INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Project-Team Estime

Parameter Estimation and Modeling in Heterogeneous Media

Rocquencourt

THEME NUM

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1. Team

Head
Jérôme Jaffré [DR, Inria]

Deputy Head
Michel Kern [CR]

Administrative Assistants (shared with project Ondes)
Sandrine Boute [until 31/3]
Sylvaine Sperte [16/2–30/11]
Héléna Kutniak [since 8/11]

INRIA Researchers
François Clément [CR]
Jean-Charles Gilbert [DR]
Jean E. Roberts [DR]

Junior Engineer
Arnaud Vodicka [until 31/8]

Scientific Advisor
Guy Chavent [University Paris 9]

External Collaborator
Hassan Kaddouri [Université du Littoral]

Visiting Scientists
Hend Ben Ameur [University of Bizerte and Lamsin-ENIT, Tunisia, 1 month]
Veerappa Gowda [Tata Institute, Bangalore, India, 1 month]
Ali Saada [Lamsin-ENIT, Tunisia, 1 month]

PhD students
Philippe Al Khoury [Cifre Auxitrol fellowship, Universities of Paris 9 and Paris 10]
Frédéric Delbos [French Institute of Petroleum, University of Paris 6]
Estelle Marchand [ANDRA fellowship, University of Paris 9 since 1/10]
Vincent Martin [ANDRA fellowship, University of Paris 9 until 31/1]
Amel Sboui [Inria fellowship, University of Paris 9]

Internships
Laïla Amir [DEA, 1/4–31/12]
Estelle Marchand [DEA, École Centrale de Lyon, 1/4–30/9]
Benaamer Bounichane [DEA, École Normale Superieure de Cachan, 1/4–30/9]

2. 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.

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 developped 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 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, telecomunication networks, shape optimization (aeronautic and tyre industry) to name a few. An outcome of this activity is also the *Modulopt library*, which gathers optimization softwares produced by the team.

3. Contracts and Grants with Industry

3.1. ANDRA

Multidomain simulation of the transport of nuclear contaminants around a nuclear waste disposal site. ANDRA is the French National Agency for Nuclear Waste Management. It provided financial support for V. Martin's and E. Marchand's PhD thesis.

4. Other Grants and Activities

4.1. National Cooperations

INRIA ARC Dynas (Dynamics of shallow water tables during heavy rainfalls), with Cermics and Cereve from Ecole Nationale des Ponts et Chaussées (Marne La Vallée) and Cemagref (Antony).

CNRS GDR Momas (Mathematical Modeling and Numerical Simulation for Deep Underground Disposal of Nuclear Waste).
Ministry of Research, ACI "Globalization of Computer Resources and Data", Project Hydrogrid, with projects Aladin and Paris at Inria-Rennes, with IMFS at Louis Pasteur University in Strasbourg, and with the "Transferts physiques et chimiques" group at UMR Geosciences, Rennes.
INRIA support for A. Vodicka, a Junior Engineer, for the study of applications of Ocaml in Scientific Computing.

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 E-Didon and is supported by INRIA.

5. Dissemination

5.1. Service to the scientific community

- F. Clément is the designer and the administrator of the ARC Dynas website. He is also the organizer of the closing Workshop held at Rocquencourt, December 6-8, 2004.
- F. Clément, J. Jaffré and P. Joly (from Ondes) were the organizers of MathGeo 04, New Trends in Mathematical and Numerical Methods for Geosciences - Direct and Inverse Problems, a conference honoring Guy Chavent held at Rocquencourt, December 9-10, 2004.
- M. Kern is the secretary of GAMNI (Groupe pour l'Avancement des Méthodes Numériques de l'Ingénieur), one of SMAI's thematic activity groups.
- M. Kern (with A. Ern and B. Sportisse, from ENPC) was the organizer of the workshop "Some problems met in numerical chemistry: hydrology, combustion, atmosphere", on December 16 at INRIA.
- M. Kern is Scientific Secretary of CNRS GDR MoMaS.
- M. Kern and Jean E. Roberts are organizing the SIAM Conference on Mathematical & Computational Issues in the Geosciences, Avignon, June 7-10, 2005.
- J. Jaffré is co-editor-in-chief (with M.F. Wheeler) of the journal Computational Geosciences
- J.E. Roberts is a member of the Editorial Board of the International Journal of Numerical Analysis and Modeling.

