INRIA

INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Project-Team Estime

Parameter Estimation and Modeling in Heterogeneous Media

Rocquencourt

THEME 4B

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1. Team

Head
Jérôme Jaffré [DR, Inria]

Deputy Head
Michel Kern [CR]

Administrative Assistant (shared with project Ondes)
Sandrine Boute

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

Junior Engineer
Arnaud Vodicka

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, 2 months]
Veerappa Gowda [Tata Institute, Bangalore, India, 1 month]
Ali Saada [Lamsin-ENIT, Tunisia, 1 month]

Postdoctoral fellows
Xavier Jonsson [Inria Postdoc at Northwestern University, USA, until 1/3]
Martial Mancip [until 30/9]

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]
Vincent Martin [ANDRA fellowship, University of Paris 9]
Amel Sboui [Inria fellowship, University of Paris 9]

Internships
Hafida Karim [DEA, University of Pau, 1/4–31/7]
Nina Khvoenkova [DEA, École Polytechnique and University of Paris 6, 1/4–31/7]
Jennifer Niessner [Master, University of Stuttgart, 15/1–15/7]

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.

7. Contracts and Grants with Industry

7.1. 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 PhD thesis.

8. Other Grants and Activities

8.1. 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).

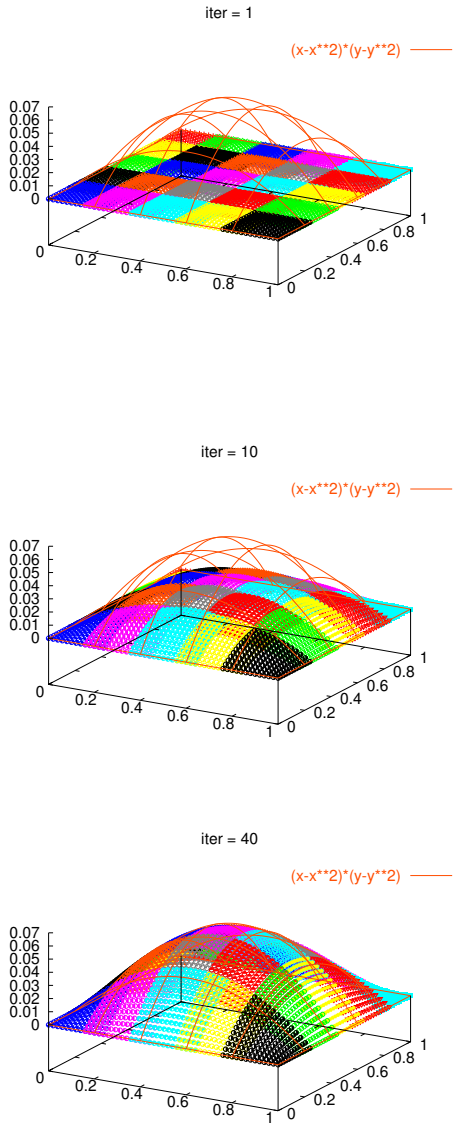

Figure 1. Resolution of the 2D Poisson's equation using Schwarz decomposition algorithm with 25 subdomains. The parallel computation is implemented with the ***OcamlP3l*** *environment and run on the 32-processor cluster of Inria at Rocquencourt. The subdomains are square and have their own color. Initial solution (top left), solution after 10 iterations (top right) and final solution after 40 iterations (bottom). The analytical solution is depicted in red.*

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.

8.2. 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.

9. Dissemination

9.1. Service to the scientific community

- F. Clément is the designer and the administrator of the ARC Dynas website.
- M. Kern is the organizer of the Rocquencourt Colloquium Rocquencourt Colloquium.
- 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 is Scientific Secretary of CNRS GDR MoMaS.
- J. Jaffré is Chief Editor (with M.F. Wheeler) of Computational Geosciences

9.2. Teaching

- Panthéon-Sorbonne University (Paris 1), DEA « Modélisation et Méthodes Mathématiques en Économie »: *Méthodes newtoniennes en optimisation avec contraintes*, 21 h., J.Ch. Gilbert.
- Pierre et Marie Curie University (Paris 6), DEA « Optimisation, Jeux et Modélisation en Économie »: *Introduction aux algorithmes de points intérieurs*, 15 h., J.Ch. Gilbert.
- University of Nanterre (Paris 10), DEA « Des Essais à la Modélisation Mécanique Thermique et Couplage »: *Interpolation et Approximation*, 9 h., P. Al Khoury.
- University of Paris 9, DESS « Mathématiques de la Décision », *Analyse Numérique*, 24 h, J. Jaffré.
- École Nationale d'Ingénieurs de Tunis (ENIT), DEA « Mathématiques Appliquées », *Volumes finis et éléments finis mixtes*, 20 h, 3 - 7 mars, J. Jaffré et J. Roberts.
- Pôle Universitaire Léonard de Vinci, *Méthodes d'approximation*, J. Roberts.
- École des Mines de Paris, 1st year, *Calcul différentiel*, 22 h, F. Clément.
- École des Mines de Paris, 1st year, *Intégration et mesure*, 30 h, V. Martin.
- École Nationale de Techniques Avancées (ENSTA), 2nd year, *Optimisation différentiable : théorie et algorithmes*, 42 h., J.Ch. Gilbert.
- École des Mines de Paris, 2nd year, *Calcul scientifique*, 17 h, M. Kern.
- University of Versailles, 1st year, *Algèbre Analyse*, 48 h., A.Sboui.

