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Activity Report 2012

Project-Team SAGE

Simulations and Algorithms on Grids for Environment

IN COLLABORATION WITH: Institut de recherche en informatique et systèmes aléatoires (IRISA)

RESEARCH CENTER
Rennes - Bretagne-Atlantique

THEME
Observation and Modeling for Environmental Sciences

Table of contents

Project-Team SAGE

Keywords: Numerical Methods, Environment, Stochastic Methods, High Performance Computing, Fluid Dynamics, Porous Fractured Media, Linear Algebra, Numerical Software Platform

Creation of the Project-Team: December 06, 2004 .

1. Members

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2. Overall Objectives

2.1. Main research areas

Numerical models are very useful for environmental applications. Several difficulties must be handled simultaneously, in a multidisciplinary context. For example, in geophysics, media are highly heterogeneous and only few data are available. Stochastic models are thus necessary. Some computational domains are complex 3D geometries, requiring adapted space discretization. Equations modeling flow and transport are transient, requiring also adapted time discretization. Moreover, these equations can be coupled together or with other equations in a global nonlinear system. These large-scale models are very time and memory consuming. High performance computing is thus required to run these types of scientific simulations. Supercomputers and clusters are quite powerful, provided that the numerical models are written with a parallel paradigm.

The team SAGE undertakes research on environmental applications and high performance computing and deals with two subjects:

1. numerical algorithms, involving parallel and grid computing,
2. numerical models applied to hydrogeology and physics.

These two subjects are highly interconnected: the first topic aims at designing numerical algorithms, which lead to high efficiency on parallel and grid architectures; these algorithms are applied to geophysical models.

Moreover, the team SAGE, in collaboration with other partners, develops the software platform H2OLab for groundwater numerical simulations in heterogeneous subsurface.

2.2. Highlights of the Year

The results of the year are focused on numerical models and simulations for flow in porous fractured media. For this subject only, the team published three papers in journals, gave an invited plenary talk and two invited talks in minisymposia. Societal and economical issues concern environment and energy, such as groundwater resources, prevention and remediation of pollution, geothermy, etc.

3. Scientific Foundations

3.1. Numerical algorithms and high performance computing

Linear algebra is at the kernel of most scientific applications, in particular in physical or chemical engineering. For example, steady-state flow simulations in porous media are discretized in space and lead to a large sparse linear system. The target size is 10^7 in 2D and 10^{10} in 3D. For transient models such as diffusion, the objective is to solve about 10^4 linear systems for each simulation. Memory requirements are of the order of Giga-bytes in 2D and Tera-bytes in 3D. CPU times are of the order of several hours to several days. Several methods and solvers exist for large sparse linear systems. They can be divided into three classes: direct, iterative or semi-iterative. Direct methods are highly efficient but require a large memory space and a rapidly increasing computational time. Iterative methods of Krylov type require less memory but need a scalable preconditioner to remain competitive. Iterative methods of multigrid type are efficient and scalable, used by themselves or as preconditioners, with a linear complexity for elliptic or parabolic problems but they are not so efficient for hyperbolic problems. Semi-iterative methods such as subdomain methods are hybrid direct/iterative methods which can be good tradeoffs. The convergence of iterative and semi-iterative methods and the accuracy of the results depend on the condition number which can blow up at large scale. The objectives are to analyze the complexity of these different methods, to accelerate convergence of iterative methods, to measure and improve the efficiency on parallel architectures, to define criteria of choice.

In geophysics, a main concern is to solve inverse problems in order to fit the measured data with the model. Generally, this amounts to solve a linear or nonlinear least-squares problem. Complex models are in general coupled multi-physics models. For example, reactive transport couples advection-diffusion with chemistry. Here, the mathematical model is a set of nonlinear Partial Differential Algebraic Equations. At each timestep of an implicit scheme, a large nonlinear system of equations arise. The challenge is to solve efficiently and accurately these large nonlinear systems.

Approximation in Krylov subspace is in the core of the team activity since it provides efficient iterative solvers for linear systems and eigenvalue problems as well. The later are encountered in many fields and they include the singular value problem which is especially useful when solving ill posed inverse problems.

3.2. Numerical models applied to hydrogeology and physics

The team Sage is strongly involved in numerical models for hydrogeology and physics. There are many scientific challenges in the area of groundwater simulations. This interdisciplinary research is very fruitful with cross-fertilizing subjects. For example, high performance simulations were very helpful for finding out the asymptotic behaviour of the plume of solute transported by advection-dispersion. Numerical models are necessary to understand flow transfer in fractured media.

The team develops stochastic models for groundware simulations. Numerical models must then include Uncertainty Quantification methods, spatial and time discretization. Then, the discrete problems must be solved with efficient algorithms. The team develops parallel algorithms for complex numerical simulations and conducts performance analysis. Another challenge is to run multiparametric simulations. They can be multiple samples of a non intrusive Uncertainty Quantification method, or multiple samples of a stochastic method for inverse problems, or multiple samples for studying the sensitivity to a given model parameter. Thus these simulations are more or less independent and are well-suited to grid computing but each simulation requires powerful CPU and memory resources.

A strong commitment of the team is to develop the scientific software platform H2OLab for numerical simulations in heterogeneous hydrogeology.

4. Application Domains

4.1. Geophysics

The team has chosen a particular domain of application, which is geophysics. In this domain, many problems require solving large scale systems of equations, arising from the discretization of coupled models. Emphasis is put on hydrogeology, but the team also investigates geodesy, heat and mass transfer in soil, and granular materials. One of the objectives is to use high performance computing in order to tackle 3D large scale computational domains with complex physical models.

4.2. Hydrogeology

This is joint work with Geosciences Rennes, University of Poitiers and CDCSP at University of Lyon. It is also done in the context of the group Momas and Andra grant.

Many environmental studies rely on modelling geo-chemical and hydrodynamic processes. Some issues concern water resources, aquifer contamination, underground waste disposal, clean-up of former waste deposits, acid mine drainage remediation. Other issues, also related to energy, concern geothermy, unconventional gas, enhanced oil recovery, underground storage of CO2, underground storage of nuclear waste.

Simulation of contaminant transport in groundwater is a highly complex problem, governed by coupled linear or nonlinear PDAEs. Moreover, due to the lack of experimental data, stochastic models are used for dealing with heterogeneity. The main objective of the team is to design and to implement efficient and robust numerical models, including Uncertainty Quantification methods.

Recent research showed that rock solid masses are in general fractured and that fluids can percolate through networks of inter-connected fractures. Fractured media are by nature very heterogeneous and multi-scale, so that homogenisation approaches are not relevant. The team develops a numerical model for fluid flow and contaminant transport in three-dimensional porous fractured media.

An important output is the parallel scientific platform H2OLab, running on clusters, grids and machines available in supercomputing centers.

5. Software

5.1. H2OLab

Participants: Thomas Dufaud, Jocelyne Erhel [correspondant], Grégoire Lecourt, Aurélien Le Gentil, Géraldine Pichot.

The software platform H2OLab is devoted to stochastic simulations of groundwater flow and contaminant transport in highly heterogeneous porous and fractured geological media. It contains a database which is interfaced through the web portal H2OWeb. It contains also software modules which can be used through the interface H2OGuilde. The platform H2OLab is an essential tool for the dissemination of scientific results. Currently, software and database are shared by the partners of the h2mno4 project (see 8.1.1). Software integrated in the platform and registered at APP are GW-UTIL, GW-NUM, PARADIS, MP-FRAC.

See also the web page http://h2olab.inria.fr.

5.2. GW-UTIL

Participants: Jocelyne Erhel, Grégoire Lecourt, Aurélien Le Gentil, Géraldine Pichot [correspondant].

- Version: version 1.0, May 2008
- APP: registered
- Programming language: C++
- See also: http://h2olab.inria.fr.
- Abstract: The software GW-UTIL allows to discretize PDE for flow and transport in aquifers and to deal with stochastic models. It contains a set of utilitary modules for geometry, input, output, random numbers, visualization, parallel computing, numerical algorithms, etc. A package is devoted to launch applications.
- Current work: refactoring.

5.3. GW-NUM

Participants: Thomas Dufaud, Jocelyne Erhel, Grégoire Lecourt, Aurélien Le Gentil, Géraldine Pichot [correspondant].

- Version: version 1.0, May 2008
- APP: registered
- Programming language: C++
- See also: http://h2olab.inria.fr.
- Abstract: The software GW-NUM is a set of generic modules to discretize PDE of flow and transport in 2D computational domains in order to deal with stochastic models. Methods for flow simulations are either Finite Volume on structured meshes or Mixed Finite Element with unstructured meshes. Method for transport simulations is a particle tracker for advection and a random walker for diffusion. Uncertainty Quantification method is Monte-Carlo. For flow computations, the involved linear system is solved by external software devoted to sparse matrices.
- Current work: refactoring.

5.4. MP-FRAC

Participants: Thomas Dufaud, Jocelyne Erhel, Aurélien Le Gentil, Géraldine Pichot [correspondant].

