INRIA

INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Project-Team SAGE

Simulations and Algorithms on Grids for Environmental Applications

Rennes - Bretagne-Atlantique

Theme : Observation and Modeling for Environmental Sciences

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2. Overall Objectives

2.1. Main research areas

The team SAGE undertakes research on high-performance computing and deals with three subjects :

- numerical algorithms, mostly for solving linear and nonlinear systems,
- large scale high performance computing, involving parallel and grid computing,
- environmental and geophysical applications, mostly in hydrogeology.

These three subjects are highly interconnected: the first topic aims at designing numerical algorithms, which will lead to high performances on parallel and grid architectures and which will be applied in geophysical models.

Moreover, the team SAGE develops a software platform for groundwater numerical simulations in heterogeneous subsurface.

3. Scientific Foundations

3.1. Numerical algorithms

The focus of this topic is the design of efficient and robust numerical algorithms in linear algebra. The main objective is to solve large systems of equations $Ax = b$, where the matrix A has a sparse structure (many coefficients are zero). High performance computing (3.2) is required in order to tackle large scale problems. Algorithms and solvers are applied to problems arising from hydrogeology and geophysics (4.1).

3.1.1. Direct linear solvers

Direct methods, based on the factorization $A = LU$, induce fill-in in matrices L and U. Reordering techniques can be used to reduce this fill-in, hence memory requirements and floating-point operations [43].

More precisely, direct methods involve two steps, first *factoring* the matrix A into the product $A = P_1LUP_2$ where P_1 and P_2 are permutation matrices, L is lower triangular, and U is upper triangular, then solving $P_1LUP_2x = b$ by processing one factor at a time. The most time consuming and complicated step is the first one, which is further broken down into the following steps :

- Choose P_1 and diagonal matrices D_1 and D_2 so that $P_1D_1AD_2$ has a "large diagonal." This helps to assure accuracy of the final solution.
- Choose P_2 so that the L and U factors of P_1AP_2 are as sparse as possible.
- Perform *symbolic analysis*, i.e. identify the locations of nonzero entries of L and U.
- Factorize P_1AP_2 into L and U.

The team worked on parallel sparse direct solvers [6].

3.1.2. Iterative linear solvers

The two main classes of iterative solvers are Krylov methods and multigrid methods.

A Krylov subspace is for example $\{x_0, Ax_0, \cdots, A^kx_0\}$. If the matrix is symmetric positive definite, the Krylov method of choice is the Conjugate Gradient; for symmetric undefinite matrices, there are mainly three methods, SYMMLQ, MINRES and LSQR. For unsymmetric matrices, it is not possible to have both properties of minimization and short recurrences. The GMRES method minimizes the error but must be restarted to limit memory requirements. The BICGSTAB and QMR methods have short recurrences but do not guarantee a decreasing residual [49], [47]. All iterative methods require preconditioning to speed-up convergence : the system $M^{-1}Ax = M^{-1}b$ is solved, where M is a matrix close to A such that linear systems $Mz = c$ are easy to solve. A family of preconditioners uses incomplete factorizations $A = LU + R$, where R is implicitely defined by the level of fill-in allowed in L and U. Other types of preconditioners include an algebraic multigrid approach, an approximate inverse or a domain decomposition [40].

Multigrid methods can be used as such or as a preconditioner. They can be either geometric or algebraic [47].

The team studies preconditioners for Krylov methods [1], [9] and uses multigrid methods.

3.1.3. Domain decomposition methods

Domain decomposition methods are hybrid methods or semi-iterative methods using iterative and direct techniques. They can be based on alternating Schwarz method when domain overlap or on Schur complement method whithout overlapping [47]. Schwarz methods can be used as preconditioners of Krylov methods or directly with an acceleration based on Aitken extrapolation. Schur methods lead to a reduced system, solved by a preconditioned Krylov method.

The team studies these various aspects of domain decomposition methods.