9.3. Conferences, Seminars, Invitations

- F. Clément, *Analyse de sensibilité et estimation de paramètres de transport pour une équation de diffusion, approche par état adjoint*, Journées Scientifiques du GDR MOMAS, Luminy, November 12-14.
- J.-Ch. Gilbert: *Fundamentals of Optimization*, three invited lectures at the "Summer School Jacques Louis Lions": *Multidisciplinary Methods for Analysis, Optimization and Control of Complex Systems*, March 17-22, Montecatini (Tuscany), Italy.
- J.-Ch. Gilbert: *Une introduction aux algorithmes de points intérieurs en optimisation*, invited lecture at the "Colloque d'Analyse Numérique CANUM-2003", La Grande Motte, France, June 2-6.
- J.-Ch. Gilbert: *Two properties of an augmented Lagrangian method for solving strictly convex quadratic programs*, 18th International Symposium on Mathematical Programming, Copenhagen, Denmark, August 18-22.
- J. Jaffré, *Flux calculation for two-phase flow in porous media*, SIAM Conference on Mathematical and Computational Issues in the Geosciences, Austin, USA, March 17-20.
- J. Jaffré, *Center for Subsurface Modeling, ICES, University of Texas at Austin, USA (Professor Mary F. Wheeler), August 4-15*
- J. Jaffré, *Université de Stuttgart, Allemagne (Professor Rainer Helmig), November 24-25*
- M. Kern: *The* COUPLEX *Models*, SIAM Conference on Mathematical and Computational Issues in the Geosciences, Austin, USA, March 17-20.
- M. Kern, *A Schwarz Waveform Relaxation Method for Convection–Diffusion Problems*, SIAM Conference on Mathematical and Computational Issues in the Geosciences, Austin, USA, March 17-20.
- M. Kern, *A Schwarz Waveform Relaxation Method for Convection–Diffusion Problems*, Rice University, Houston, USA, March 21.
- M. Kern, *Simulation of density driven flow: Model formulation and a Corba based distributed implementation*, Moscow, June 21-22.
- M. Kern, *Simulation of density driven flow Model formulation and a Corba based distributed implementation*, special day on "Calcul Scientifique et le GRID" september 18.
- M. Kern, *Couplage de code pour l'écoulement et le transfert de polluants en milieu géologique : une approche par composants logiciels*, special days "Applications, Algorithmique et Ordonnancement pour la grille", Bordeaux, september 24-15.
- M. Kern, *Méthodes numériques pour le transport réactif*, Journées Scientifiques du GDR MOMAS, Luminy, November 12-14.
- V. Martin, *Parallel domain decomposition with OcamlP3l: a local refinement method*, Journées Scientifiques du GDR MOMAS, Luminy, November 12-14.
- V. Martin, *Domain decomposition for flow simulation around a waste disposal site: direct simulation versus code coupling using OcamlP3l*, (with F. Clément, A. Vodicka, R. Di Cosmo and P. Weis), 5th Intern. Conf. on Supercomputing in Nuclear Applications, SNA'2003, Paris, September 22-24.
- V. Martin, *Numerical modeling of flow in porous media with faults*, SIAM Conference on Mathematical and Computational Issues in the Geosciences, Austin, USA, March 17-20.
- V. Roberts, organization of the minisymposium *Flow in porous media with fractures*, SIAM Conference on Mathematical and Computational Issues in the Geosciences, Austin, USA, March 17-20
- J. Roberts, *Center for Subsurface Modeling, ICES, University of Texas at Austin, USA (Professor Mary F. Wheeler), August 4-15*
- J. Roberts, *Université de Stuttgart, Allemagne (Professor Rainer Helmig), November 3-4*
- A. Sboui, *Raffinement en temps par sous-domaine pour la convection en milieu poreux*, Journées Scientifiques du GDR MOMAS, Luminy, November 12-14.

9.4. Software Distribution

- Distribution of optimization codes from the MODULOPT library (in collaboration with Claude Lemaréchal, NUMOPT project). The distribution is only made on demand, through the Web page of the library (http://www-rocq.inria.fr/estime/modulopt/index.html). We list below the laboratories and researchers to which the codes have been sent.