- Version: version 1.0, May 2008
- APP: registered
- Programming language: C++
- See also: http://h2olab.inria.fr.
- Abstract: The software MP-FRAC aims at modelling and simulating numerically flow in a fractured aquifer. The physical domain is a network of fractures, either deterministic or stochastic, with a permeability field either deterministic or stochastic. The software computes the velocity field in the aquifer, by assuming that the medium is saturated and that flow is steady-state. Physical equations are stochastic PDEs, handled by a Monte-Carlo method. This non intrusive approach generates a set of random samples, which are used for simulations. Then, the software analyzes statistically the flow in the stochastic case. The objective is to characterize hydraulic properties in Discrete Fracture Networks. The software MP-FRAC handles a simulation corresponding to one sample, whereas Monte-Carlo method is implemented in a generic way by the software GW-NUM. The software is specific of the physical model (Discrete Fracture Network) and of the application (steady-state flow). Generic numerical methods to discretize PDE are implemented in the software GW-NUM.
- Current work: refactoring and design of libraries.

5.5. PARADIS

Participants: Jocelyne Erhel, Grégoire Lecourt, Aurélien Le Gentil, Géraldine Pichot [correspondant].

- Version: version 1.0, May 2008
- APP: registered
- Programming language: C++
- See also: http://h2olab.inria.fr/.
- Abstract: The software PARADIS aims at modelling and simulating numerically flow in a porous aquifer and transport by convection-diffusion of an inert solute. The porous medium is heterogeneous, with a stochastic or deterministic permeability field. A first step computes the velocity filed in the aquifer, by assuming that the medium is saturated and that flow is steady-state. A second step computes the distribution of solute concentration, by assuming a transport by convection and by molecular diffusion. Physical equations are stochastic PDEs, handled by a Monte-Carlo method and discretized by numerical methods. This non intrusive approach generates a set of random samples, which are used for simulations. Then, the software analyzes statistically the flow in the stochastic case. The objectives are to determine asymptotic laws of transport, to characterize pre-asymptotic behavior and to define global laws.

  The software PARADIS handles a simulation corresponding to one sample, whereas Monte-Carlo method is implemented in a generic way by the software GW-NUM. The software is specific of the physical model (heterogeneous porous medium) and of the application (steady-state flow then transport with macro-dispersion). Generic numerical methods to discretize PDE are implemented in the software GW-NUM.
- Current work: refactoring and design of libraries.

5.6. GRT3D

Participants: Édouard Canot, Jocelyne Erhel [correspondant], Souhila Sabit.

- Version: version 1.0, April 2011
- APP: registered
- Programming language: C
- Abstract: Reactive transport modeling has become an essential tool for understanding complex environmental problems. It is an important issue for MoMaS partners (see section 8.1.7), in particular Andra (see section 7.1). We have developed a method coupling transport and chemistry, based on a method of lines such that spatial discretization leads to a semi-discrete system of algebraic differential equations (DAE system). The main advantage is to use a complex DAE solver, which controls simultaneously the timestep and the convergence of Newton algorithm. Another approach, called SIA, is to use a fixed-point method to solve the nonlinear system at each timestep.

  The software suite GRT3D has four executable modules:
  - SIA1D: Sequential Iterative Approach for 1D domains;
  - GDAE1D: Global DAE approach for 1D domains;
  - SNIA3D: Sequential Non Iterative Approach for 1D, 2D or 3D domains.
  - GDAE3D: Global DAE approach for 1D, 2D or 3D domains.
- Current work: extension of the chemistry module and reduction of CPU time.

5.7. GPREMS

Participants: Édouard Canot, Jocelyne Erhel [correspondant].

- Version: version 1.0, May 2008
- APP: registered
- Programming language: C++
- See also: http://www.irisa.fr/sage/.
- Abstract: GPREMS implements a robust hybrid solver for large sparse linear systems that combines a Krylov subspace method as accelerator with a Schwarz-based preconditioner. This preconditioner uses an explicit formulation associated to one iteration of the multiplicative Schwarz method. The Newton-basis GMRES, which aims at expressing a good data parallelism between subdomains is used as accelerator.

5.8. DGMRES

Participant: Jocelyne Erhel [correspondant].

- Version: version 1.0, June 2011
- APP: distributed with the free software PETSC
- Programming language: C
- See also: http://www.irisa.fr/sage/.
- Abstract: DGMRES implements a preconditioner based on adaptive deflation, which can be used with any preconditioner for the GMRES algorithm.

5.9. AGMRES

Participant: Jocelyne Erhel [correspondant].

- Version: version 1.0, November 2011
- APP: distributed with the free software PETSC
- Programming language: C
- See also: http://www.irisa.fr/sage/.
- Abstract: AGMRES implements an augmented subspace approach, based on adaptive deflation, which can be used with any preconditioner for the GMRES algorithm. It also implements a Newton basis for enhancing parallelism.

5.10. PPAT: pseudo-spectrum

Participants: Édouard Canot [corresponding author], Bernard Philippe.

PPAT (Parallel PATh following software) is a parallel code, developed by D. Mezher, W. Najem (University of Saint-Joseph, Beirut, Lebanon) and B. Philippe. This tool can follow the contours of a functional from $\mathbb{C}$ to $\mathbb{R}^+$. The present version is adapted for determining the level curves of the function $f(z) = \sigma_{\min}(A - zI)$ which gives the pseudospectrum of matrix A.

The algorithm is reliable: it does not assume that the curve has a derivative everywhere. The process is proved to terminate even when taking into account roundoff errors. The structure of the code spawns many independent tasks which provide a good efficiency in the parallel runs.

The software can be downloaded under the GPL licence from: http://sourceforge.net/projects/ppat.

5.11. MUESLI: Scientific computing

Participant: Édouard Canot [corresponding author].

Doing linear algebra with sparse and dense matrices is somehow difficult in scientific computing. Specific libraries do exist to deal with this area (*e.g.* BLAS and LAPACK for dense matrices, SPARSKIT for sparse ones) but their use is often awful and tedious, mainly because of the large number of arguments which must be used. Moreover, classical libraries do not provide dynamic allocation. Lastly, the two types of storage (sparse and dense) are so different that the user must know in advance the storage used in order to declare correctly the corresponding numerical arrays.

MUESLI is designed to help in dealing with such structures and it provides the convenience of coding in Fortran with a matrix-oriented syntax; its aim is therefore to speed-up development process and to enhance portability. It is a Fortran 95 library split in two modules: (i) FML (Fortran Muesli Library) contains all necessary material to numerically work with a dynamic array (dynamic in size, type and structure), called `mfArray`; (ii) FGL (Fortran Graphics Library) contains graphical routines (some are interactive) which use the `mfArray` objects.

MUESLI includes some parts of the following numerical libraries: Arpack, Slatec, SuiteSparse, Triangle, BLAS and LAPACK.

Linux is the platform which has been used for developing and testing MUESLI. Whereas the FML part (numerical computations) should work on any platform (*e.g.* Win32, Mac OS X, Unix), the FGL part is intended to be used only with X11 (*i.e.* under all UNIXes).

Last version of MUESLI is 2.6.6 (2012-08-29). More information can be found at: http://people.irisa.fr/Edouard.Canot/muesli

5.12. CANARD: BEM for surface flows

Participant: Édouard Canot [corresponding author].

When dealing with non-linear free-surface flows, mixed Eulerian-Lagrangian methods have numerous advantages, because we can follow marker particles distributed on the free-surface and then compute with accuracy the surface position without the need of interpolation over a grid. Besides, if the liquid velocity is large enough, Navier-Stokes equations can be reduced to a Laplace equation, which is numerically solved by a Boundary Element Method (BEM); this latter method is very fast and efficient because computing occur only on the fluid boundary. This method has been applied to the spreading of a liquid drop impacting on a solid wall and to the droplet formation at a nozzle; applications take place, among others, in ink-jet printing processes.

The code used (CANARD) has been developped with Jean-Luc Achard (LEGI, Grenoble) for fifteen years and is used today mainly through collaborations with Carmen Georgescu at UPB (University Polytechnica of Bucarest, Romania), and with Alain Glière (CEA-LETI, Grenoble).

6. New Results

6.1. Parallelism and convergence in iterative linear solvers

6.1.1. Generation of Krylov subspace bases

Participant: Bernard Philippe.

This work was done in collaboration with L. Reichel, from University of Kent, USA (see 8.3.1).

It is published in a journal [19].

Many problems in scientific computing involving a large sparse square matrix A are solved by Krylov subspace methods. This includes methods for the solution of large linear systems of equations with A, for the computation of a few eigenvalues and associated eigenvectors of A, and for the approximation of nonlinear matrix functions of A. When the matrix A is non-Hermitian, the Arnoldi process commonly is used to compute an orthonormal basis for a Krylov subspace associated with A. The Arnoldi process often is implemented with the aid of the modified Gram–Schmidt method. It is well known that the latter constitutes a bottleneck in parallel computing environments, and to some extent also on sequential computers. Several approaches to circumvent orthogonalization by the modified Gram–Schmidt method have been described in the literature, including the generation of Krylov subspace bases with the aid of suitably chosen Chebyshev or Newton polynomials. We review these schemes and describe new ones. Numerical examples are presented.

