Project-Team Estime

Parameter Estimation and Modeling in Heterogeneous Media

Rocquencourt

Activity Report

2004
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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]
- Hélène 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 computing. 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 developed to estimate at the same time the zonation and the values of the hydraulic transmissivities in groundwater 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, telecommunication 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).
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.
- 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


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


*Analyse de sensibilité et estimation de paramètres pour des problèmes en géohydrologie*, Rencontre ForPro-MoMaS, ISTIL, Lyon, October 27.


*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.


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


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


Doctoral dissertations and Habilitation theses


Articles in referred journals and book chapters


Publications in Conferences and Workshops


Internal Reports


Miscellaneous
