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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

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Project-Team SAGE

Keywords: Environment, Scientific Computation, High Performance Computing, Numerical Methods, Fluid Dynamics, Porous Media

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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

- The team Sage, with the LMNO at the University of Caen, was chosen by the scientific committee ddm.org to organize the 21th international conference on Domain Decomposition (DD21) in Rennes, 25-29 June 2012 (co-chair J. Erhel and T. Sassi).
- The software GPREMS and the modules DGMRES, AGMRES are now used by the SME Fluorem (Lyon) to solve large linear systems. The CPU time was reduced from 12 hours in 2007 to 15 minutes in 2011. Very large systems, which were intractable in 2007, are now solved in 10 hours.

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 to solve 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 aquifer contamination, underground waste disposal, underground storage of nuclear waste, land-filling of waste, clean-up of former waste deposits. 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. Rock media are thus interesting for water resources as well as for the underground storage of CO2. 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 fractured media.

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

5. Software

5.1. H2OLab

Participants: Jocelyne Erhel [correspondant], Aurélien Le Gentil, Géraldine Pichot, Baptiste Poirriez, Nadir Soualem.

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 software and a database which are interfaced through the web portal H2OWEB. The platform H2OLab is an essential tool for the dissemination of scientific results. Currently, software and database are shared by the partners of the Micas project (see 8.1.2). 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, Aurélien Le Gentil, Géraldine Pichot [correspondant], Baptiste Poirriez, Nadir Soualem.

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

- Version: version 1.0, May 2008
- APP: registered
- Programming language: C++

5.3. GW-NUM

Participants: Jocelyne Erhel, Aurélien Le Gentil, Géraldine Pichot [correspondant], Baptiste Poirriez, Nadir Soualem.

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

- Version: version 1.0, May 2008
- APP: registered
- Programming language: C++

5.4. MP-FRAC

Participants: Jocelyne Erhel, Aurélien Le Gentil, Géraldine Pichot [correspondant], Baptiste Poirriez, Nadir Soualem.

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

- Version: version 1.0, May 2008
- APP: registered
- Programming language: C++

5.5. PARADIS

Participants: Jocelyne Erhel, Aurélien Le Gentil, Géraldine Pichot [correspondant], Baptiste Poirriez, Nadir Soualem.

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

- Version: version 1.0, May 2008
- APP: registered
- Programming language: C++

5.6. GRT3D

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

Reactive transport modeling has become an essential tool for understanding complex environmental problems. It is an important issue for MoMaS partners (see section 8.1.1), 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 three executable modules:

- SIA1D: Sequential Iterative Approach for 1D domains;
- GDAE1D: Global DAE approach for 1D domains;
- GDAE3D: Global DAE approach for 1D, 2D or 3D domains.

- Version: version 1.0, April 2011
- APP: registered
- Programming language: C

5.7. GPREMS

Participants: Édouard Canot, Jocelyne Erhel [correspondant], Désiré Nuentsa Wakam, Nadir Soualem.

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.

See also the web page http://www.irisa.fr/sage/.

- Version: version 1.0, May 2008
- APP: registered
- Programming language: C++

5.8. DGMRES

Participants: Jocelyne Erhel [correspondant], Désiré Nuentsa Wakam.

DGMRES implements a preconditioner based on adaptive deflation, which can be used with any preconditioner for the GMRES algorithm. It is distributed with the free software PETSC.

See also the web page http://www.irisa.fr/sage/.

- Version: version 1.0, June 2011
- APP: distributed with PETSC
- Programming language: C

5.9. AGMRES

Participants: Jocelyne Erhel [correspondant], Désiré Nuentsa Wakam.

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. It will be distributed with the free software PETSC.

See also the web page http://www.irisa.fr/sage/.

- Version: version 1.0, November 2011
- APP: soon distributed with PETSC
- Programming language: C

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 2.5.2 (29 nov 2011). More information can be found at: http://www.irisa.fr/sage/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 is 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 Krylov methods

Participants: Édouard Canot, Jocelyne Erhel, Désiré Nuentsa Wakam, Bernard Philippe.

This work is done in the context of the Cinemas2 and the Libraero contracts, 7.2 and 8.1.3. It is also done in collaboration with the joint INRIA/ NCSA laboratory on petascale computing.

A Ph-D thesis was defended this year [12].

6.1.1. Some properties of Krylov methods

Participant: Jocelyne Erhel.

A survey was presented at a conference and published in a book chapter [37] [24].

Solving a linear system is at the heart of many scientific and engineering applications. Generally, this operations is the most time and memory consuming part of the simulation. This paper focuses on some properties of Krylov iterative methods. Iterative methods of Krylov type require less memory than direct methods, but the number of iterations increases rapidly with the size of the system. The convergence rate and the accuracy of the results depend on the condition number which can blow up at large scale. Therefore, it is essential to combine these methods with a preconditioner; the idea is to solve another system, close to the original one, but which is easier to solve; also, on parallel computers, it must be scalable. In Krylov iterative methods, the matrix is not transformed but the kernel operation is the matrix-vector product; thus it is possible to use matrix-free versions without storing the matrix. However, preconditioning will sometimes require the matrix. Krylov methods are described in many books. In this survey, we choose the framework of polynomial and projection methods. We first give general properties. Then, we study specific methods for the three different types of matrices: the case of SPD matrices is analyzed first, followed by the case of symmetric indefinite matrices. The general case of nonsymmetric matrices is studied with the description of several Krylov methods. Finally, some practical issues, preconditioning and parallelism are discussed.