6.1.2. Parallel Adaptive Deflated GMRES

Participants: Jocelyne Erhel, Bernard Philippe.

This work was done in the context of the joint Inria/ NCSA laboratory on petascale computing (see 8.3.7), and the c2sexa project (see 8.1.3). Computations were done with GENCI supercomputers (see 8.1.6), using the software GPREMS, AGMRES, DGMRES (see 5.7, 5.8, 5.9).

It was presented at two conferences [30] [29], is published in proceedings [39] and is submitted (in revision) to a journal [46]. The algorithms are implemented in the software DGMRES and AGMRES, which are freely available in the PETSC repository.

The GMRES iterative method is widely used as Krylov subspace accelerator for solving sparse linear systems when the coefficient matrix is nonsymmetric and indefinite. The Newton basis implementation has been proposed on distributed memory computers as an alternative to the classical approach with the Arnoldi process. The aim of our work here is to introduce a modification based on deflation and augmented techniques. This approach builds an augmented subspace or a preconditioning matrix in an adaptive way to accelerate the convergence of the restarted formulation. It can be combined with preconditioning methods based for example on domain decomposition. In our numerical experiments, we show the benefits of our method to solve large linear systems.

6.1.3. Memory efficient hybrid algebraic solvers for linear systems arising from compressible flows

Participants: Jocelyne Erhel, Bernard Philippe.

This work was done in collaboration with FLUOREM company, in the context of the joint Inria/ NCSA laboratory on petascale computing (see 8.3.7) and the C2S@EXA project (see 8.1.3). Computations were done with GENCI supercomputers (see 8.1.6), using the software GPREMS, AGMRES, DGMRES (see 5.7, 5.8, 5.9).

It has been published in a journal [18].

This paper deals with the solution of large and sparse linear systems arising from design optimization in Computational Fluid Dynamics. From the algebraic decomposition of the input matrix, a hybrid robust direct/iterative solver is often defined with a Krylov subspace method as accelerator, a domain decomposition method as preconditioner and a direct method as subdomain solver. The goal of this paper is to reduce the memory requirements and indirectly the computational cost at different steps of this scheme. To this end, we use a grid-point induced block approach for the data storage and the partitioning part, a Krylov subspace method based on the restarted GMRES accelerated by deflation, a preconditioner formulated with the restricted additive Schwarz method and an aerodynamic/turbulent fields split at the subdomain level. Numerical results are presented with industrial test cases to show the benefits of these choices.

6.1.4. Efficient parallel implementation of the fully algebraic multiplicative Aitken-RAS preconditioning technique

Participant: Thomas Dufaud.

This work was done in collaboration with D. Tromeur-Dervout, from ICJ, University of Lyon and has been published in a journal [14].

This paper details the software implementation of the ARAS preconditioning technique [48], in the PETSc framework. Especially, the PETSc implementation of interface operators involved in ARAS and the introduction of a two level of parallelism in PETSc for the RAS are described. The numerical and parallel implementation performances are studied on academic and industrial problems, and compared with the RAS preconditioning. For saving computational time on industrial problems, the Aitken's acceleration operator is approximated from the singular values decomposition technique of the RAS iterate solutions.

6.1.5. An algebraic multilevel preconditioning framework based on information of a Richardson process

Participant: Thomas Dufaud.

This work was done in the context of the C2S@EXA project (see 8.1.3).

It has been presented at a conference [23] and submitted to the proceedings.

A fully algebraic framework for constructing coarse spaces for multilevel preconditioning techniques is proposed. Multilevel techniques are known to be robust for scalar elliptic Partial Differential Equations with standard discretization and to enhance the scalability of domain decomposition method such as RAS preconditioning techniques. An issue is their application to linear system encountered in industrial applications which can be derived from non-elliptic PDEs. Moreover, the building of coarse levels algebraically becomes an issue since the only known information is contained in the operator to inverse. Considering that a coarse space can be seen as a space to represent an approximated solution of a smaller dimension than the leading dimension of the system, it is possible to build a coarse level based on a coarse representation of the solution. Drawing our inspiration from the Aitken-SVD methodology, dedicated to Schwarz methods, we proposed to construct an approximation space by computing the Singular Value Decomposition of a set of iterated solutions of the Richardson process associated to a given preconditioner. This technique does not involve the knowledge of the underlying equations and can be applied to build coarse levels for several preconditioners. Numerical results are provided on both academic and industrial problems, using two-level additive preconditioners built with this methodology.

6.2. Parallel numerical algorithms

6.2.1. High Performance Scientific Computing

Participant: Bernard Philippe.

This work was done in collaboration with several authors, from US, Greece, etc. (see 8.3.1 and 8.2.1).

A book appeared on this subject in 2012 [45] and a chapter of this book is devoted to a historical perspective [44].

This comprehensive text/reference, inspired by the visionary work of Prof. Ahmed H. Sameh, represents the state of the art in parallel numerical algorithms, applications, architectures, and system software. Articles in this collection address solutions to various challenges arising from concurrency, scale, energy efficiency, and programmability. These solutions are discussed in the context of diverse applications, ranging from scientific simulations to large-scale data analysis and mining.
As exascale computing is looming on the horizon while multicore and GPU's are routinely used, we survey the achievements of Ahmed H. Sameh, a pioneer in parallel matrix algorithms. Studying his contributions since the days of Illiac IV as well as the work that he directed and inspired in the building of the Cedar multiprocessor and his recent research, unfolds a useful historical perspective in the field of parallel scientific computing.

6.2.2. Counting eigenvalues in domains of the complex field

Participant: Bernard Philippe.

This work is done in collaboration with E. Kamgnia, from the University of Yaounde 1, Cameroon, in the context of the MOMAPLI project at LIRIMA (see 8.3.5).

It is accepted for publication in a journal [15], and was presented in conferences [31], [32], [38], [40].

A procedure for counting the number of eigenvalues of a matrix in a region surrounded by a closed curve is presented. It is based on the application of the residual theorem. The quadrature is performed by evaluating the principal argument of the logarithm of a function. A strategy is proposed for selecting a path length that insures that the same branch of the logarithm is followed during the integration. Numerical tests are reported for matrices obtained from conventional matrix test sets.

The procedure is now combined with the PPAT methodology (see 5.10). A list of triangles is built for overlapping the boundary of the pseudo-spectra. From the list of vertices, a closed polygonal line is defined and the number of enclosed eigenvalues is determined.

6.2.3. Ratio-Based Parallel Time Integration

Participant: Jocelyne Erhel.

This work is done in in the context of the MODNUM project (see 8.3.2), in collaboration with American University of Beirut (AUB), Lebanon.

It was presented at a conference [41] and is submitted to the proceedings. It was also presented at a seminar of Inria Rennes.

Because time-integration of time-dependent problems is inherently sequential, time parallelism aims mainly at reducing the computational time of some real-time evolutionary problems and may be done through predictor-corrector schemes.

We apply the rescaling method onto initial value problems having an explosive or oscillatory solution, in infinite time. We show how a relevant choice of the end-of-slice condition and the time-rescaling factor might lead to rescaled systems having a uniform convergence to a limit problem. This property provides much better predictions and enhances the relevance of RaPTI that consists mainly of (i) the little sequential computations it involves (predictions and corrections are done in parallel), (ii) the relatively low communication cost it induces and (iii) the similarity of the computation on all slices yielding similar computational times on all processors. Hence, significant speed-ups are achieved. This is illustrated on two problems: a non-linear diffusion-reaction problem having an explosive solution, and a membrane problem having an oscillatory and explosive solution.

6.3. Numerical models and simulations applied to physics

6.3.1. Heat transfer modeling in saturated porous media

Participant: Édouard Canot.

This work is done in the context of the ARPHYMAT project (see 8.3.3) and the MODNUM project (see 8.3.2), in collaboration with Archeosciences, IPR and Lebanese International University (LIU), Lebanon. It was also done in the context of Caroline Thoux's internship (L3, INSA Rennes).

This work is published in [17].

In this paper, the authors introduce a robust numerical strategy to estimate the temperature dependent heat capacity, thermal conductivity and porosity of a saturated porous medium, basing on the knowledge of heating curves at selected points in the medium. In order to solve the inverse problem, we use the least squares criterion (in which the sensitivity coefficients appear), leading to a system of ordinary differential equations (ODE). At the stage of numerical computations, we propose a new global approach, based on the method of lines and ordinary differential equations solvers, combined with a modified Newton method to deal with the nonlinearities presented in the system of coupled equations.

Concerning strong thermal transfer in saturated porous media, the LHA method (Latent Heat Accumulation) is able to take into account phase changes by considering heat accumulation at the local level. The explicit knowledge of the cells which are changing their state allows the build of the liquid-gas interface position. A 2D configuration has been considered, together with a structured mesh but without refinement. The validation of this new method has been checked by making comparison between numerical results and an analytical solution.

6.3.2. Granular materials

Participant: Édouard Canot.

This work is done in collaboration with IPR and is published in [11].