3.1.4. Linear least-squares problems

For linear least-squares problems $\min_x \|Ax - b\|$, direct methods are based on the normal equations $A^TAx = A^Tb$, using either a Cholesky factorization of A^TA or a QR factorization of A, whereas the most common Krylov iterative method is LSQR. If the discrete problem is ill-posed, regularization like Tychonov or a Truncated Singular Value Decomposition (TSVD) is required [45], [39]. For large matrices, the so-called complete factorization is also useful. The first step is a pivoted QR factorization, followed by a second factorization $A = U \begin{pmatrix} T & 0 \\ 0 & E \end{pmatrix} V^T$ where U and V are orthogonal matrices and E is a matrix neglectable with respect to the chosen threshold. Such a decomposition is a robust rank-revealing factorization and it provides for free the Moore-Penrose Generalized Inverse. Recently, efficient QR factorization software libraries became available but they do not consider column or row permutations based on numerical considerations since the corresponding orderings often end up with a non tractable level of fill-in.

The team studies iterative Krylov methods for regularized problems, as well as rank-revealing QR factorizations.

3.1.5. Nonlinear problems and time integration

Nonlinear methods to solve $F(x) = 0$ include fixed-point methods, nonlinear stationary methods, secant method, Newton method [48], [42], [46]. The team studies Newton-Krylov methods, where the linearized problem is solved by a Krylov method [3], Broyden methods, Proper Orthogonalization Decomposition methods.

Another subject of interest is time decomposition methods. The idea is to divide the time interval into subintervals, to apply a timestep in each subinterval and to apply a nonlinear correction at both ends of subintervals. This can be applied to explosive or oscillatory problems.

3.1.6. Eigenvalue problems

Let us consider the problem of computing some extremal eigenvalues of a large sparse and symmetric matrix A. The Davidson method is a subspace method that builds a sequence of subspaces, which the initial problem is projected on. At every step, approximations of the sought eigenpairs are computed : let V_m be an orthonormal basis of the subspace at step m and let (λ, z) be an eigenpair of the matrix $H_m = {V_m}^T A V_m$; then the Ritz pair $(\lambda, x = V_m z)$ is an approximation of an eigenpair of A. The specificity of the method comes from how the subspace is augmented for the next step. In contrast to the Lanczos method, which is the method to refer to, the subspaces are not Krylov subspaces, since the new vector $t = x + y$ which will be added to the subspace is obtained by an acceleration procedure : the correction y is obtained by an exact Newton step (Jacobi-Davidson method) or an inexact Newton step (Davidson method). The behavior of the Davidson method is studied in [4] while the Jacobi-Davidson method is described in [50]. These methods bring a substantial improvement over the Lanczos method when computing the eigenvalues of smallest amplitude. For that reason, the team considered Davidson method to compute the smallest singular values of a matrix B by applying them to the matrix $B^T B$ [4].

3.1.7. Robust algorithms for characterizing spectra

In several applications, the eigenvalues of a nonsymmetric matrix are often needed to decide whether they belong to a given part of the complex plane (e.g. half-plane of the negative real part complex numbers, unit disc). However, since the matrix is not exactly known (at most, the precision being the precision of the floating point representation), the result of the computation is not always guaranteed, especially for ill-conditioned eigenvalues. Actually, the problem is not to compute the eigenvalues precisely, but to characterize whether they lie in a given region of the complex field. For that purpose the notion of ϵ-spectrum or equivalently the notion of pseudospectrum was simultaneously introduced by Godunov [44] and Trefethen [51]. Several teams proposed softwares to compute pseudospectra, including the SAGE team with the software PPAT [8], described in Section 5.1.

3.2. High-Performance Computing

The focus of this topic is the development of parallel algorithms and software. The objectives are to solve large scale equations in linear algebra (3.1) and to use high performance computing for dealing with problems arising from hydrogeology and geophysics (4.1).

3.2.1. Parallel sparse linear algebra

Algorithms have been described above (3.1). The team works on the development of parallel software for iterative solvers (PCG, GMRES, subdomain method), least-squares solvers (QR factorization). The team also compares existing solvers. The target is Giga-systems with billions (10^9) of unknowns.

3.2.2. Parallel spatial discretization

Our applications in hydrogeology and geophysics (4.1) are in the framework of Partial Differential Algebraic Equations (PDAE). We usually discretize time by a classical one-step or multi-step scheme and space by a Finite Element Method or a similar method. To get a fully parallel implementation, it is necessary to parallelize the matrix computation and generation. A common approach is to divide the computational domain into subdomains. Once the matrix is computed, it is used in linear solvers. The challenge is to reduce communication between the two phases. Recently, we have also investigated particle methods and we have developed a parallel particle tracker.