6.1.2. Generation of Krylov subspace bases

Participant: Bernard Philippe.

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

It has been 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.

6.1.3. Parallel preconditioned GMRES with Multiplicative Schwarz

Participants: Édouard Canot, Jocelyne Erhel, Désiré Nuentsa Wakam, Bernard Philippe.

This work was published in a journal [18].

This paper presents a robust hybrid solver for 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 aim at expressing a good data parallelism between subdomains is used as accelerator. In the first part of this paper, we present the pipeline parallelism that is obtained when the multiplicative Schwarz preconditioner is used to build the Krylov basis for the GMRES method. This is referred as the first level of parallelism. In the second part, we introduce a second level of parallelism inside the subdomains. For Schwarz-based preconditioners, the number of subdommains is kept small to provide a robust solver. Therefore, the linear systems associated to subdomains are solved efficiently with this approach. Numerical experiments are performed on several problems to demonstrate the benefits of using these two levels of parallelism in the solver, mainly in terms of numerical robustness and global efficiency.

6.1.4. Adaptive deflation in preconditioned GMRES algorithm using a combined preconditioning

Participants: Jocelyne Erhel, Désiré Nuentsa Wakam, Bernard Philippe.

This work has been presented at a conference and a workshop [35], [27] and submitted to the proceedings of DD20 [45]. The software module DGMRES is integrated in the Petsc distribution.

Many scientific libraries are currently based on the GMRES method as a Krylov subspace iterative method for solving large linear systems. The restarted formulation known as GMRES(m) has been extensively studied and several approaches have been proposed to reduce the negative effects due to the restarting procedure. A common effect in GMRES(m) is a slow convergence rate or a stagnation in the iterative process. In this situation, it is less attractive as a general solver in industrial applications. In this work, we propose an adaptive deflation strategy which retains useful information at the time of restart to avoid stagnation in GMRES(m) and improve its convergence rate. We give a parallel implementation in the PETSc package. The provided numerical results show that this approach can be effectively used in the hybrid direct/iterative methods to solve large-scale systems.

6.1.5. Adaptive deflation in preconditioned GMRES algorithm using an augmented subspace

Participants: Jocelyne Erhel, Désiré Nuentsa Wakam, Bernard Philippe.

This work has been presented at a conference [31] and submitted to the journal ETNA [46].

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 techniques. This approach builds an augmented subspace in an adaptive way to accelerate the convergence of the restarted formulation. In our numerical experiments, we show the benefits of using this implementation with hybrid direct/iterative methods to solve large linear systems.

6.1.6. Using deflated preconditioned GMRES for industrial CFD problems

Participant: Désiré Nuentsa Wakam.

This work has been submitted to the journal Computers and Fluids [47].

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.

6.2. 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.

A book will appear on this subject in 2012 [39] and a chapter of this book is devoted to a historical perspective [38].

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 [38]. 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. *Updating the Diagonalization of a Symmetric Matrix*

Participant: Bernard Philippe.

This work is done in the context of the DIAMS project.

Two methods are compared : Jacobi method and first order correction of the spectral projectors [25],[26].

6.2.3. *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.

It has been submitted to a journal [43].

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.

6.2.4. *Rescaling for time integration*

Participant: Jocelyne Erhel.

This work is done in collaboration with N. Makhoul and N. Nassif, from the American University of Beirut, Lebanon.

It is published in a journal [17].

This paper considers the mathematical framework of a sliced-time computation method for explosive solutions to systems of ordinary differential equations: $Y(t) \in \mathbb{R}^k : \frac{dY}{dt} = F(Y),\ 0 < t,\ Y(0) = Y_0$, that have **finite or infinite explosion time**. The method used generates automatically a sequence of non uniform slices $\{[T_{n-1}, T_n] | n \geq 1\}$ determined by an end-of-slice condition that controls the growth of the solution within each slice. It also uses rescaling of the variables, whereas: $t = T_{n-1} + \beta_n s$ and $Y(t) = Y(T_{n-1}) + D_n Z_n(s)$, $D_n \mathbb{R}^{k \times k}$ and β_n being respectively an invertible diagonal matrix and a rescaling time factor. Thus, the original system is transformed into a sequence of slices-dependent initial-value shooting problems: $\frac{dZ_n}{ds} = G_n(Z_n),\ 0 < s \leq s_n,\ Z_n(0) = 0$. A suitable selection of β_n and D_n leads the rescaled systems to verify a concept of **uniform similarity**, allowing to disable the extreme stiffness of the original ODE problem. Then, on each time slice, the uniformly rescaled systems are locally solved using a 4^{th} order explicit Runge-Kutta scheme, within a computational tolerance of ϵ_{loc}. After sequentially implementing the local solver on a total of N slices, a global tolerance ϵ_{glob} would result in approximating the solution $Y(t)$ of the original system.
The proper definition of Uniform Similarity leads to deriving, under a stability assumption, a relationship between ϵ_{loc}, ϵ_{glob} and N. Numerical experiments are conducted for infinite and finite times explosive discrete reaction diffusion problems. These experiments validate the theoretical results and attest for the efficiency of the method in terms of stability and high accuracy.