We first studied the granular flows by the "discrete elements" method in silo geometries. By changing the micro-mechanical properties of the grains (restitution and friction) we showed that they had a significant influence on the flow discharge. Although models such as "discrete elements" provide access to all the individual properties of the grains, they have one major drawback: the computation time is very important that prohibits the modeling of geophysical and industrial situations. To overcome this problem, we used the "continuous medium" approach, which consider that the granular medium studied follows a rheology recently proposed in the literature. After discussing the numerical implementation, we have studied this rheology for steady and fully developed flows with a semi-analytical method in two configurations: a shear cell and a channel. This allowed us to highlight the differences between a granular medium and a Newtonian fluid.

6.4. Models and simulations for flow and transport in porous media

6.4.1. Flow and transport in highly heterogeneous porous medium

Participants: Jocelyne Erhel, Grégoire Lecourt, Géraldine Pichot.

This work is done in the context of the H2MNO4 project (see 8.1.1), the H2OGUILDE project (see 8.1.4), the HEMERA project (see 8.1.2). Computations are partly done with GENCI supercomputers (see 8.1.6), using the platform H2OLab (see 5.1) and the software GWNUM, GWUTIL, PARADIS (see 5.3, 5.2, 5.5).

This work was done in collaboration with A. Beaudoin, from University of Poitiers (Pprime) and J.-R. de Dreuzy, from Geosciences Rennes (who is on leave until 2013 at UPC, Barcelona, Spain, see 8.2.1). It is also done in collaboration with A. Debussche, from ENS-Cachan-Rennes/Ipso Inria team. It was also done in the context of Grégoire Lecourt's internship (M2, INSA Rennes).

It has been presented at a conference (plenary talk) [26] and a paper is submitted to a journal.

Models of hydrogeology must deal with both heterogeneity and lack of data. We consider in this paper a flow and transport model for an inert solute. The conductivity is a random field following a stationary log normal distribution with an exponential or Gaussian covariance function, with a very small correlation length. The quantities of interest studied here are the expectation of the spatial mean velocity, the equivalent permeability and the macro spreading. In particular, the asymptotic behavior of the plume is characterized, leading to large simulation times and in turn to large physical domains. Uncertainty is dealt with a classical Monte Carlo method, which turns out to be very efficient, thanks to the ergodicity of the conductivity field and to the very large domain. These large scale simulations are achieved by means of high performance computing algorithms and tools.

6.4.2. Solving flow equations in highly heterogeneous porous medium

Participant: Thomas Dufaud.

This work was done in collaboration with L. Berenguer and D. Tromeur-Dervout, from University of Lyon (ICJ).

It is published in a journal [12].

This paper is devoted to the acceleration by Aitken's technique of the convergence of the Schwarz domain decomposition method applied to large scale 3D problems with non separable linear operators. These operators come from the discretization of groundwater flow problems modeled by the linear Darcy equation, where the permeability field is highly heterogeneous and randomly generated. To be computationally efficient, a low-rank approximation of the Aitken's formula is computed from the singular value decomposition of successive iterated solutions on subdomains interfaces. Numerical results explore the efficiency of the solver with respect to the random distribution parameters, and specific implementations of the acceleration are compared for large scale 3D problems. These results confirm the numerical behavior of the methodology obtained on 2D Darcy problems [49].

6.4.3. *Transport in discontinuous porous medium*

Participants: Lionel Lenôtre, Géraldine Pichot.

This work was done in collaboration with A. Lejay, from Inria Nancy, in the context of the H2MNO4 project (8.1.1).

It is published in a journal [16].

We propose new Monte Carlo techniques for moving a diffusive particle in a discontinuous media. In this framework, we characterize the stochastic process that governs the positions of the particle. The key tool is the reduction of the process to a Skew Brownian Motion (SBM). In a zone where the coefficients are locally constant on each side of the discontinuity, the new position of the particle after a constant time step is sampled from the exact distribution of the SBM process at the considered time. To do so, we propose two different but equivalent algorithms: a two-steps simulation with a stop at the discontinuity and a one-step direct simulation of the SBM dynamic. Some benchmark tests illustrate their effectiveness.

6.4.4. *Adaptive stochastic collocation method for an elliptic problem with random data*

Participants: Jocelyne Erhel, Mestapha Oumouni.

This work is done in collaboration with Z. Mghazli, from the university of Kenitra, Morocco, in the context of the joint PhD supervision and the HYDRINV project (see 8.3.8,8.3.4).

This work has been presented at two conferences [43] [42].

Stochastic collocation methods are frequently used for elliptic equations with random coefficients. However, sparse grid methods are quite expensive and adaptive approaches are designed to save computations.

6.4.5. *Reactive transport*

Participants: Édouard Canot, Jocelyne Erhel, Souhila Sabit.

This work is done in the context of the MOMAS GNR (8.1.7), the contract with Andra (7.1) and the C2S@EXA project (see 8.1.3). Computations use the software GRT3D (see 5.6).

It has been presented at a conference and a workshop [35] [36].

Modeling reactive transport of contaminants in porous media is a complex time-dependent problem, due to combining the difficulties of modeling transport and chemistry, especially the coupling between them. In this work, we are interested to solve this type of coupling. Several methods have been developed for the resolution for solving this type problem. We choose to solve this problem by a global approach, which considers all the equations as a whole system of differential algebraic equations (DAE), which come from the spatial-only discretization of the equations (method of lines). This approach uses implicit schemes, which imply solving many large linear systems with the Jacobian matrix. The differential algebraic system (DAE) is solved by the solver IDA Sundials. Our new technique is implemented in the GRT3D software; we have observed that the CPU time increases very fast with the size of the system. Our aim is thus to reduce this computation time. Profiling tools have shown that an important part of this computation is due to the linear solving related to the Jacobian matrix. We focus our effort on improving this part, by exploiting the 3x3 block-structure of the Jacobian matrix, via a Gaussian block elimination technique. Our simulations are performed on academic test cases, which involve few chemical components (4 to 5) for both 1D and 2D geometries, giving a number

of unknowns up to 72000. First results have shown that our technique is very promising, because the CPU time is reduced by approximately 40 After this part, we eliminated the tracer in our test cases. In GRT3D-SL software, we calculated the concentrations directly without using the Logarithms and with this software, we have reduced the CPU time to 50 %.

6.5. Models and simulations for flow in porous fractured media

This work is done in collaboration with J.-R. de Dreuzy, from Geosciences Rennes (who is on leave until 2013 at UPC, Barcelona, Spain, see 8.2.1). It is done in the context of the GEOFRAC project (see 8.1.5), the H2OGUILDE project (see 8.1.4), the HEMERA project (see 8.1.2), and the Joint Laboratory for Petascale Computing (see 8.3.7). Computations are partly done with GENCI supercomputers (see 8.1.6), using the platform H2OLab (see 5.1) and the software GWNUM, GWUTIL, MPFRAC (see 5.3, 5.2, 5.4).

6.5.1. Influence of fracture scale heterogeneity on the flow properties of three-dimensional Discrete Fracture Networks

Participant: Géraldine Pichot.

This work is published in a journal [21].

While permeability scaling of fractured media has been so far studied independently at the fracture- and network- scales, we propose a numerical analysis of the combined effect of fracture-scale heterogeneities and the network-scale topology. The analysis is based on 2×10^6 discrete fracture network (DFNs) simulations performed with highly robust numerical methods. Fracture local apertures are distributed according to a truncated Gaussian law, and exhibit self-affine spatial correlations up to a cutoff scale L_c. Network structures range widely over sparse and dense systems of short, long or widely-distributed fracture sizes and display a large variety of fracture interconnections, flow bottlenecks and dead-ends. At the fracture scale, accounting for aperture heterogeneities leads to a reduction of the equivalent fracture transmissivity of up to a factor of 6 as compared to the parallel plate of identical mean aperture. At the network scale, a significant coupling is observed in most cases between flow heterogeneities at the fracture and at the network scale. The upscaling from the fracture to the network scale modifies the impact of fracture roughness on the measured permeability. This change can be quantified by the measure α_2, which is analogous to the more classical power-averaging exponent used with heterogeneous porous media, and whose magnitude results from the competition of two effects: (i) the permeability is enhanced by the highly transmissive zones within the fractures that can bridge fracture intersections within a fracture plane; (ii) it is reduced by the closed and low transmissive areas that break up connectivity and flow paths.

6.5.2. Synthetic benchmark for modeling flow in 3D fractured media

Participants: Jocelyne Erhel, Géraldine Pichot.

This work is published in a journal [22].

Intensity and localization of flows in fractured media have promoted the development of a large range of different modeling approaches including Discrete Fracture Networks, pipe networks and equivalent continuous media. While benchmarked usually within site studies, we propose an alternative numerical benchmark based on highly-resolved Discrete Fracture Networks (DFNs) and on a stochastic approach. Test cases are built on fractures of different lengths, orientations, aspect ratios and hydraulic apertures, issuing the broad ranges of topological structures and hydraulic properties classically observed. We present 18 DFN cases, with 10 random simulations by case. These 180 DFN structures are provided and fully documented. They display a representative variety of the configurations that challenge the numerical methods at the different stages of discretization, mesh generation and system solving. Using a previously assessed mixed hybrid finite element method (Erhel et al., 2009a), we systematically provide reference flow and head solutions. Because CPU and memory requirements stem mainly from system solving, we study direct and iterative sparse linear solvers. We show that the most cpu-time efficient method is a direct multifrontal method for small systems, while conjugate gradient preconditioned by algebraic multrigrid is more relevant at larger sizes. Available results can be used further as references for building up alternative numerical and physical models in both directions of improving accuracy and efficiency.