3.2.3. Software components for coupled problems

Our applications are quite often multi-physics models, where nonlinear coupling occurs. Our objective is to design software components, which provide a great modularity and flexibility for using the models in different contexts. The main numerical difficulty is to design a coupling algorithm with parallel potentiality.

3.2.4. Grid computing for stochastic simulations

In our applications, we use stochastic modelling in order to take into account geophysical variability. From a numerical point of view, it amounts to run multiparametric simulations. The objective is to use the power of grid computing. The target architecture is a heterogeneous collection of parallel clusters, with high-speed networks in clusters and slower networks interconnecting the clusters.

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 investigates also geodesy, submarine acoustics, geological rock formation and heat transfer in soil. 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 Le Havre and CDCSP at University of Lyon. It is also done in the context of GdR 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 wastes, 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 nuclear wastes. 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 fracture networks.

The output is a parallel scientific platform running on clusters and on experimental computational grids. Simulations of several test cases assess the performance of the software.

5. Software

5.1. 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.

5.2. 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.

MUESLI supports all free Fortran compilers currently available (INTEL-ifort, GNU-gfortran, FSF-g95). 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 2.0.4 (15 october 2009). More information can be found at: http://www.irisa.fr/sage/edouard/canot/muesli/

5.3. 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).

5.4. H2OLAB: numerical simulations in hydrogeology

Participants: Jocelyne Erhel [corresponding author], Baptiste Poirriez, Nadir Soualem.

Website: http://h2olab.inria.fr

The software-platform H2OLab is developed in collaboration with J.-R. de Dreuzy, from Geosciences, university of Rennes 1, with A. Beaudoin, from the University of Le Havre and with D. Tromeur-Dervout, from the University of Lyon.

The platform H2OLab (previously Hydrolab) aims at modeling flow and transport of solute in highly heterogeneous porous or fractured media [29]. Numerical models currently include steady-state flow in saturated media and transport by advection-diffusion. Physical models can be either a porous medium or a network of fractures. For flow equations, H2OLab uses a mixed finite element method or a finite volume method and it includes a particle tracker for transport equations. The platform is organized in software components and relies as far as possible on existing free libraries, such as sparse linear solvers. Because the target is large computational domains, the platform makes use of high performance computing and all modules have a parallel version. The target is currently clusters with distributed memory and grid architectures. The code is written in C++ and uses the MPI library for parallel computing. Most modules are fully generic so that they can be used by any application within the platform. The platform is currently implemented on Windows systems and on Linux systems as well. The objective is to develop a free software available on the Web; it is managed using Gforge of Inria; four components are registered at the APP: PARADIS, MP_FRAC, GW_NUM, GW_UTIL.

6. New Results

6.1. Numerical algorithms and high performance computing

6.1.1. Rank-Revealing QR factorization

Participant: Bernard Philippe.

That work is done in cooperation with Laura Grigori, from the team Grand Large at INRIA Saclay, and with Frédéric Guyomarc'h, from the team Dart at INRIA Lille.

We have developed an algorithm to compute a rank revealing sparse QR factorization. The algorithm consists of first a standard QR factorization performed with standard high performance routines like MA49, and a second part based on incremental condition number estimation ICE. The goal of the procedure is to solve rank-deficient linear least-squares problems without appealing to a truncated SVD which is too expensive. The existing MATLAB code is adapted to dense matrices. A sparse version is still under development.

6.1.2. Generation of Krylov subspace bases

Participant: Bernard Philippe.

This work is carried out in cooperation with Lothar Reichel during his visits to Rennes and during B. Philippe's visit to Kent State University.

Methods for generating bases for Krylov subspaces, especially in the case of nonsymmetric matrices, are the kernels of GMRES or Arnoldi algorithms. The usual procedure, which consists in computing an orthonormal basis through the Arnoldi procedure, is not well adapted to parallel computing. The direct computation of a monomial basis times a vector, which then is orthogonalized at once, is more suitable for parallel computation. However, propagated round-off errors lead to untractable computations as soon as the condition number of the computed basis reaches some threshold. Our goal is to follow two directions to generate well-conditioned bases: (i) the Newton bases with Leja ordered shifts: this approach was first introduced by L. Reichel and his co-authors several years ago and has been used many times by researchers from the SAGE team; (ii) the use of orthogonal polynomials: these polynomials already been used for defining iterative linear solvers, the problem of ellipse fitting, which is required to define the polynomials, is easier to solve for the present application. In a submitted paper [37], we develop the two approaches and provide some mathematical estimates of their effectiveness. We conclude with a few numerical experiments.