6.3. Numerical models and simulations applied to physics

6.3.1. *Heat and mass transfer in soil and prehistoric fires*

Participant: Édouard Canot.

This work is done in the context of the Arphymat project, in collaboration with Archeosciences, IPR and Lebanese International University (LIU), Lebanon.

This work is published in a journal [16].

This paper is devoted to the simulation of water forced evaporation in a porous saturated medium in a 3D-axisymmetric domain by resolution of partial differential algebraic equations (PDAE) that are encountered in different engineering applications. The goal of this paper is an attempt to present effective realizations, in order to determine the minimal duration of burning for prehistoric occupations. This multidisciplinary work includes scientists in Mathematics, Physics and Archaeology. The model proposed here couples the heat conduction in a water saturated soil with the water steam flow in the medium. We propose an efficient and robust global numerical method, based on a method of lines and differential algebraic equations (DAE) solvers, combined with a Newton method using a powerful sparse linear solver. After a brief overview of classes for numerical techniques applied for moving boundary problems, the Apparent Heat Capacity method (AHC) is used, and in order to validate our codes, a comparison with experiments is done.

Recent work concerns the optimal choice of the temperature interval across which the phase change occurs in the apparent capacity method, because we have to make a compromise between the smoothness of the solution and its accuracy.

6.3.2. Rheology of granular systems flowing out of silo

Participant: Édouard Canot.

This work is done in the framework of a project funded by the Region Bretagne. A PhD thesis (Merline Djouwe-Tankeo), coadvised with Patrick Richard, who is from the Physics Institute at the University of Rennes (IPR), started in February 2009 and will be defended in January 2012.

It has been presented at a conference [36] and a paper is submitted.

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 transport in porous media

6.4.1. Transport in highly heterogeneous porous medium

Participants: Jocelyne Erhel, Géraldine Pichot, Nadir Soualem.

This work is done in collaboration with A. Beaudoin, from University of Poitiers (Pprime) and J.-R. de Dreuzy, from Geosciences Rennes. It is done in the context of the Micas project (8.1.2).

It has been presented at a conference and a paper is in preparation [28].

We study the transport of an inert species in a 2D heterogeneous porous medium via a Random Walk Particle Tracking (RWPT) method. The main objective is to derive the macroscopic properties of the transport by the means of Monte-Carlo simulations in large domains. Conditions to reach asymptotic macro-dispersion coefficients are given. We also present our on-going research about the RWPT method in presence of discontinuities within the domain.

6.4.2. Transport in discontinuous porous medium

Participants: Jocelyne Erhel, Géraldine Pichot.

This work is done in collaboration with A. Lejay, from Inria Nancy. It is done in the context of the Micas project (8.1.2).

It is published in the proceedings of a conference and submitted in a journal [30], [44].

We study a diffusion process in a 1D discontinuous medium using a random walk approach. Our main contribution is to encompass two existing numerical methods in the unified framework of the Skew Brownian Motion. This theoretical approach allows to detail and justify the derived algorithms. Numerical simulations are performed on two test cases to show that the algorithms can deal with the discontinuity in the diffusion coefficient.

6.4.3. Reactive transport

Participants: Édouard Canot, Jocelyne Erhel, Souhila Sabit, Nadir Soualem.

This work is done in the context of the MOMAS GNR (8.1.1) and the contract with Andra (7.1).

It has been presented at a workshop and a paper is in preparation [33]. The software GRT3D (see section 5.6) is described in a report [48].

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 nonlinear iterations [53]. Analysis done with several numerical experiments showed that most of CPU time is spent in solving the linear systems of Newton iterations. We have reduced this computational time by reducing the size of the system; numerical experiments with large 2D domains show the efficiency.

6.5. Models and simulations for flow in fractured media

This work is done in collaboration with J.-R. de Dreuzy, from the department of Geosciences at the University of Rennes 1 (who is on leave until 2013 at UPC, Barcelona, Spain). It is done in the context of the Micas project (8.1.2).

A Ph-D thesis was defended this year [13].

6.5.1. Domain decomposition method for flow in 3D networks of fractures

Participants: Jocelyne Erhel, Baptiste Poirriez.

This work was presented at a conference and published in the proceedings of another conference [29], [32]. A paper is in preparation.

This paper aims at solving efficiently the linear system arising from flow computations in Discrete Fracture Networks (DFN). We define a partition of fractures into connected sets and apply a Schur domain decomposition method. Conjugate Gradient is preconditioned by Neumann-Neumann and deflation. Preliminary results with one network show the ability of our method to reduce both the number of iterations and the computational time.

6.5.2. Mortar method for flow in 3D networks of fractures

Participants: Jocelyne Erhel, Géraldine Pichot.

This work is published in a journal [20].