6.5.3. Robust numerical methods for solving flow in stochastic fracture networks

Participants: Jocelyne Erhel, Géraldine Pichot.

This work is published in a journal [20] and was presented at a conference (plenary talk) [33].

Working with random domains requires the development of specific and robust numerical methods to be able to solve physical phenomena whatever the generated geometries. Hydrogeology is a typical area of application where one has to face uncertainty about the geometry and the properties of the domain since the available information on the underground media is local, gathered through in-situ experiments with outcrops and wells. From measurements, statistical laws are derived that allow the generation of natural-like random media. The focus of this talk will concern flow in discrete fracture networks. The parameters governing the fractures lengths, shapes, orientations, positions as well as their hydraulic conductivity are stochastic. Our objective is to design robust numerical methods to solve Poiseuille's flow in large and heterogeneous stochastic fracture networks. The first part deals with the meshing strategies required to obtain a good quality mesh for any generated networks. The second part is devoted to numerical techniques to solve the flow equations. A Mortar-like method to deal with nonconforming meshes at the fracture intersections is presented as well as a Schur complement approach to solve the linear system of interest in parallel.

6.5.4. Deflation and Neumann-Neumann Preconditionner for Schur Domain Decomposition Method

Participants: Jocelyne Erhel, Géraldine Pichot.

This work was presented at a conference [34]. A paper is in preparation.

We study a domain decomposition method, which takes advantages from both the direct method and the Preconditioned Conjugate Gradient (PCG). This Schur method reduces the global problem to an interface problem, with a natural domain decomposition based on fractures or fracture packs. We propose an original approach for optimizing the algorithm and a global preconditioning of deflation type. Since the Schur complement S is spd, we apply PCG to solve the linear system $Sx = b$. We use the classical Neumann-Neumann (NN) preconditioner. To gain in efficiency, we use only one Cholesky factorization of the subdomain matrices for the preconditionning and the conjugate gradient steps. We also define a coarse space, based on the subdomain definition, to apply a deflation preconditioner. We do a theoretical complexity study of our algorithm. We use this study, with the numerical data, to compute experimental complexity. We compare the results between several combination for the preconditioner. Then, we confront our results with existing solvers.

6.5.5. Flow in complex 3D geological fractured porous media

Participants: Thomas Dufaud, Jocelyne Erhel, Géraldine Pichot.

This work was presented at a conference [24].

This communication focuses on numerical techniques to compute flow in complex 3D geological fractured porous media, where water can flow both in the rock matrix and in the fractures. This study is an extension of the models designed in the teams SAGE and POMDAPI. The numerical model deals with steady-state flow for single phase and incompressible fluid. In the rock matrix, the flow is governed by Darcy's law, while the flow in the fractures is governed by Poiseuille's law. For both, the law of mass conservation is verified. In a first part, we present the model. Then we propose a test case and its discretization considering a Mixed Hybrid Finite Element Method.

7. Bilateral Contracts and Grants with Industry

7.1. ANDRA: Numerical methods for reactive transport

Participants: Édouard Canot, Jocelyne Erhel, Souhila Sabit.

Title: Numerical methods for reactive transport.

Time: three years from October 2010.
Partner: ANDRA Coordination: J. Erhel, with G. Pépin (ANDRA)

8. Partnerships and Cooperations

8.1. National Initiatives

8.1.1. ANR-MN: H2MNO4 project

Participants: Thomas Dufaud, Jocelyne Erhel, Grégoire Lecourt, Aurélien Le Gentil, Lionel Lenôtre, Géraldine Pichot.

Contract with ANR, program Modèles Numériques
Duration: four years from November 2012.
Title: Original Optimized Object Oriented Numerical Model for Heterogeneous Hydrogeology.
Coordination: Jocelyne Erhel and Géraldine Pichot, with Fabienne Cuyollaa.
Partners: Geosciences Rennes, University of Poitiers, University of Lyon 1, Andra, Itasca.
Web page: http://www.irisa.fr/sage/
Abstract: The project H2MNO4 will develop numerical models for reactive transport in heterogeneous media. It defines six mathematical and computational challenges and three applications for environmental problems with societal impact (see 6.4.1, 6.4.3, 5.1).

8.1.2. Inria Large Wingspan intiative: HEMERA project

Participants: Jocelyne Erhel, Géraldine Pichot.

Title: Hemera
Duration: from September 2010.
Coordination: C. Perez, GRAAL team.
Partners: 22 Inria teams.
Webpage: http://www.grid5000.fr/mediawiki/index.php/Hemera
Abstract: Hemera is an Inria Large Wingspan project, started in 2010, that aims at demonstrating ambitious up-scaling techniques for large scale distributed computing by carrying out several dimensioning experiments on the Grid'5000 infrastructure, at animating the scientific community around Grid'5000 and at enlarging the Grid'5000 community by helping newcomers to make use of Grid'5000.

The team Sage is the leader of the Scientific Challenge Hydro: Multi-parametric intensive stochastic simulations for hydrogeology. The objective is to run multiparametric large scale simulations (see 6.4.1, 6.5).

8.1.3. Inria Large Wingspan intiative: C2S@EXA project

Participants: Édouard Canot, Thomas Dufaud, Jocelyne Erhel, Géraldine Pichot, Souhila Sabit.

Title: C2S@EXA
Duration: from January 2012.
Coordination: S. Lanteri, Nachos team.
Partners: Inria teams working on HPC; external partners: ANDRA and CEA.
Webpage: http://www-sop.inria.fr/c2s_at_exa/
Abstract: The C2S@Exa Inria large-scale initiative is concerned with the development of numerical modeling methodologies that fully exploit the processing capabilities of modern massively parallel architectures in the context of a number of selected applications related to important scientific and technological challenges for the quality and the security of life in our society (see 6.1.2, 6.1.3, 6.1.5, 6.4.5). The team participated in the first workshop France-Brazil on HPC (Nice, July 2012).

8.1.4. Inria Technological development actions: H2OGuilde project

Participants: Jocelyne Erhel, Aurélien Le Gentil, Géraldine Pichot.

Title: H2OGuilde
Duration: October 2011 - October 2013.
Coordination: J. Erhel and G. Pichot.
Partner: Charles Deltel, SED Inria Rennes
Webpage: http://www.irisa.fr/sage/
Abstract: The project H2OGuilde aims at developing an interface for the platform H2OLab (see 5.1) and at designing software libraries with a large academic diffusion (see 6.4.1,6.5, 8.1.1).

8.1.5. Inria Collaborative Research Action: GEOFRAC project

Participants: Thomas Dufaud, Jocelyne Erhel, Géraldine Pichot.

Title: GEOFRAC
Duration: June 2011-June 2013.
Coordinator: J. Erhel and G. Pichot.
Partners: Pomdapi and Gamma3 Inria teams, Géosciences Rennes.
Webpage: http://www.irisa.fr/sage/geofrac/
Abstract: In the last twenty years, the interest of geological fractured rocks has been renewed by a variety of energy-related applications, such as carbonate oil reservoirs, geothermic energy production, geological storage of high level nuclear waste, geological sequestration of CO2. Fractures are highly permeable pathways within a less pervious but more porous medium generally called matrix. The discrete modeling of fractures faces at least two challenging numerical issues. First, the fracture and matrix phases have very different hydraulic properties. Permeability is at least two orders of magnitude larger in the fractures than in the matrix. Second, the fracture structure complexity yield intricate geometrical configurations difficult to mesh. We propose to address these limitations by developing new numerical methods (see 6.5, 5.1).

8.1.6. GENCI: project on advanced linear solvers

Participants: Édouard Canot, Jocelyne Erhel, Grégoire Lecourt, Aurélien Le Gentil, Géraldine Pichot.

Title: Scalabilité de méthodes numériques pour l'hydrogéologie
Duration: 2012
Coordination: J. Erhel and G. Pichot.
Webpage: http://www.genci.fr/
Abstract: To run large scale simulations, we defined a project, based on the software H2OLab, AGMRES, GRT3D and MUESLI (see 5.1, 5.9, 5.6, 5.11). We obtained and used computing time on machines located at Idris supercomputing center (see 6.1.2, 6.1.3, 6.4.1, 6.5).

8.1.7. GNR MOMAS: project on reactive transport

Participants: Jocelyne Erhel, Souhila Sabit.

Webpage: http://momas.univ-lyon1.fr/

The working group MOMAS includes many partners from CNRS, Inria, universities, CEA, ANDRA, EDF and BRGM. It covers many subjects related to mathematical modeling and numerical simulations for nuclear waste disposal problems.