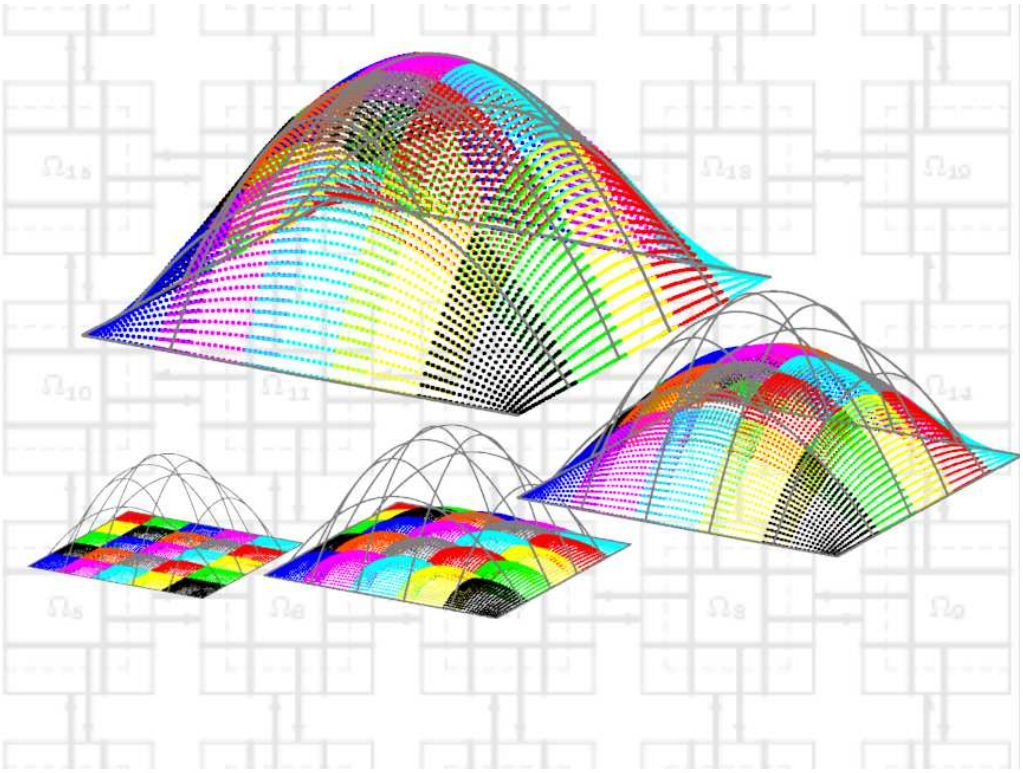

Figure 1. Image used for the cover of the CD-Rom of free softwares distributed by INRIA (December 2004). It shows four iterations towards the resolution of the 2D Poisson's equation using Schwarz decomposition algorithm with 25 subdomains. Automatic parallelism on the INRIA cluster was obtained with the OCamlP3l environment. The same OCaml module is used to compute the image displaying the communications between subdomains (in the background). This is a collaboration with project Cristal.

5.2. Teaching

F. Clément École des Mines de Paris. 1st year: *Differential Calculus*, 22 h

J. Ch. Gilbert Université Panthéon-Sorbonne (Paris I), DEA Modélisation et Méthodes Mathématiques en Économie, *Méthodes newtoniennes en optimisation avec contraintes*, 21 h/y.
ENSTA, 2nd year, *Optimisation différentiable : théorie et algorithmes*, 42 h/y.