The simulation of flow in fractured media requires handling both a large number of fractures and a complex interconnecting network of these fractures. Networks considered in this paper are 3D domains made up of 2D fractures intersecting each other and randomly generated. Due to the stochastic generation of fractures, intersections can be highly intricate. The numerical method must generate a mesh and define a discrete problem for any Discrete Fracture Network (DFN). A first approach [51] is to generate a conforming mesh and to apply a mixed hybrid finite element method. However the resulting linear system becomes very large when the network contains many fractures. Hence a second approach [52] is to generate a non conforming mesh, using an independent mesh generation for each fracture. Then a Mortar technique applied to the mixed hybrid finite element method deals with the non-matching grids. When intersections do not cross nor overlap, pairwise Mortar relations for each intersection are efficient [52]. But for most of random networks, discretized intersections involve more than two fractures. In this paper, we design a new method generalizing the previous one and applicable for stochastic networks. The main idea is to combine pairwise Mortar relations with additional relations for the overlapping part. This method still ensures the continuity of fluxes and heads and still yields a symmetric positive definite linear system. Numerical experiments show the efficiency of the method applied to complex stochastic fracture networks. We also study numerical convergence when reducing the mesh step. This method makes it easy to perform mesh optimization and appears as a very promising tool to simulate flow in multiscale fracture networks.

6.6. Uncertainty quantification in hydrogeoloy

This work is done in collaboration with A. Debussche, from ENS-Cachan-Rennes and Ipso INRIA team. It is done in the context of the Micas project (8.1.2).

A PhD thesis was defended this year [11].

6.6.1. Strong and weak error estimates for elliptic partial differential equations with random coefficients

Participant: Julia Charrier.

This work has been presented at a workshop and is published in a journal [23], [14].

We consider the problem of numerically approximating the solution of an elliptic partial differential equation with random coefficients and homogeneous Dirichlet boundary conditions. We focus on the case of a lognormal coefficient, we have then to deal with the lack of uniform coercivity and uniform boundedness with respect to the randomness. This model is frequently used in hydrogeology. We approximate this coefficient by a finite dimensional noise using a truncated Karhunen-Loève expansion. We give then estimates of the corresponding error on the solution, both a strong error estimate and a weak error estimate, that is to say an estimate of the error commited on the law of the solution. We obtain a weak rate of convergence which is twice the strong one. Besides this, we give a complete error estimate for the stochastic collocation method in this case, where neither coercivity nor boundedness are stochastically uniform. To conclude, we apply these results of strong and weak convergence to two classical cases of covariance kernel choices: the case of an exponential covariance kernel on a box and the case of an analytic covariance kernel, yielding explicit weak and strong convergence rates.

6.6.2. Numerical analysis of a multilevel Monte Carlo method for elliptic PDEs with random coefficients

Participant: Julia Charrier.

This work has been presented at a conference and is submitted in a journal [42], [22].

We consider a finite element approximation of elliptic partial differential equations with random coefficients. Such equations arise, for example, in uncertainty quantification in subsurface flow modelling. Models for random coefficients frequently used in these applications, such as log-normal random fields with exponential covariance, have only very limited spatial regularity, and lead to variational problems that lack uniform coercivity and boundedness with respect to the random parameter. In our analysis we overcome these challenges by a careful treatment of the model problem almost surely in the random parameter, which then enables us to prove uniform bounds on the finite element error in standard Bochner spaces. These new bounds can then be used to perform a rigorous analysis of the multilevel Monte Carlo method for these elliptic problems that lack full regularity and uniform coercivity and boundedness. To conclude, we give some numerical results that confirm the new bounds.

6.6.3. *Numerical analysis of the advection-diffusion of a solute in random media*

Participant: Julia Charrier.

This work is submitted in a journal [41].

We consider the problem of numerically approximating the solution of the coupling of the flow equation in a random porous medium, with the advection-diffusion equation. More precisely, we present and analyse a numerical method to compute the mean value of the spread of a solute introduced at the initial time, and the mean value of the macro-dispersion, defined at the temporal derivative of the spread. We propose a Monte-Carlo method to deal with the uncertainty, i.e. with the randomness of the permeability field. The flow equation is solved using finite element. The advection-diffusion equation is seen as a Fokker-Planck equation, and its solution is approximated thanks to a probabilistic particular method. The spread is indeed the expected value of a function of the solution of the corresponding stochastic differential equation, and is computed using an Euler scheme for the stochastic differential equation and a Monte-Carlo method. Error estimates on the mean spread and on the mean dispersion are established, under various assumptions, in particular on the permeability random field.

6.6.4. *Model reduction for a 1D stochastic elliptic PDE*

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 Co-Advise and Hydromed projects (8.2.1,8.3.4).

This work has been presented at a conference and published in a journal [15] [34].

In this paper, we present an efficient method to approximate the expectation of the response of a one-dimensional elliptic problem with stochastic inputs. In conventional methods, the computational effort and cost of the approximation of the response can be dramatic. Our method presented here is based on the Karhunen–Loève (K-L) expansion of the inverse of the diffusion parameter, allowing us to build a base of random variables in reduced numbers, from which we construct a projected solution. We show that the expectation of this projected solution is a good approximation, and give an a priori error estimate. A numerical example is presented to show the efficiency of this approach.

6.6.5. *Inverse problems in hydrogeology*

Participant: Sinda Khalfallah.

This work is done in collaboration with A. ben Abda, from LAMSIN, Tunisia, in the context of the Hydromed and Co-Advise projects (8.2.1, 8.3.4). It is also done in collaboration with B. T. Johansson, from University of Birmingham, GB.