6.1.3. C++ interface to sequential and parallel solvers

Participants: Jocelyne Erhel, Désiré Nuentsa Wakam, Nadir Soualem.

This work is done in the context of the Cinemas2 and the Libraero contracts, 7.1.3 and 7.1.4. It is the subject of training for the student Frédéric Wang (master 1).

Modern sequential and parallel solvers are complex. Implementation of these codes and their connexion to home made software require substantial efforts. We have built a C++ interface to the following sequential and parallel solvers:

- Sequential SuperLU and UMFPACK
- SuperLU_DIST
- Hypre
- Mumps

Design and implementation of this module allow to define a set of general C++ classes to solve linear systems using parallel computing features. The most common sparse storage scheme matrix have been implemented, and conversion operators have been defined according to input data waited by the different solvers. This library covers basic linear algebra operations on matrices and vectors using C++ overloading operators(+, -, *, transpose, etc ...). A list of experiments has been done on Grid'5000 clusters using MPICH2 implementation. Matrices have been judiciously chosen in the DataBase MatrixMarket. Documentation and code sources are available and have been hosted in Inria Gforge source manager.

6.1.4. Solution of large linear systems arising from fluid dynamics

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

This work is done in the context of the Cinemas2 and the Libraero contracts, 7.1.3 and 7.1.4.

We have pursued our work of finding efficient parallel solvers for large linear systems coming from fluid dynamics simulations. Solvers under consideration implement direct, iterative or domain decomposition methods and most of them are freely available packages. As each solver has its own interface to link with, we have designed a unified toolbox that helped us to link uniformely with any of the package under study (See section 6.1.3). Among the solvers used, we had our parallel GMRES with Schwarz preconditioner (See section 6.1.5). The numerical tests performed have revealed that this parallel preconditioner is competitive among other domain decomposition methods. However, it still suffers from poor scalability. So we have investigated ways to improve this aspect by using some multilevel techniques (See section 6.1.6). The results of this work has been presented at international conferences [22], [33].

6.1.5. Parallel Multiplicative Schwarz preconditioner for GMRES: software GPREMS

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

That work is done in cooperation with E. Kamgnia, from the University of Yaoundé, Cameroon. It is also done in the context of the Cinemas2 and the Libraero contracts, 7.1.3 and 7.1.4.

We have pursued the work on a parallel version of the GMRES method preconditioned by Multiplicative Schwarz [25].

Software called GPREMS has been documented and will be available for free download, as soon as it will be registered at APP.

6.1.6. A two-level parallelism in GPREMS

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

This work is done in the context of the Cinemas2 and the Libraero contracts, 7.1.3 and 7.1.4.

In this work, we are improving the perfomance of the parallel solver presented at the section 6.1.5. As this preconditioner is based on domain decomposition method, the matrix of the linear system is algebraically splitted into several submatrices. The classical scheme is to assign a subdomain/submatrix to a compute node of the parallel computer. Then at each application of the preconditioner, each node has to solve a linear system associated with a subdomain. Usually, the reduced local systems are solved with a sequential solver. But depending on the size of the global matrix, the local matrices can be very large. Also, the total time to solve the global system depends heavily on the time to solve (accurately or not) those local systems. On the other hand, an increase of the number of subdomains leads often to an increase of the overall number of iterations to reach the solution of the global system. In our approach, we have chosen a reasonable number of subdomains. For the local systems, instead of using a sequential solver, we have applied a parallel solver internally to each node to keep all the cores busy. The communication among the cores are enhanced by using the appropriate MPI implementation [41]. The results of this work have been discussed during several workshops [23], [24].

6.1.7. Parallel-in-time integration

Participants: Jocelyne Erhel, Noha Makhoul.

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

The rescaling methodology generates a sequence of time slices governed by an End-of-slice condition and uses a change of variables. The sequential implementation of the rescaling technique on monotonous problems of global time existence, has shown the existence of a relation between the initial values on successive time slices (ratio property). It was the basic idea for devising a prediction procedure, based on this ratio property, yielding the *Ratio-based Parallel Time Integration* (RaPTI) algorithm.