8.2. European Initiatives

8.2.1. Collaborations with Major European Organizations

UPC: Universitat Politècnica de Catalunya-UPC, Institute of Environmental Assessment and Water Research (Spain)

numerical simulations in hydrogeology, reactive transport in heterogeneous media, upscaling, scientific software platform (see 5.1, 6.4.1, 6.5).

UFZ: Helmholtz Centre for Environmental Research-UFZ, Hydrogeology group (Germany)

numerical simulations in hydrogeology, flow in porous fractured media, scientific software platform

HPCLab: University of Patras, High Performance Information Systems Laboratory (Greece)

cooperation with B. Philippe in editing a book, in writing a book, and in common research on low rank approximations of matrix functions (see 6.2.1).

ERCIM: working group on numerical algorithms, high performance computing.

8.3. International Initiatives

8.3.1. Inria International Partners

University of Kent (USA)

Krylov methods (see 6.1.1)

University of Purdue (USA)

High Performance Scientific Computing (see 6.2.1)

8.3.2. Cedre (Lebanon): MODNUM project

Participants: Édouard Canot, Jocelyne Erhel, Bernard Philippe.

Program: CEDRE Lebanon

Title: Modélisation numérique pour des applications libanaises

Inria principal investigator: Jocelyne Erhel and Bernard Philippe

International Partner (Institution - Laboratory - Researcher): American University of Beirut (Lebanon)

Duration: Jan 2012 - Dec 2013

Abstract: the project deals with numerical parallel algorithms and with applications to archaeology.

8.3.3. ECOS Sud (Argentina): ARPHYMAT project

Participant: Édouard Canot.

Program: COFECUB

Title: Processus de formation et transformation de structures de combustion archéologique

Inria principal investigator: Édouard CANOT

International Partner (Institution - Laboratory - Researcher): University of Buenos Aires (Argentina)

Duration: Jan 2012 - Dec 2014

Abstract: the project concerns numerical simulations of prehistoric fires and comparison with archaeological data in South America.

8.3.4. Inria Euro Med 3+3: HYDRINV project

Participants: Amine Abdelmoula, Édouard Canot, Jocelyne Erhel, Sinda Khalfallah, Bernard Philippe.

Program: Euromediterranean 3+3

Title: Direct and inverse problems in subsurface flow and transport

Coordination: H. ben Ameur, ENIT, Tunisia and J. Jaffré, Inria, Paris

Inria-Rennes principal investigator: Jocelyne Erhel

International Partners (Institution - Laboratory - Researcher):

Université Ibn Tofail - Faculté des Sciences de Kénitra (Morocco) - Laboratoire Interdisciplinaire en Ressources Naturelles et en Environnement - Zoubida Mghazli

Ecole Nationale d'Ingénieurs de Tunis (Tunisia) - Laboratoire de Modélisation en Hydraulique et Environnement - Rachida Bouhlila

Universidad de Sevilla (Spain) - Department Ecuaciones Diferenciales y Anâlisis Numérico - Tomas Chacon Rebollo

Universitat Politècnica de Catalunya (Spain) - Department of Geotechnical Engineering and Geo-Sciences - Xavier Sànchez Vila

University Centre of KHEMIS MILIANA (Algeria) - Laboratoire de l'Energie et des Systèmes Intelligents - Mohammed Hachama

Ecole Mohammadia d'Ingénieurs (Morocco) - LERMA - Rajae Aboulaich

Ecole Nationale d'Ingénieurs de Tunis (Tunisia) - Laboratoire de Modélisation Mathématique et Numérique dans les Sciences de l'Ingénieur - Hend Ben Ameur

Duration: Jan 2012 - Dec 2015

Abstract: The management of water resources is a problem of great importance in all countries, and is particularly acute around the Mediterranean sea. The goal is to find a reasonable balance between these resources and demand while preserving the quality of water. Towards this goal it is essential to understand and simulate flow and transport in the subsurface. The science corresponding to this topic is hydrogeology. Since models become more and more complicated and quantitative answers must be given, numerical modeling become more and more sophisticated and mathematicians must also be involved. This project brings together hydrogeologists and mathematicians from France, Spain, Algeria, Morocco and Tunisia in order to develop, analyze, and validate numerical methods for several problems arising from modeling flow and transport in the subsurface. The emphasis is put on direct nonlinear problems (air-water flow, density driven flow related to salinization, transport with chemistry) and on inverse problems.

8.3.5. LIRIMA laboratory: MOMAPLI team (Cameroon)

Participant: Bernard Philippe.

Program: Laboratoire International de Recherche en Informatique et Mathématiques Appliquées

Title: Modélisation Mathématique et Applications

Inria principal investigator: Bernard Philippe

International Partner (Institution - Laboratory - Researcher): University of Yaounde, Cameroon - Norbert Noutchegueme

Duration: 2010-2013

See also: http://www.lirima.uninet.cm/index.php/recherche/equipes-de-recherche/momappli

Abstract: The team deals with high performance scientific computing, with a focus on reliable tools for localizing eigenvalues of large sparse matrices (see 6.2.2).

8.3.6. LIRIMA laboratory: EPIC team (Tunisia)

Participants: Amine Abdelmoula, Bernard Philippe, Jocelyne Erhel, Sinda Khalfallah.

Program: Laboratoire International de Recherche en Informatique et Mathématiques Appliquées

Title: Problèmes Inverses et Contrôle

Inria principal investigator: Houssem Haddar, Defi team

International Partner (Institution - Laboratory - Researcher): ENIT, University of Tunis, Tunisia - LAMSIN - Amel ben Abda

Duration: 2011-2013

See also: http://www.lirima.uninet.cm/index.php/recherche/equipes-de-recherche/epic

Abstract: The team deals with nonlinear and inverse problems.

8.3.7. Joint Laboratory for Petascale Computing (USA)

Participant: Jocelyne Erhel.

Program: Joint Laboratory for Petascale Computing

Inria principal investigator: Franck Cappello and Laura Grigori, Grand Large team

International Partner (Institution - Laboratory - Researcher): University of Illinois at Urbana-Champaign, USA - Marc Snir and Bill Gropp

Duration: 2011-2013

See also: http://jointlab.ncsa.illinois.edu/

abstract: The team works on deflation methods and their integration into the software PETSc (see 6.1.2) and on domain decomposition methods (see 6.5.4). The team Sage participated in the workshop organized in June in Rennes (France).

8.3.8. Joint supervision of M. Oumouni's PhD (Morroco)

Program: International joint supervision of PhD agreement

Title: Méthodes numériques et leur analyse pour la résolution des équations de l'écoulement et de transport en milieux poreux hétérogènes et aléatoires

Inria principal investigator: Jocelyne Erhel

International Partner (Institution - Laboratory - Researcher): University Ibn Tofail - Faculté des Sciences de Kénitra (Morocco) - Zoubida Mghazli

Duration: Jan 2009 - Aug 2012

Abstract: see 6.4.4.

8.3.9. Joint supervision of S. Khalfallah's PhD (Tunisia)

Program: International joint supervision of PhD agreement

Title: Contribution à l'analyse mathématique et numérique de quelques problèmes issus de l'hydrogéologie

Inria principal investigator: Jocelyne Erhel

International Partner (Institution - Laboratory - Researcher): Ecole Nationale d'Ingénieurs de Tunis - LAMSIN (Tunisia) - Amel ben Abda

Duration: 2010 - 2013

Abstract: The objective is to solve data completion problems applied to hydrogeology (see 8.3.4, 8.3.6).

8.3.10. Joint supervision of A. Abdelmoula's PhD (Tunisia)

Program: International joint supervision of PhD agreement

Title: Résolution de problèmes inverses en géodésie physique

Inria principal investigator: Bernard Philippe

International Partner (Institution - Laboratory - Researcher): Ecole Nationale d'Ingénieurs de Tunis - LAMSIN (Tunisia) - Maher Moakher

Duration: 2005 - 2013

Abstract: The objective is to compute a set of point-mass which generate an a priori given gravitational field (see 8.3.4, 8.3.6).

8.4. International Research Visitors

8.4.1. Visits of International Scientists

- Basile Louka, 3 weeks, December 2011-January 2012; see 8.3.5.
- Norbert NOUTCHEGUEME, 2 weeks, January 2012; see 8.3.5.
- Stratis Gallopoulos, 1 week in January 2012 and 1 week in December 2012; see 6.2.1, 8.2.1.
- Ahmed Sameh, 1 week in January 2012 and 1 week in December 2012; see 6.2.1, 8.3.1.
- Emmanuel Kamgnia, 2.5 months, March-April 2012 and December; see 8.3.5, 6.2.2.
- Dani Mezher, 1 week, March 2012.
- Nabil Nassif, 1.5 month, June-July 2012; see 6.2.3.
- Noha Makhoul, 1 week, July 2012; see 6.2.3.
- Myriam El Fergougui, 1 month, March 2012.

8.4.2. Internships

- Salwa Mansour, 1.5 month, June-August 2012; see 8.3.2, 6.3.1.
- Mestapha Oumouni, 1.5 month, May-June 2012; see 8.3.8, 6.4.4.

