Project-Team Estime

Parameter estimation and modeling in heterogeneous media

Paris - Rocquencourt

Theme : Observation and Modeling for Environmental Sciences
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1. Team

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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 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 two-phase flow are studied.

Interphase problems for two-phase flow in porous media: Two-phase 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 two-phase 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 fully 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 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 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 $F(x)^T G(x) = 0$, $F(x) \geq 0$, and $G(x) \geq 0$, where $F$ and $G : \mathbb{R}^n \rightarrow \mathbb{R}^n$ 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. 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. Modulopt

- \texttt{SQP1ab} (version 0.4.4: February 2009): 250 downloads in 2010.

4. New Results

4.1. Coupling transport with Chemistry

We have achieved significant progresses for the simulation of reactive transport phenomena. B. Gueslin and M. Kern have completed the simulation of a water–gas system, including several aqueous species and minerals, designed by IFP-Energies Nouvelles, in the framework of the SHPCO2 ANR project. A snapshot of the concentrations of some species is shown on figure 1.

Figure 1. Species concentration for the dissolution of CO2. Upper left: CO2 gas, upper right: calcite, lower left: pH, lower right: chloride (tracer)

The figure shows the initial gas bubble dissolving in water, with a corresponding increase in pH, and calcite dissolution.
5. Contracts and Grants with Industry

5.1. 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 of *infeasible* convex quadratic optimization problems using the augmented Lagrangian approach [10] and
- on the solution of the optimization of the electricity production under uncertainties, using the progressive hedging algorithm.

5.2. Grants with Industry

ANDRA

1. Phuong Hoang Thi Thao’s PhD began in October her PhD thesis on subdomain time stepping formulated as a time and space domain decomposition problem. Her thesis is supported by a contract between INRIA and ANDRA.

2. Another contract between INRIA and ANDRA concerns M. Kern’s consulting support on high performance computing.

5.3. National Initiatives


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, Ecole des Mines de St Etienne and BRGM.

5.4. International Initiatives

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.

Estime is also associated with LIRNE-Equipe d’ingénierie mathématiques, université Ibn Tofail, 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.

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.

5.5. Exterior research visitors

A. Taakili, Univ. of Errachidia (Marrocco), 09/09/2010 to 30/07/2010.

A. Fumagalli, PhD student, MOX, Politecnico di Milano (Itlay), 06/09/2010 to 24/09/2010.
6. Dissemination

6.1. Animation of the scientific community

M. Kern is a member of the Scientific Board of Groupement MoMaS.
M. Kern is a member of the Scientific Board of UNIT, l’Université Numérique Ingénierie et Technologie.

6.2. Teaching

I. Ben Gharbia:
  – Université Paris Dauphine, License 2nd year, Calcul matriciel, 54 h.
  – Université Paris Dauphine, License 1st year, Linear algebra, 39 h.

A. Chiche: ENSTA, 2nd year, Optimisation différentiable – théorie et algorithmes, 26 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, Eléments 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. Conferences, Seminars, Invitations

I. Ben Gharbia


Comportement et usage de l’algorithme de Lagrangien augmenté dans le cas d’un problème quadratique convexe non-réalisable, Groupe de travail de l’équipe Commands (Inria-Ensta-Cmap-CNrs), Journée des doctorants, Paris, France, 18 juin 2010.


J. Jaffré
– One week visit to Prof. Zoubida Mghazli, université Ibn Tofail, Kenitra, Maroc (PHC Volubilis).

M. Kern
– (with L. Amir, A. Taakili) Reactive transport in porous media, visit to MOX, Politecnico di Milano (Italy), April 14 2010.
– (with A. Michel) organized the SHPCO2 workshop, St Lambert des Bois (France), June 14-15 2010 (30 participants, 15 invited talks).
– (with L. Amir, B. Gueslin) Coupled formulations and coupling algorithms for reactive transport in porous media, DyCap Workshop "Microbiology and Reactive Transport in the Capillary Fringe", University of Heidelberg, (Germany), October 7-8, 2010, invited lecture.
– (with B. Gueslin) Coupled formulations and coupling algorithms for reactive transport in porous media, seminar at LMA, Université Technologique de Compiègne (France), November 16, 2010.
– Comment calcule un ordinateur ?, pedagogical presentation to first year university students, Université René Descartes, Paris (France), September 17, 2010.

J. E. Roberts
– (with N. Frih, V. Martin and A. Saada) Some numerical results for modeling fractures as interfaces with nonconforming grids (poster presentation), 2010 InterPore Conference and Annual, College Station,Texas, USA, March 15-17, 2010.
– Single phase flow in porous media with fractures modeling Forchheimer fractures as interfaces (with Peter Knabner) and organized with Z. Mghazli the minisymposium Méthodes et Outils pour les Milieux Poreux, 2ième Congrès de la Société Marocaine de Mathématiques Appliquées (SM2A), Rabat, Maroc, 28-30 juin 2010.
– One week visit to Prof. Zoubida Mghazli, université Ibn Tofail, Kenitra, Maroc (PHC Volubilis).
7. Bibliography

Publications of the year

Articles in International Peer-Reviewed Journal


International Peer-Reviewed Conference/Proceedings


Scientific Books (or Scientific Book chapters)


Research Reports


Other Publications