RaPTI Algorithm starts with running the rescaling method sequentially on n_s slices and computing the ratios of the successive initial values until their stabilization, up to a given computational tolerance. Then, the stabilized ratios are used for predicting the initial values of the solution on the remaining slices and thus, allowing a parallel-in-time integration [13]. Unlike the other parallel-in-time algorithms, RaPTI does not involve any sequential computation on the coarse grid (except for the first slices) and generates time slices with a varying size. The similarity properties of the rescaled problems have been studied in a theoretical way and have shown the existence of limit problems that could be used for improving the prediction procedure. Moreover, a method of extrapolation based on the previous values of the starting values of the solution and taking into consideration their limit value have been devised and led to much better predictions and a very quick convergence. RaPTI Algorithm has been intensively experimented, on an eight core machine using Parallel Matlab Toolbox, on the following problems:

- A membrane problem of which the solution is explosive in infinite time and in an oscillatory way.
- A reaction-Diffusion problem of which the solution is explosive in infinite time.
- A satellite trajectory in a J_2 perturbed motion.

The results are very encouraging, showing a big improvement of the parallel efficiency.

6.1.8. Multiparametric Monte-Carlo simulations using clusters and computational grids

Participant: Jocelyne Erhel.

This work is done in the context of the Micas contract, 7.1.2.

In hydrogeology, the description of the underground properties is very poor, mainly due to its complex heterogeneity and to the lack of measures. As a consequence, we rely on stochastic models of geometrical and physical properties. We have identified three levels of distributed and parallel computing. At the simulation level, we choose to define distributed memory algorithms and to rely on the MPI library for communications between processors. The intermediate level is the Uncertainty Quantification non intrusive method, currently Monte-Carlo. Our objective is to design a facility for running the set of random simulations by choosing either a parallel approach with MPI or a distributed approach with a grid middleware. At the multiparametric level, we choose a distributed approach as is done in most projects on computational grids. We have done some numerical experiments with the first two levels, using MPI [30].

6.2. Numerical models and simulations applied to physics

6.2.1. Inverse problems in geodesy

Participants: Amine Abdelmoula, Bernard Philippe.

This work is done in collaboration with M. Moakher, from ENIT, Tunisia, in the context of the co-advise project, 7.2.2.

The geoid is the level surface of the earth attraction at the sea level. That surface is obtained as a correction of a regular surface by fitting existing mesures. The problem ends up with a large structured generalized least squares problem. Therefore, we plan to apply our algorithms on QR factorizations (6.1.1).

The main research direction on which we now focus, is the determination of an equivalent mass system which can generate a given geoid. The mathematical definition of the problem is expressed as a non-linear least-squares problem in the Hilbert space of harmonic functions. The most difficult aspect comes from the fact that, in order to be useful, the least-squares problem must be expressed on a limited region of the earth. We propose for that purpose to use Slepian's approach. Now we aim at tuning the minimizing procedure in the code.

6.2.2. Heat transfer in soil and prehistoric fires

Participants: Édouard Canot, Mohamad Muhieddine.

Mohamad Muhieddine began his PhD thesis in October 2006 on the subject: "Numerical simulations of prehistoric fires", co-advised by Ramiro March (ArcheoSciences, Rennes). This project takes place in the archeological/human sciences program: "Man and fire: towards a comprehension of the evolution of thermal energy control and its technical, cultural and paleo-environmental consequences". Both physical and numerical approach is used to understand the functioning mode and the thermal history of the studied structures. The main topic of this thesis concerns the simulation of forced evaporation of water in a saturated soil.

2D and 3D-axisymmetric configurations of this physical problem have been solved, using the Apparent Capacity Method. Emphasis is put on performance: the Jacobian matrix is stored in a sparse structure and the Newton iterations (inside the BDF method) are solved by the UMFPACK part of the SuiteSparse package. All these modifications are done inside MUESLI, giving an easy-to-use programming interface for the user.

In addition, we have investigated the heat conduction in a real 3D saturated porous medium. In term of numerics, the discretization is based on the hybrid mixed finite element method in space and a semi-implicit scheme in time. To solve this problem we have modified `TRACES` (Transport of RadioActive Elements in Subsurface, 2004, P. Ackerer and H. Hoteit, IMFS, Université de Strasbourg) which is a computer program for the simulation of flow reactive transport in saturated porous media. This work has been presented to the MAMERN'09 conference[32].