J. Jaffré Université Paris-Dauphine, DESS Mathématiques de la décision (Master level), *Numerical Analysis: Numerical Solution of Large Systems*, 18 hours
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. Roberts (since 2000).

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,
École Polytechnique, teaching assistant for *Modeling and Simulation Projects*, applied mathematics section, 4th year students, 20 hours.

J. Roberts École Supérieure d'Ingénieurs Léonard de Vinci, *Approximation methods*, 4th year students, 40 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

P. Al Khoury *Line search global strategies for nonlinear least-squares problems based on curvature and projected curvature*, Inverse Problems, Design and Optimization (IPDO) Symposium, Rio de Janeiro, Brazil, March 17-19.

F. Clément *Analyse de sensibilité et estimation de paramètres de transport pour une équation de diffusion, approche par état adjoint*, Séminaire du DEN/DM2S/SFME/MTMS, CEA, Saclay, June 8, 2004.
Analyse de sensibilité et estimation de paramètres pour des problèmes en géohydrologie, Rencontre ForPro-MoMaS, ISTIL, Lyon, October 27.

J.Ch. Gilbert *A dedicated constrained optimization method for 3D reflection tomography*, 66th EAGE Conference & Exhibition, Paris, June 7 (with F. Delbos and D. Sinoquet).
On the solution of convex quadratic optimization problems by augmented Lagrangian and active set methods, premier Congrès Canada-France des Sciences Mathématiques, Toulouse, July 12, invited talk.

J. Jaffré *Numerical Flux Calculation For Two-phase Flow in Porous Media*, International Conference on Nonlinear Phenomena, Indian Institute of Science, Bangalore, India, January 5-10, 2004, Invited lecture.
Méthodes numériques pour les écoulements en milieu poreux, Ecole Geomeca, Chambery, 29-30 novembre 2004.

M. Kern *Using Scilab to Solve Inverse Problems for Ordinary Differential Equations*, Scilab 2004 Conference, INRIA, Rocquencourt, December 2-3, 2004.

E. Marchand *About the Pressure in Two-Phase Slightly Compressible Flow Equations*, Workshop DYNAS '04, INRIA, Rocquencourt, December 6-8.

J. Roberts *Two-phase Flow in Porous Media With Fractures*, International Conference on Nonlinear Phenomena, Indian Institute of Science, Bangalore, India, January 5-10, 2004, Invited lecture.
Numerical methods for two-phase flow in a porous medium with two rock-types, 13th Conference on Mathematics for Industry (ECMI-2004), Eindhoven, The Netherlands, June 2004.

5.4. Consulting

- J.Ch. Gilbert is a consultant for the Institut Français du Pétrole and supervises the PhD thesis of Frédéric Delbos, which aims at taking constraints into account in seismic tomography techniques for the reconstitution of the subsoil. He had also consulting activities for Michelin at Clermont-Ferrand.
- M. Kern was a consultant for ANDRA (French National Agency for Nuclear Waste Management, until May 31).
- J. Jaffré is a member of the Scientific Advisory Board of ANDRA, the French agency for nuclear waste management and of CIPR, the Center for Integrated Petroleum Research at the university of Bergen.

6. Bibliography

Books and Monographs

[1] A. BOURGEAT, M. KERN, EDS. *Simulation of transport around a nuclear waste disposal site: the* COUPLEX *test cases*, Special Issue of the Journal Computational Geosciences, Vol.8, No 2, 2004.

Doctoral dissertations and Habilitation theses

[2] V. MARTIN. *Simulations multidomaines des écoulements en milieu poreux*, Ph. D. Thesis, Université de Paris 9, 2004.

Articles in referred journals and book chapters

[3] ADIMURTHI, J. JAFFRÉ, VEERAPPA GOWDA. *Godunov-type methods for conservation laws with a flux function discontinuous in space*, in "SIAM Journal in Numerical Analysis", 2004, p. 179-208.