8.4.3. Visits to International Teams

- B. Philippe, 2 weeks, February 2012, University of Yaoundé I, Cameroon; see 8.3.5, 6.2.2.
- B. Philippe, 2 weeks, May 2012, Purdue University, USA; see 8.3.1, 6.2.1.
- B. Philippe, 1 week, December 2012, ENIT, Tunisia; see 8.3.6, 8.3.4, 8.3.10.

9. Dissemination

9.1. Scientific Animation

9.1.1. Conferences and networks

- the team Sage organized, with the LMNO, the international conference on Domain Decomposition methods DD21 (Rennes, France, June 2012). Chair J. Erhel (with T. Sassi, University of Caen); members of the organizing committee É. Canot and G. Pichot; webmaster N. Soualem and A. Le Gentil; local coordination E. Blin and F. Cuyollaa.
- G. Pichot is a member of the organizing committee of the SMAI 2013 conference (Seignosse, France, May 2013).
- J. Erhel is a member of the scientific committee of the SMAI 2013 conference (Seignosse, France, May 2013).
- J. Erhel is a member of the scientific committee of the MAMERN'13 conference (Granada, Spain, April 2013).

- J. Erhel is a member of the international advisory committee of the parallel CFD conferences (Atlanta, USA, May 2012 and Changsha, Hunan, China, May 2013).
- J. Erhel is a member of the steering committee of the Réseau National des Systèmes Complexes.

9.1.2. Editorial Boards

- B. Philippe is one of the four chief-editors of the electronic journal ARIMA (revue Africaine de la Recherche en Informatique et Mathématiques Appliquées).
- B. Philippe is managing editor of the electronic journal ETNA (Electronic Transactions on Numerical Analysis).
- J. Erhel is member of the editorial board of ETNA.
- J. Erhel is member of the editorial board of ESAIM:Proceedings.
- J. Erhel is member of the editorial board of Interstices.
- J. Erhel is member of the editorial board of Mathematics of Planet Earth 2013, un jour-une brève.

9.1.3. Inria committees

- É. Canot is member of the CUMI (Commission des Utilisateurs de Moyens Informatiques), of Inria-Rennes, from September 2007.
- É. Canot is member of the CHS (Commission Hygiène et Sécurité), of Inria-Rennes, from September 2010.
- J. Erhel is member of the Comité Technique d'Etablissement Public of Inria.
- J. Erhel is member of Conseil d'Administration of Inria.
- J. Erhel participates in the working group of Inria Rennes on project management (first meeting, December 2012).

9.2. Teaching - Supervision - Juries

9.2.1. Teaching

A. Abdelmoula is teaching assistant (permanent position) in computer science at the University of Tunis, Tunisia.

S. Khalfallah is teaching assistant (permanent position since September 2012) in mathematics at the University of Kairouan, Tunisia.

M. Oumouni: TP in mathematics at the University of Kenitra, Morocco.

L. Lenôtre is teaching assistant (contrat doctoral avec mission d'enseignement) in mathematics at the University of Rennes 1.

A. Le Gentil: Master M1; title: TP d'analyse, conception et programmation orientée objets; 26 hours; INSA, Rennes, France.

J. Erhel: Master M2; title: Cours de modélisation et calcul scientifique; 12 hours; INSA, Rennes, France.

É. Canot: Master M2; title: TP de modélisation et calcul scientifique; 12 hours; INSA, Rennes, France.

9.2.2. PhD supervision

PhD: M. Djouwe Tankeo, University of Rennes 1, 20 January 2012, advisors P. Richard with É. Canot.

PhD in progress: S. Sabit, University of Rennes 1, October 2010, advisors J. Erhel with É. Canot.

PhD in progress: S. Khalfallah, University of Rennes 1 and University of Tunis, October 2009, co-advisors J. Erhel and A. ben Abda.

PhD in progress: M. Oumouni, University of Rennes 1 and University of Kenitra, October 2009, co-advisors J. Erhel and Z. Mghazli.

PhD in progress: A. Abdelmoula, University of Rennes 1 and University of Tunis, October 2005, co-advisors B. Philippe and M. Moakher.

PhD in progress: L.-B. Nguenang, University of Yaounde 1, October 2011, advisors E. Kamgnia with B. Philippe.

PhD in progress: L. Lenôtre, University of Rennes 1, October 2012, co-advisors A. Lejay (Inria Nancy) and J. Erhel, with G. Pichot.

9.2.3. Boards of examiners

- HdR: J.-Y. L'Excellent, ENS Lyon, Computer Science, September 2012. Reviewer J. Erhel.
- PhD: S. Duminil, Université du Littoral Côte d'Opale in Calais, Mathematics, July 2012. Reviewer J. Erhel.
- PhD: H. Alcin, University of Nice, Mathematics, December 2012. Chair J. Erhel.
- PhD: M. Rousseau, ENPC in Paris, Mathematics, December 2012. Chair J. Erhel.

9.3. Popularization

- J. Erhel is the scientific coordinator of the website Interstices (since June 2012). See http:http://www.interstices.info.
- J. Erhel gave a talk about numerical models for hydrogeology at lycée Descartes, Rennes, in March 2012 [47]. Video recording at http://videos.rennes.inria.fr/#descartes.
- J. Erhel is member of the editorial board of Mathematics of Planet Earth 2013, un jour-une brève. See http://mpt2013.fr/.

10. Bibliography

Major publications by the team in recent years

[1] K. BURRAGE, J. ERHEL. *On the performance of various adaptive preconditioned GMRES*, in "Numerical Linear Algebra with Applications", 1998, vol. 5, p. 101-121.

[2] J. CARRAYROU, J. HOFFMANN, P. KNABNER, S. KRÄUTLE, C. DE DIEULEVEULT, J. ERHEL, J. VAN DER LEE, V. LAGNEAU, K. MAYER, K. MACQUARRIE. *Comparison of numerical methods for simulating strongly non-linear and heterogeneous reactive transport problems. The MoMaS benchmark case.*, in "Computational Geosciences", 2010, vol. 14, n^{o} 3, p. 483-502.

[3] P. CHARTIER, B. PHILIPPE. *A Parallel Shooting Technique for Solving Dissipative ODE's, Part 1: Theoretical Analysis; Part 2: Numerical Implementation*, in "Computing", 1993, vol. 51, n^{o} 3-4, p. 209-236.

[4] R. CHOQUET, J. ERHEL. *Newton-GMRES algorithm applied to compressible flows*, in "International Journal for Numerical Methods in Fluids", 1996, vol. 23, p. 177-190.

[5] M. CROUZEIX, B. PHILIPPE, M. SADKANE. *The Davidson Method*, in "SIAM, Journal on Scientific and Statistical Computing", 1994, vol. 15:1, p. 62-76.

[6] J. ERHEL, S. RAULT. *Algorithme parallèle pour le calcul d'orbites : Parallélisation à travers le temps*, in "Technique et science informatiques", 2000, vol. 19, n^{o} 5.

[7] H. HOTEIT, J. ERHEL, R. MOSÉ, B. PHILIPPE, P. ACKERER. *Numerical Reliability for Mixed Methods Applied to Flow Problems in Porous Media*, in "Computational Geosciences", 2002, vol. 6, p. 161-194.

[8] M. MUHIEDDINE, É. CANOT, R. MARCH, R. DELANNAY. *Coupling heat conduction and water-steam flow in a saturated porous medium*, in "International Journal for Numerical Methods in Engineering", 2011, vol. 85, n^{o} 11, p. 1390-1414 [*DOI :* 10.1002/NME.3022], http://hal.inria.fr/inria-00540366/en.

[9] Y. SAAD, M. YEUNG, J. ERHEL, F. GUYOMARC'H. *A deflated version of the Conjugate Gradient Algorithm*, in "SIAM Journal on Scientific Computing", 2000, vol. 21, n^{o} 5, p. 1909-1926.

[10] J.-R. DE DREUZY, A. BEAUDOIN, J. ERHEL. *Asymptotic dispersion in 2D heterogeneous porous media determined by parallel numerical simulations*, in "Water Resource Research", 2007, vol. 43, n^{o} W10439, doi:10.1029/2006WR005394.

Publications of the year

Doctoral Dissertations and Habilitation Theses

[11] M. DJOUWE MEFFEJA. *Simulation et modélisation de milieux granulaires confinés*, University of Rennes 1, January 2012.

Articles in International Peer-Reviewed Journals

[12] L. BERENGUER, T. DUFAUD, D. TROMEUR-DERVOUT. *Aitken's acceleration of the Schwarz process using singular value decomposition for heterogeneous 3D groundwater flow problems*, in "Computers and Fluids", 2012, http://dx.doi.org/10.1016/j.compfluid.2012.01.026.

[13] J. CHARRIER. *Strong and weak error estimates for elliptic partial diffrential equations with random coefficients*, in "SIAM Journal on numerical analysis", 2012, vol. 50(1), p. 216-246.

[14] T. DUFAUD, D. TROMEUR-DERVOUT. *Efficient parallel implementation of the fully algebraic multiplicative Aitken-RAS preconditioning technique*, in "Advances in Engineering Software", 2012, vol. 53, p. 33-44, http://dx.doi.org/10.1016/j.advengsoft.2012.07.005.