Recently, we have introduced a robust numerical strategy to estimate temperature dependent thermal capacity, thermal conductivity and the porosity of a saturated porous medium, based on the knowledge of heating curves at selected points in the medium. In order to solve the inverse problem, the least squares criterion (in which the sensitivity coefficients appear) has been used. We have proposed a new global approach to solve the system of coupled equations. This work has been presented to the NASCA'09 conference[35].

All the work is presented in the thesis defended in October by M. Muhieddine[10]. Other publication associated to this work: [12].

6.2.3. *Rheology of granular systems flowing out of silo*

Participant: Édouard Canot.

This work is in the framework of a project funded by the Region Bretagne. A PhD thesis began in February 2009, coadvised with Patrick Richard, who is from the Physics Institute at the University of Rennes (IPR). The study concerns the rheology of granular media flowing out of a silo. The two objectives are (i) to understand the rheological properties of such kind of granular flows and especially the effect of the micro mechanical characteristics, and (ii) to determine the most efficient ways to decompact and to unblock these systems. We expect that the results will help the understanding of the jamming transition which is of fundamental interest for discrete matter.

We expect to carry out and compare numerical simulations and experiments of granular flows; the method used is based on molecular dynamics.

6.3. Numerical models and simulations applied to hydrogeology

6.3.1. *Reactive transport*

Participant: Jocelyne Erhel.

This work is done in the context of the MOMAS GNR (7.1.1).

Reactive transport models are complex nonlinear Partial Differential Algebraic Equations (PDAE), coupling the transport engine with the reaction operator. We consider here chemical reactions at equilibrium. We have pursued our work on a global approach, based on a method of lines and a DAE solver. We have developed a software in C, dealing with 1D, 2D and 3D domains, implementing our global approach. For large computational domains, it is necessary to reduce the cost of the sparse solver. Indeed, it is possible to reduce the number of unknowns by eliminating some of them. We have run experiments with several test cases in 1D and 2D, in order to show the accuracy of our software and to analyze its efficiency. In particular, we have pursued our work on the benchmark proposed by Momas. Publications related to this work are [15], [28], [14], [20], [19].

6.3.2. *Flow and transport in highly heterogeneous porous medium*

Participants: Jocelyne Erhel, Nadir Soualem.

This work is done in collaboration with A. Beaudoin, from the University of le Havre and J.-R. de Dreuzy, from the department of Geosciences at the University of Rennes 1. It is done in the context of the Micas contract (7.1.2).

We have pursued our work for simulating flow and solute transport in 2D domains, where the permeability field is highly heterogeneous and is a random field [31]. Numerical analysis of PARADIS (Parallel Dispersion) is the subject of internship for Ibrahim Zangré (master 1).

We have checked the mesh size influence on the coupled problem:

$$\epsilon v = -K\nabla H \quad , \quad s\frac{\partial H}{\partial t} + \nabla.(\epsilon v) = q \tag{1}$$

where the first equation is Darcy Law and the second one the mass conservation. Numerical methods are based on Finite Volume Element method for flow equations and it includes a particle tracker for the following transport equation:

$$\frac{\partial C}{\partial t} + \nabla.(\epsilon v C) - \nabla.(D \nabla C) = 0. \tag{2}$$

where:

- C : solute concentration , with initial condition given by (C_0)
- D : dispersion tensor

Stochastic computations are performed by using a Monte Carlo method. We have shown the good behaviour of the scheme when the mesh grid size is refined, using the following criteria

$$\frac{\lambda}{L} \sim 500 \tag{3}$$

where λ is the correlation length and L the domain size length.

Numerical experiments illustrate ergodicity properties of the physical quantities. All tests have been performed on Grid'5000 clusters.

6.3.3. Flow in 3D networks of fractures

Participants: Jocelyne Erhel, Baptiste Poirriez.

This work is done in collaboration with J.-R. de Dreuzy and G. Pichot, from the department of Geosciences at the University of Rennes 1. It is done in the context of the Micas contract (7.1.2).

We have pursued our work for simulating flow in a 3D network of interconnected plane fractures

Discrete Fracture Networks are complex 3D structures with 2D domains intersecting each other. A challenge comes with the meshing of such networks, where the mesh must be of good quality and must not contain too many cells. We have designed a method to generate a mesh of good quality [11], [21]. It is based on a conforming discretization of intersections, in the sense that each intersection has a unique 3D discrete representation. It also relies on a unique mesh step for all fractures. However, the number of cells can be large, especially if the network contains large fractures as well as small fractures.

