P. 105, 78153 Le Chesnay cedex, France, March 2009, to appear in Transport in Porous Media, Technical report.

[15] J. ZHANG, G. CHAVENT, J. JAFFRÉ. *Estimating nonlinearities in twophase flow in porous media*, n° 6892, INRIA, B.P. 105, 78153 Le Chesnay cedex, France, March 2009, Technical report.

Other Publications

[16] H. BEN AMEUR, G. CHAVENT, F. CLÉMENT, P. WEIS. *Image Segmentation with optimal Control Techniques*, 2009, in preparation.

[17] I. BEN GHARBIA, J. GILBERT, J. JAFFRÉ. *A liquid-gas system with hydrogen dissolution formulated as a complementary problem*, 2009, poster presented at Journées scientifiques du GNR MOMAS, CIRM, Marseille, 23-25 novembre.

[18] S. BOLDO, F. CLÉMENT, J.-C. FILLIÂTRE, M. MAYERO, G. MELQUIOND, P. WEIS. *Formal Proof of a Wave Equation Resolution Program: the Method Error*, 2009, in preparation.

[19] A. CHICHE, J. GILBERT. *On the behavior of the augmented Lagrangian algorithm on an infeasible convex quadratic optimization problem*, 2009, in preparation.

[20] F. DELBOS, E. ECHAGÜE, J. GILBERT. *Interpolation, regression, and update of models made of sum of squares of polynomials*, 2009, in preparation.

[21] F. DELBOS, J. GILBERT, N. METLA, D. SINOQUET. *A nonsmooth Newton approach for solving nonlinear optimization problems*, 2009, in preparation.