[15] E. KAMGNIA, B. PHILIPPE. *Counting eigenvalues in domains of the complex field*, in "Electronic Transactions on Numerical Analysis", October 2012, n^{o} RR-7770, accepted for publication, http://hal.inria.fr/hal-00634065/en.

[16] A. LEJAY, G. PICHOT. *Simulating diffusion processes in discontinuous media: a numerical scheme with constant time steps*, in "Journal of Computational Physics", August 2012, vol. 231, n^{o} 21, p. 7299-7314 [*DOI :* 10.1016/J.JCP.2012.07.011], http://hal.inria.fr/hal-00649170.

[17] M. MUHIEDDINE, É. CANOT, R. MARCH. *Heat transfer modeling in saturated porous media and identification of the thermophysical properties of the soil by inverse problem*, in "Applied Numerical Mathematics", 2012, vol. 62, p. 1026-1040 [*DOI :* 10.1016/J.APNUM.2012.02.008], http://hal.inria.fr/hal-00757211.

[18] D. NUENTSA WAKAM, F. PACULL. *Memory efficient hybrid algebraic solvers for linear systems arising from compressible flows*, in "Computers and Fluids", 2012, vol. online.

[19] B. PHILIPPE, L. REICHEL. *On the generation of Krylov subspace bases*, in "Applied Numerical Mathematics (APNUM)", 2012, vol. 62, n^{o} 9, p. 1171-1186.

[20] G. PICHOT, J. ERHEL, J.-R. DE DREUZY. *A generalized mixed hybrid mortar method for solving flow in stochastic discrete fracture networks*, in "SIAM Journal on scientific computing", 2012, vol. 34(1), p. B86-B105, http://hal.inria.fr/insu-00681662.

[21] J.-R. DE DREUZY, Y. MEHEUST, G. PICHOT. *Influence of fracture scale heterogeneity on the flow properties of three-dimensional Discrete Fracture Networks*, in "Journal of Geophysical Research", 2012.

[22] J.-R. DE DREUZY, G. PICHOT, B. POIRRIEZ, J. ERHEL. *Synthetic benchmark for modeling flow in 3D fractured media*, in "Computers & Geosciences", 2012, in press [*DOI :* 10.1016/J.CAGEO.2012.07.025], http://hal.inria.fr/hal-00735675.

Invited Conferences

[23] T. DUFAUD. *An algebraic multilevel preconditioning framework based on information of a Richardson process*, in "21st International Conference on Domain Decomposition Methods (DD21)", Rennes, France, June 2012, organizer of a minisymposium.

[24] T. DUFAUD. *On a numerical method to compute flow in complex 3D geological fractured porous media*, in "3 ème Conférence Internationale de la Société Marocaine de Mathématiques Appliquées (SM2A)", Marrakech, Maroc, September 2012, invited in a minisymposium.

[25] J. ERHEL. *MICAS: Modelling and Intensive Computation for Aquifer Simulations*, in "Grand colloque STIC 2012 (ANR)", Lyon, January 2012, Invited contribution and poster.

[26] J. ERHEL. *PARADIS: modélisation stochastique du transport de soluté dans un milieu hétérogène*, in "CANUM 2012", 2012, invited plenary talk.

[27] J. ERHEL. *Solving linear systems arising from flow simulations in 3D Discrete Fracture Networks*, in "The Seventh Workshop of the Inria-Illinois Joint Laboratory on Petascale Computing", Rennes, France, June 2012, invited talk.

[28] M. HASSINE, M. JAOUA, S. SABIT. *Plasma boundary reconstruction using topological asymptotic expansion*, in "Inverse Problems, Control and Shape Optimization", Paris, France, April 2012, invited poster.

[29] D. NUENTSA WAKAM, J. ERHEL. *A parallel augmented GMRES algorithm*, in "3rd Dolomites Workshop on Constructive Approximation and Applications (DWCAA12)", Alba di Canazei, Italy, September 2012, invited talk in a minisymposium.

[30] D. NUENTSA WAKAM, J. ERHEL. *Parallel deflated GMRES with the Newton basis*, in "SIAM Conference on Applied Linear Algebra", Spain, June 2012, invited in a minisymposium.

[31] B. PHILIPPE, E. KAMGNIA, L. B. NGUENANG. *A parallel method for counting eigenvalues of a large sparse matrix in the complex plane*, in "PMAA2012", Birbek University of London, 2012.

[32] B. PHILIPPE. *Counting eigenvalues in pseudospectra*, in "3rd Dolomites Workshop on Constructive Approximation and Applications(DWCAA12)", Alba di Canazei, 2012.

[33] G. PICHOT. *On robust numerical methods for solving flow in stochastic fracture networks*, in "21st International Conference on Domain Decomposition Methods", Rennes, France, June 2012, invited plenary talk.

[34] B. POIRRIEZ, J. ERHEL. *Deflation and Neumann-Neumann Preconditionner for Schur Domain Decomposition Method*, in "21st International Conference on Domain Decomposition Methods (DD21)", Rennes, France, June 2012, invited talk in a minisymposium.

[35] S. SABIT, J. ERHEL, É. CANOT. *Méthodes Numériques de transport réactif : approche globale DAE*, in "3 ème Conférence Internationale de la Société Marocaine de Mathématiques Appliquées (SM2A)", Marrakech, Maroc, Sept 2012, invited in a minisymposium.

[36] S. SABIT, J. ERHEL, É. CANOT. *Numerical methods of reactive transport: global approach DAE*, in "First BrazilFrance workshop on High performance computing and scientific data management driven by highly demanding applications", Nice, France, July 2012, invited talk.

International Conferences with Proceedings

[37] T. DUFAUD, D. TROMEUR-DERVOUT. *ARAS2 preconditioning technique for CFD industrial cases*, in "Proceedings of international conference on domain decomposition (DD20)", LNCSE, Springer, 2012.

[38] E. KAMGNIA, L. B. NGUENANG, B. PHILIPPE. *Some efficient methods for computing the determinants of large sparse matrices*, in "11th African Conference on Research in Computer Science and Applied Mathematics (CARI'2012)", Algiers, 2012.

[39] D. NUENTSA WAKAM, J. ERHEL, W. GROPP. *Parallel Adaptive Deflated GMRES*, in "Proceedings of international conference on domain decomposition (DD20)", LNCSE, Springer, 2012.

Conferences without Proceedings

[40] E. KAMGNIA, B. PHILIPPE. *Counting eigenvalues in pseudospectra*, in "Congrès de méthodes numériques et modélisation", Tunis, December 2012.

[41] N. MAKHOUL-KARAM, N. NASSIF, J. ERHEL. *Ratio-Based Parallel Time Integration*, in "21st International Conference on Domain Decomposition Methods (DD21)", Rennes, France, June 2012, accepted contribution.

[42] M. OUMOUNI, J. ERHEL, Z. MGHAZLI. *Méthode des grilles clairsemées anisotrope et adaptative pour un prblème elliptique stochastique*, in "3 ème Conférence Internationale de la Société Marocaine de Mathématiques Appliquées (SM2A)", Marrakech, Maroc, Septembre 2012.

[43] M. OUMOUNI, J. ERHEL, Z. MGHAZLI. *Une Méthode de collocation adaptative pour un problème elliptique à coefficients aléatoires*, in "CANUM 2012", Superbesse, France, May 2012.

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[44] K. GALLIVAN, E. GALLOPOULOS, A. GRAMA, B. PHILIPPE, E. POLIZZI, Y. SAAD, F. SAIED, D. SORENSEN. *Parallel Numerical Computing from Illiac IV to Exascale: The Contributions of Ahmed H. Sameh*, in "High-Performance Scientific Computing - Algorithms and Applications", M. BERRY, K. GALLIVAN, E. GALLOPOULOS, A. GRAMA, B. PHILIPPE, Y. SAAD, F. SAIED (editors), Springer, 2012.

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[45] M. BERRY, K. GALLIVAN, E. GALLOPOULOS, A. GRAMA, B. PHILIPPE, Y. SAAD, F. SAIED (editors). *High-Performance Scientific Computing - Algorithms and Applications*, Springer, 2012.

Research Reports

[46] D. NUENTSA WAKAM, J. ERHEL. *Parallelism and robustness in GMRES with the Newton basis and the deflated restarting*, Inria, 2012, n^{o} RR-7787 (v2), submitted to ETNA, in revision, http://hal.inria.fr/inria-00638247/en.

Scientific Popularization

[47] J. ERHEL. *Des modèles numériques pour analyser les nappes phréatiques*, in "A la découverte de la recherche", lycée Descartes, 2012.

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[48] T. DUFAUD, D. TROMEUR-DERVOUT. *Aitken's acceleration of the restricted additive Schwarz preconditioning using coarse approximations on the interface*, in "C. R. Math. Acad. Sci. Paris", 2010, vol. 348, n^{o} 13-14, p. 821–824, http://dx.doi.org/10.1016/j.crma.2010.06.021.

[49] D. TROMEUR-DERVOUT. *Meshfree adaptive Aitken-Schwarz domain decomposition with application to Darcy flow*, in "Comput Sci Eng Technol", 2009, vol. 21, p. 217-250.