This work has been submitted to a journal [40].

This work is an initial study of a numerical method for identifying multiple leak zones in saturated unsteady flow. Using the conventional saturated groundwater flow equation, the leak identification problem is modelled as a Cauchy problem for the heat equation and the aim is to find the regions on the boundary of the solution domain where the solution vanishes, since leak zones corresponds to null pressure values. To reconstruct the solution to the Cauchy problem in a stable way, we modify and employ an iterative regularizing method proposed recently. In this method, one solves mixed well-posed problems (obtained by changing the boundary conditions) for the heat operator as well as for its adjoint, to get a sequence of approximations to the original Cauchy problem. The mixed problems are solved using a Finite element method (FEM), and the numerical results obtained show that the leak zones can be accurately identified also when there is noise in the data.

7. Contracts and Grants with Industry

7.1. ANDRA: Numerical methods for reactive transport

Participants: Jocelyne Erhel, Souhila Sabit.

Contract with ANDRA
Time: three years from October 2010.
Title: Numerical methods for reactive transport.

See sections 6.4.3, 4.2, 8.1.1.

7.2. competitive cluster LUTB: CINEMAS2 project

Participants: Denis Billon, Jocelyne Erhel, Désiré Nuentsa Wakam.

Contract with Région Rhône Alpes.
Time: three years from May 2007, extended until October 2011.
Title: Conception Interactive par simulation Numérique des Ecoulements couplées à des Méthodes d'optimisation par Algorithmes Spécifiques.
Coordinator: Ecole Centrale de Lyon.
Partners: INSA Lyon, University of Lyon, Plastic Omnium, Valeo, Renault Trucks.

See sections 6.1, 5.7 and grant LIBRAERO, section 8.1.3.

8. Partnerships and Cooperations

8.1. National Initiatives

8.1.1. 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. We coordinate the project entitled "numerical models and simulations for transport by advection diffusion of chemical species with kinetic and equilibrium reactions."

See sections 6.4.3, 4.2, 7.1.

8.1.2. ANR-CIS: MICAS project

Participants: Julia Charrier, Jocelyne Erhel, Aurélien Le Gentil, Géraldine Pichot, Baptiste Poirriez, Nadir Soualem.

Contract with ANR, program CIS
Time: four years from January 2008.
Title: Modelling and Intensive Computation for Aquifer Simulations.
Coordinator: Sage.
Partners: Geosciences Rennes, University of Le Havre, University of Lyon 1.
Web page: http://www.irisa.fr/sage/micas

See sections 6.4, 6.5, 6.6, 5.1, 4.2.

8.1.3. ANR-RNTL: LIBRAERO project

Participants: Denis Billon, Jocelyne Erhel, Désiré Nuentsa Wakam.

Contract with ANR, program RNTL
Time: three years from October 2007.
Title: Large Information Base for the Research in AEROdynamics.
Coordinator: FLUOREM, Lyon.
Partners: LMFA, Ecole Centrale de Lyon; CDCSP, University of Lyon; Sage team.

This work is done in the context of the CINEMAS2 project, section 7.2.

See section 6.1, 5.7.

8.1.4. GENCI: project on advanced linear solvers

Participants: Édouard Canot, Désiré Nuentsa Wakam, Jocelyne Erhel, Aurélien Le Gentil, Baptiste Poirriez, Nadir Soualem, Géraldine Pichot.

Webpage: http://www.genci.fr/

To run large simulations, we defined a project, based on H2OLab and GPREMS, accepted by Genci. We got accounts on the cluster IBM Power 6 located at IDRIS. In 2011, we obtained and used hours.

See sections 5.1 and 5.7.

8.1.5. INRIA Large Wingspan intiative: HEMERA project

Participants: Jocelyne Erhel, Nadir Soualem, Géraldine Pichot.

Title: Hemera
Time: from September 2010.
Coordinator: C. Perez, GRAAL team.
Partners: 22 INRIA teams.
Webpage: http://www.grid5000.fr/mediawiki/index.php/Hemera

Hemera is an INRIA Large Wingspan project, started in 2010, that aims at demonstrating ambitious upscaling 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. Experiments have been conducted on Grid'5000 in 2011, in collaboration with D. Balouek, engineer in team GRAAL, Lyon. They show that our approach based on a two-level parallelism for Monte-Carlo simulations is quite efficient.

See sections 6.4, 6.5, 6.6, 8.1.2, 5.1.

8.2. European Initiatives

8.2.1. Marie Curie program: Co-Advise project

Participants: Jocelyne Erhel, Sinda Khalfallah, Mestapha Oumouni, Bernard Philippe.

Type of project: COADVISE Project supported by the European Commission [Seventh Framework Programme - Marie Curie Actions 'People' International Research Staff Exchange Scheme (IRSES)].
Time: It started in February 2009 for a duration of 36 months.

The project aims at supporting and strenghtening the different existing collaboration actions between Europe and Mediterranean Partner Countries. The structuring action of the programme consists in co-advising PhD students between the two sides of the Mediterranean Sea. The project is coordinated by INRIA Centre de Recherche Sophia Antipolis. There are 5 partners in Tunisia, 2 partners in Morocco, 1 partner in Algeria, 1 partner in Italy, 1 partner in Spain and 1 partner in France.