[4] P. AL KHOURY, G. CHAVENT, F. CLÉMENT, P. HERVÉ. *Inversion of spectroscopique data of CO_2 radiation*, in "Inverse Problems in Science and Engineering", to appear, 2005.

[5] A. BOURGEAT, M. KERN, S. SCHUMACHER, J. TALANDIER. *The COUPLEX Test Cases: Nuclear Waste Disposal Simulation*, in "Computational Geosciences", Special Issue: Simulation of Transport Around a Nuclear Waste Disposal Site: The COUPLEX Test Cases (Editors: Alain Bourgeat and Michel Kern), vol. 8, n^o 2, 2004, p. 83-98.

[6] V. BOUYER, I. DARBORD, P. HERVÉ, G. BAUDIN, C. L. GALLIC, F. CLÉMENT, G. CHAVENT. *Shock to detonation transition of nitromethane: time-resolved emission spectroscopy measurements*, in "Combustion and Flame", submitted to, 2004.

[7] G. CHAVENT. *Curvature steps and geodesic moves for nonlinear least squares descent algorithms*, in "Inverse Problems in Science and Engineering", vol. 12, 2004, p. 173-191.

[8] F. DELBOS, J. GILBERT. *Global linear convergence of an augmented Lagrangian algorithm for solving convex quadratic optimization problems*, in "Journal of Convex Analysis", 2005.

[9] F. DELBOS, J. GILBERT, R. GLOWINSKI, D. SINOQUET. *Constrained optimization in seismic reflection tomography: an SQP augmented Lagrangian approach*, in "Geophysical Journal International", 2005.

[10] J. GILBERT, C. GONZAGA, E. KARAS. *Examples of ill-behaved central paths in convex optimization*, in "Mathematical Programming", 2005.

[11] J. JAFFRÉ, V. MARTIN, J. E. ROBERTS. *Modelling Fractures and Barriers as Interfaces for Flow in Porous Media*, in "SIAM J. Scient. Comp.", to appear, 2004.

[12] T. SCHAAF, G. CHAVENT, M. MEZGHANI. *Refinement indicators for optimal selection of geostatical realizations using the gradual deformation method*, in "Mathematical Geology", vol. 36, 2004, p. 425-445.

[13] A. YOUNES, P. ACKERER, G. CHAVENT. *From mixed finite elements to finite volumes for elliptic PDEs in two and three dimensions*, in "International Journal in Numerical Methods for Engineering", vol. 59, 2004, p. 365-388.

Publications in Conferences and Workshops

[14] P. AL KHOURY, G. CHAVENT. *Line search global strategies for nonlinear least-squares problems based on curvature and projected curvature*, in "Inverse Problems, Design and Optimization Symposium", H. R. B. ORLANDE (editor)., March 2004.

Internal Reports

[15] F. CLÉMENT, N. KHVOENKOVA, A. CARTALADE, P. MONTARNAL. *Analyse de sensibilité et estimation de paramètres de transport pour une équation de diffusion, approche par état adjoint*, Rapport de Recherche, n° 5132, Inria, Rocquencourt, France, 2004, http://www.inria.fr/rrrt/rr-5132.html.

[16] F. CLÉMENT, R. DI COSMO, Z. LI, V. MARTIN, A. VODICKA, P. WEIS. *Parallel Programming with the OcamlP3l System. Applications to Numerical Code Coupling*, Rapport de Recherche, n° 5131, Inria, Rocquencourt, France, 2004, http://www.inria.fr/rrrt/rr-5131.html.

Miscellaneous

[17] M. GANDER, L. HALPERN, M. KERN. *A Schwarz Waveform Relaxation Method for Convection–Diffusion Problems*, contract report, 2004.

[18] E. MARCHAND. *Méthode de Newton pour un écoulement eau/air en hydrogéologie*, 2004, Travail de Fin d'Études, École Centrale de Lyon.