  - N1CG1 (strictly convex quadratic optimization by a dynamically BFGS preconditioned conjugate gradient): meteorological forcast with a 4D-var model (ARMA, Service Météorologique du Canada, Pierre Gauthier).
  - M1QN3 (large scale unconstrained optimization): teledetection in a vegetation model (INRA à Avignon, Frédéric Baret, Claire Lauvernet); satellite data assimilation to recover aerosol information (Laboratoire d'Optique Atmosphérique, Olivier Boucher); parameter estimation in an oceanic ecosystem model (Woods Hole Oceanographic Institution, USA, Jeffrey Dusenberry); two body problem (Reading University, GB, Laura Stanton, M.J. Baines); predictability of dynmaical systems with application to the atmosphere and the ocean (Courant Institute of Mathematical Sciences, Richard Kleeman); subproblem resolution appearing in a Lagrangian relaxation approach in convex optimization (France Télécom R&D, Adam Ouorou); atmospheric pollution simulation at a regional scale (Laboratoire LISA, UMR 7583, Université Paris XII, Laurent Menut); estimates of global and European CH4 emissions, using ground based and satellite observations of atmospheric CH4 mixing ratios (Institute for Environment and Sustainability, Joint Research Centre, European Commission, Ispra, Italy, Peter Bergamaschi); 4-dimensional variational data assimilation in the model of the ocean (International Arctic Research center, Alaska, Fairbaks, USA, Gleb Panteleev).
  - N2QP1 (strictly convex quadratic optimization with bounds): portfolio optimization (Laboratoire Probabilité et Modèles Aléatoires, Université Paris VI-Paris VII, Huyên Pham); wave propagation in a fissured medium (Laboratoire SINETICS, EdF Clamart, T. Fouquet).

9.5. 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.
- M. Kern is a consultant for ANDRA (French National Agency for Nuclear Waste Management).
- J. Jaffré is a member of the Scientific Advisory Board of ANDRA.

10. Bibliography

Articles in referred journals and book chapters

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[2] A. BOURGEAT, M. KERN, S. SCHUMACHER, J. TALANDIER. *The Couplex Models.* in « Computational Geosciences », to appear.

[3] G. CHAVENT, J. JAFFRÉ, J. ZHANG. *Estimating nonlinearities in multiphase flow in porous media.* B. SPORTISSE, F.-X. LE DIMET, editors, in « Inverse Problems », Springer, to appear.

[4] F. CLÉMENT, R. DI COSMO, Z. LI, V. MARTIN, A. VODICKA, P. WEIS. *Parallel programming with the OcamlP3l system, with applications to coupling numerical codes.* in « J. Functional Programming », submitted.

[5] W. HUNDSDORFER, J. JAFFRÉ. *Implicit-explicit time stepping with spatial discontinuous finite elements.* in « Applied Numerical Mathematics », volume 6, 2003, pages 523-543.

[6] J. JAFFRÉ, V. MARTIN, J. ROBERTS. *Modeling fractures and barriers as interfaces for flow in porous media.* in « SIAM J. on Scientific Computing », to appear.

[7] J. NIESSNER, R. HELMIG, H. JACOBS, J. ROBERTS. *Interface Condition and Exact Linearization in the Newton Iterations for Two-Phase Flow in Heterogeneous Porous Media.* submitted.

[8] P. AL KHOURY, G. CHAVENT, F. CLÉMENT, P. HERVÉ. *Inversion of spectroscopic data of CO_2 radiation.* in « Inverse Problems in Engineering », submitted, previously released as Proc. of the 4th Internat. Conf. on Inverse Problems in Engineering, 2002.

Publications in Conferences and Workshops

[9] A. BOURGEAT, M. KERN, S. SCHUMACHER, J. TALANDIER. *the* COUPLEX *Test Cases: Models and Lessons.* in « Proc. of the 5th Internat. Conf. on Supercomputing in Nuclear Applications », 2003.

[10] F. CLÉMENT, V. MARTIN, A. VODICKA, R. DI COSMO, P. WEIS. *Domain decomposition with local refinement for flow simulation around a nuclear waste disposal: direct computation and simulation using code couplng with OcamlP3l.* in « Proc. of the 5th Internat. Conf. on Supercomputing in Nuclear Applications », 2003.

Internal Reports

[11] F. CLÉMENT, A. VODICKA, R. DI COSMO, P. WEIS. *Couplage de codes numériques, parallélisme et langages de haut niveau.* Rapport de Recherche, number 4825, Inria, Rocquencourt, France, 2003, http://www.inria.fr/rrrt/rr-4825.html.

[12] F. DELBOS, J. GILBERT. *Global linear convergence of an augmented Lagrangian algorithm for solving convex quadratic optimization problems.* Technical report, number 5028, INRIA, 2003, http://www.inria.fr/rrrt/rr-5028.html.

[13] F. DELBOS, J. GILBERT, R. GLOWINSKI, D. SINOQUET. *Constrained optimization in reflection tomography: an augmented Lagrangian SQP approach.* Technical report, Institut Français du Pétrole, 2003.

[14] J. ERHEL, M. KERN. *Méthodes numériques pour le transport réactif.* Technical report, INRIA, 2004, to appear.

[15] M. GANDER, L. HALPERN, M. KERN. *A Schwarz Waveform Relaxation Method for Convection–Diffusion Problems.* Technical report, INRIA, 2004, to appear.

[16] M. MANCIP, M. KERN. *Simulation of density driven flow: Model formulation and a Corba based distributed implementation.* Technical report, INRIA, 2004, to appear.

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