In 2011, two PhD students visited the Sage team during 6 months each: Sinda Khalfallah, Tunisia; Mestapha Oumouni, Morocco.

See sections 8.3.4, 6.6.

8.2.2. European collaborations

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.

UFZ: Helmholtz Centre for Environmental Research-UFZ, Hydrogeology group (Germany)
numerical simulations in hydrogeology, flow in porous fractured media, scientific software platform.

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.

ERCIM working group
numerical algorithms, high performance computing.

8.3. International Initiatives

8.3.1. Visits of International Scientists

- E. Gallopoulons, professor University of Patras, Greece, 2 months, January-March
- E. Kamgnia, professor University of Yaounde 1, Cameroon, 2 months, March
- D. Sorensen, professor University of Rice, USA, 1 week, May
- M. Muhieddine, associate professor University of , Lebanon, 2 weeks, June
- F.-Z. Nouri, professor University Badji Mokhtar, Algeria, 2 weeks, December

8.3.2. Internship

- F. Saceh, PhD student, University Badji Mokhtar, Algeria, 3 months, April-July
- M. ben Refifa, Master student, ENIT, Tunisia, 3 months, May-July
- L.-B. Nguenang, PhD student, University of Yaounde 1, Cameroon, 4 months, November 2011-February 2012

8.3.3. Visits to international laboratories

- É. Canot, University Badji Mokhtar, Algeria, 1 week, April
- B. Philippe, University Badji Mokhtar, Algeria, 1 week, October
- É. Canot, University of Yaounde 1, Cameroon, 1 week, November

8.3.4. INRIA Euro-Mediterranean Program: HYDROMED project

Participants: Édouard Canot, Jocelyne Erhel, Sinda Khalfallah, Mestapha Oumouni.

Title: Inverse problems in hydrogeology
Time: 2009 - 2011
Coordination: LAMSIN, Tunis, Tunisia.
Partners: Rabat (Morocco), Kenitra (Morocco), Annaba (Algeria), Tunis (Tunisia), Naples (Italy), Barcelona (Spain), Paris and Rennes.
Webpage: http://www.lamsin.rnu.tn/

The project deals with the numerical simulation of groundwater flow and the transport of pollutants. A workshop was organized in Tunis, in December 2011. See sections 8.3.1, 8.2.1, 6.6.

8.3.5. LIRIMA network: MOMAPLI team

Participant: Bernard Philippe.

Title: Modélisation Mathématique et Applications
Time: 2010-2013
Partner: University of Yaounde, Cameroon.

The project deals with high performance scientific computing. See sections 8.3.1, 8.3.3, 6.2.3.

8.3.6. LIRIMA network: EPIC team

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

Time: 2011-2013
Partner: ENIT, University of Tunis, Tunisia.

The project deals with nonlinear problems and inverse problems. See sections 8.3.1, 6.6.

8.3.7. LIRIMA network: CSPE team

Participants: Édouard Canot, Bernard Philippe.

Title: Calcul Scientifique pour des Problèmes en Environnement
Time: 2010-2011
Partner: University of Annaba, Algeria.

The project deals with the numerical simulation of fluid flows. See sections 8.3.1, 8.3.3.

8.3.8. INRIA and UIUC: Joint Laboratory for Petascale Computing

Participants: Désiré Nuentsa Wakam, Jocelyne Erhel.

Webpage: http://jointlab.ncsa.illinois.edu/

The team Sage participated in the workshop organized in June at Grenoble (France).

The team works on deflation methods and their integration into the software PETSc. See sections 6.1, 5.7.

9. Dissemination

9.1. Animation of the scientific community

9.1.1. Program and organizing committees

- the team Sage organizes the international conference on Domain Decomposition methods DD21 (Rennes, June 2012). Chair J. Erhel (with T. Sassi, University of Caen); organizing committee É. Canot, G. Pichot; webmaster N. Soualem, A. Le Gentil; local coordination F. Cuyollaa (with E. Blin).
- J. Erhel organized with D. Tromeur-Dervout a mini-symposium at the international conference ParCFD (Barcelona, Spain, May 2011).
- G. Pichot organized with M. Kern a mini-symposium at the international conference SIAM on Geosciences (Long Beach, USA, March 2011).

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). He was a thematic editor of the special issue after the international conference CARI'2010 (Volume 14, 2011).
- 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 Interstices.

9.1.3. INRIA and University 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 2007.
- J. Erhel was member and secretary of the Comité de Gestion Local of AGOS at INRIA-Rennes, until December 2011.
- J. Erhel was member of Comité Technique Paritaire of INRIA, until November 2011. She is now member of the Comité Technique d'Etablissement Public of INRIA.
- J. Erhel is member of Comité de Concertation of INRIA.
- J. Erhel is member of Conseil d'Administration of INRIA.
- J. Erhel participated in the working group on the assistants' activities.

9.2. Teaching and supervision

9.2.1. Teaching

- A. Abdelmoula is teaching assistant (permanent position) in computer science at the University of Tunis, Tunisia.
- J. Charrier was teaching assistant (monitrice) in mathematics at ENS-Cachan-Rennes, until August.
- D. Nuentsa Wakam was teaching assistant (moniteur) in computer science at faculty of law, University of Rennes 1, until August.
- B. Poirriez was teaching assistant (ATER) in computer science at INSA, Rennes, until August.

Master: B. Philippe taught one module "Krylov methods for solving large linear systems", 10 hours, M2, University of Annaba, Algeria.

9.2.2. PhD supervision

PhD: J. Charrier, ENS Cachan Bretagne, 12 July 2011, advisors A. Debussche with J. Erhel.

PhD: D. Nuentsa Wakam, University of Rennes 1, 7 December 2011, advisors J. Erhel with É. Canot.

PhD: B. Poirriez, University of Rennes 1, 20 December 2011, advisor J. Erhel.

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

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

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

see also section 8.3.1.

9.2.3. internship supervision

see section 8.3.1.

9.3. Scientific popularization

9.3.1. Articles for the general public

- J. Erhel wrote a paper entitled "Un algorithme pour mettre en rang une équipe de football", in Intestices, July, [50]. See http://interstices.info/
- J. Erhel and J.-R. de Dreuzy wrote a paper entitled "des pollutions suivies à la trace", in Intestices, September, [49]. See http://interstices.info/algo-football

10. Bibliography

Major publications by the team in recent years

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Doctoral Dissertations and Habilitation Theses

[11] J. CHARRIER. *Analyse numérique d'équations aux dérivées partielles à coefficients aléatoires, applications à l'hydrogéologie*, École normale supérieure de Cachan - ENS Cachan, July 2011, http://hal.inria.fr/tel-00625092/en.

[12] D. NUENTSA WAKAM. *Parallélisme et robustesse dans les solveurs hybrides pour grands systèmes linéaires: Application à l'optimisation en dynamique des fluides*, University of Rennes 1, 2011.

[13] B. POIRRIEZ. *Etude et mise en oeuvre d'une méthode de sous-domaines pour la modélisation de l'écoulement dans des réseaux de fractures en 3D*, University of Rennes 1, 2011.

Articles in International Peer-Reviewed Journal

[14] J. CHARRIER. *Strong and weak error estimates for elliptic partial diffrential equations with random coefficients*, in "SIAM Journal on numerical analysis", 2012, to appear.

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[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, to appear.

Invited Conferences

[21] É. CANOT. *Suivi d'interfaces fluides par la méthode des éléments frontières*, in "Workshop of the University of Annaba", 2011, invited in a workshop.

[22] J. CHARRIER. *Numerical analysis of a multilevel Monte Carlo method for elliptic PDEs with random coefficients*, in "European Numerical Mathematics and Advanced Applications (ENUMATH 2011)", September 2011, invited in a mini-symposium.

[23] J. CHARRIER. *Weak and strong error estimates for elliptic PDE with random coefficients*, in "Applied Mathematics and Statistics (AMSTAT Seminars), Warwick Mathematics Institute", November 2011, invited talk.

[24] J. ERHEL. *Some Properties of Krylov Projection Methods for Large Linear Systems*, in "PARENG'2011", Ajaccio, France, May 2011, invited plenary talk.

[25] F. JÉZÉQUEL, B. PHILIPPE. *Correction d'une décomposition spectrale approchée pour une matrice symétrique*, in "20ème Anniversaire du Laboratoire d'Etude et de Recherche en Mathématiques Appliquées", Rabat, June 2011.

[26] F. JÉZÉQUEL, B. PHILIPPE. *Updating the Diagonalization of a Symmetric Matrix*, in "Festkolloquium Parallel Computing: Algorithms, Applications and architectures", Salzburg, June 2011.

[27] D. NUENTSA WAKAM, J. ERHEL, W. GROPP. *About deflated Parallel GMRES*, in "fith workshop of the INRIA-Illinois Joint Laboratory on Petascale Computing", Grenoble, June 2011, invited talk.

[28] G. PICHOT, A. BEAUDOIN, J. CHARRIER, N. SOUALEM, J. ERHEL, J.-R. DE DREUZY, M. KERN. *Simulation of Transport in 2D Heterogeneous Porous Media via a Random Walk Particle Tracking method*, in "2011 SIAM Conference on Mathematical and Computational Issues in the Geosciences", 2011, organization of a mini-symposium.

[29] B. POIRRIEZ, J. ERHEL, G. PICHOT. *Schur Complement Preconditioning for Flow Simulation in 3D Discrete Fracture Networks*, in "2011 SIAM Conference on Mathematical and Computational Issues in the Geosciences", 2011, invited in a mini-symposium.

International Conferences with Proceedings

[30] J. ERHEL, A. LEJAY, G. PICHOT. *Comparison of some lagrangian schemes for the simulation of diffusion in discontinuous media*, in "Proceedings of the 4th International Conference on Approximation Methods and Numerical Modelling in Environment and Natural Resources (MAMERN'11)", B. AMAZIANE, D. BARRERA, H. MRAOUI, M. RODRIGUEZ, D. SBIBIH (editors), EUG, 2011, p. 319-322, invited in a mini-symposium.

[31] D. NUENTSA WAKAM, J. ERHEL, É. CANOT. *Robustness in hybrid algebraic solvers for large linear systems*, in "Proceedings of 23th International Conference on Parallel Computational Fluid Dynamics (Parallel CFD 2011)", Barcelona Supercomputing Center, 2011, 5 pages, invited in a mini-symposium, http://parcfd2011.bsc.es/.

[32] B. POIRRIEZ, J. ERHEL. *Flow computations in 3D Discrete Fracture Networks using a Domain Decomposition Method*, in "Proceedings of the 4th International Conference on Approximation Methods and Numerical Modelling in Environment and Natural Resources (MAMERN'11)", B. AMAZIANE, D. BARRERA, H. MRAOUI, M. RODRIGUEZ, D. SBIBIH (editors), EUG, 2011, p. 603-606, invited in a mini-symposium.

Conferences without Proceedings

[33] J. ERHEL, M. KERN. *MoMaS: 10 years of reactive transport*, in "Journées scientifiques du GNR MOMAS", Marseille, France, November 2011.

[34] J. ERHEL, Z. MGHAZLI, M. OUMOUNI. *Calcul de l'espérance de la solution d'une EDP stochastique unidimensionnelle à l'aide d'une base réduite*, in "TAM-TAM'11: 5ième colloque maghrébin de Mathématiques Appliquées.", Sousse, Tunisie., April 2011.

[35] D. NUENTSA WAKAM, J. ERHEL, É. CANOT. *Deflated GMRES with Multiplicative Schwarz Preconditioner: A Challenge of Robustness and Parallelism*, in "The Twentieth International Conference on Domain Decomposition Methods", La Jolla, California, USA, February 2011, contributed talk.

[36] M. TANKEO, P. RICHARD, É. CANOT. *Simulation of granular flow in channel*, in "2nd Int. Conference on Material Modelling", Paris, France, Sept 2011, contributed talk.

Scientific Books (or Scientific Book chapters)

[37] J. ERHEL. *Some Properties of Krylov Projection Methods for Large Linear Systems*, in "Computational Technology Reviews", P. IVANYI, B. TOPPING (editors), Saxe-Coburg Publications, 2011, vol. 3, p. 41-70.

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

Books or Proceedings Editing

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

Research Reports

[40] A. BEN ABDA, B. JOHANSSON, S. KHALFALLAH. *Leak identification in saturated unsteady flow via a Cauchy problem for the heat equation and iterative regularization.*, ENIT, 2011, In revision, submitted to Journal of Scientific Computing.

[41] J. CHARRIER. *Numerical analysis of the advection-diffusion of a solute in random media*, INRIA, March 2011, n^{o} RR-7585, http://hal.inria.fr/inria-00581244/en.

[42] J. CHARRIER, R. SCHEICHL, A. TECKENTRUP. *Finite element error analysis of elliptic PDEs with random coefficients and its application to multilevel Monte Carlo methods*, University of Bath, March 2011, n^{o} 2/11, http://www.bath.ac.uk/math-sci/BICS.

[43] E. KAMGNIA, B. PHILIPPE. *Counting eigenvalues in domains of the complex field*, INRIA, October 2011, n^{o} RR-7770, http://hal.inria.fr/hal-00634065/en.

[44] A. LEJAY, G. PICHOT. *Simulating diffusion processes in discontinuous media: a numerical scheme with constant time steps*, INRIA, 2011, submitted to Journal of Computational Physics.

[45] D. NUENTSA WAKAM, J. ERHEL, W. GROPP. *Parallel Adaptive Deflated GMRES*, INRIA, San Diego, USA, 2011, in revision, submitted to proceedings of DD20.

[46] D. NUENTSA WAKAM, J. ERHEL. *Parallelism and Robustness in GMRES with the Newton basis and the deflated restarting*, INRIA-7787, November 2011, n^{o} RR-7787, http://hal.inria.fr/inria-00638247/en.

[47] D. NUENTSA WAKAM, F. PACULL. *Memory efficient and robust hybrid algebraic solvers for large CFD linear systems*, INRIA, 2011, submitted to computers and fluids.

[48] S. SABIT, N. SOUALEM. *Suite Logicielle GRT3D (Global Reactive Transport 3D)*, INRIA, 2011.

Scientific Popularization

[49] J. ERHEL, J.-R. DE DREUZY. *Des pollutions suivies à la trace*, in "Interstices", 2011.

[50] J. ERHEL. *Un algorithme pour mettre en rang une équipe de football*, in "Interstices", 2011.

References in notes

[51] J. ERHEL, J.-R. DE DREUZY, B. POIRRIEZ. *flow simulations in three-dimensional Discrete Fracture Networks*, in "SIAM Journal on Scientific Computing", 2009, vol. 31, n^{o} 4, p. 2688-2705 [*DOI :* DOI:10.1137/080729244], http://dx.doi.org/10.1137/080729244.

[52] G. PICHOT, J. ERHEL, J.-R. DE DREUZY. *A mixed hybrid Mortar method for solving flow in discrete fracture networks*, in "Applicable Analysis", 2010, vol. 89, n^{o} 10, p. 1629-1643.

[53] C. DE DIEULEVEULT, J. ERHEL, M. KERN. *A global strategy for solving reactive transport equations*, in "Journal of Computational Physics", 2009, vol. 228, p. 6395-6410 [*DOI :* DOI: 10.1016/J.JCP.2009.05.044], http://www.sciencedirect.com/science/article/B6WHY-4WGDR6C-1/2/ada7965dcd6096984365876b64411966.