We address this difficulty with two different approaches: we investigate efficient parallel sparse linear solvers and we introduce non-matching discretizations of intersections.

We have run several simulations using different solvers. We have tested a direct solver, UMFPack, and the following ones from the Hypre library :

- a multigrid solver, BoomerAMG;
- PCG preconditioned by BoomerAMG.

They have shown some limits for our problems. The direct solver is limited by memory usage when the system size increases: it cannot exceed 10 millions of unknowns. The iterative solvers have also some drawbacks. They can solve larger problems (up to 20 millions of unknowns) but they are less efficient than UmfPack. Moreover, for some cases, boomerAMG fails to converge. PCG is more stable but even less efficient than BoomerAMG. The results of these simulations were presented at SIAM GS 09 [27].

We expect to overcome these limits by using domain decomposition methods, which combine the benefits of iterative and direct solvers. Currently we are implementing a Schur method, and use a direct solver in sub-domains, thus for small systems, and PCG at the interface. The major challenge is to find a suitable two-level preconditioning method, acting at the local and the global levels. We are testing Neumann-Neumann for local preconditioning and either deflation or coarse-grid correction for global preconditioning, with different subspace definitions. Linear systems associated with discrete fracture networks have a sparsity structure strongly dependent on the network geometry. We are using this structure to carry out the domain decomposition.

We have developed a software in Matlab in order to validate our approach. This required to export some geometrical and structural data from the software MPFRAC in the platform H2OLab. The next step will be to implement the algorithm in the platform. Then we will design a parallel version, based on the domain decomposition.

The other idea is to generate a 2D mesh in each fracture with possibly different mesh steps from one fracture to another and to apply interface conditions using a mortar method. We use a mixed hybrid finite element method which allows to eliminate the flux unknowns. It appears that this method is well adapted for integrating a mortar method. We have developed a software integrated in the platform H2OLab. We have applied our mortar method to various fracture networks and compared it with the method using matching grids. Results show a fairly good accuracy of the mortar method [34], [36].

6.3.4. Uncertainty Quantification methods

Participants: Julia Charrier, Jocelyne Erhel, Mestapha Oumouni.

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 contract (7.1.2). Study of stochastic finite element methods is the subject of internship for Hélène Philippe (master 1). In our applications described above, we use stochastic models and rely on uncertainty quantification methods. We use Monte-Carlo methods (see section 6.1.8) and study other UQ methods based on stochastic finite element methods.

We have worked on error estimation of our method applied to the flow and transport/diffusion equations in heterogeneous porous media. We have proved, under regularity conditions, the convergence of the Monte Carlo method and given an upper bound for the errors comitted by estimating the spreading and the macro-dispersion of the solute:

$$\sup_{t\in[O,T]} ||Er||_{L^2L^2} \leq C(\frac{1}{\sqrt{N}} + \frac{1}{\sqrt{M}} + \Delta t + h|lnh|)$$

where N is the number of realizations of the permeability field, M the number of particles for each realization of the permeability field, Δt the mesh of the time discretisation for the computation of the particles trajectories and h the mesh of the spatial discretization for the computation of the velocity field. This work was presented in two workshops [17], [18], and a paper is in preparation.

After a bibliographic work on stochastic spectral finite elements methods, we realized a numerical comparison between Monte Carlo method and stochastic spectral method for the flow equation in one dimensionnal heterogeneous porous media. This was the subject of internship for Hélène Philippe. We have investigated the convergence rates for the two methods, and the dependency of this convergence rate with respect to the value of the correlation length. This work will be continued with the flow/transport equation.

An approach has emerged as useful and current tool to address the curse of dimensionality experienced by stochastic spectral finite element methods, called sparse grids stochastic collocation method. It uses global polynomials in the stochastic space to interpolate the solution. These sparse grids are a subset of the full tensor product grids. There are several orders of magnitude reduction in the number of collocation points required to achieve the same level of accuracy as with the full grid, under some smoothness of parameters. We have studied an adaptive sparse grid collocation strategy, using piecewise multi-linear hierarchical basis functions to locally approximate the solution in stochastic and physical space. A hierarchical surplus is used

as an error indicator to automatically detect the discontinuity region in the stochastic space and to adaptively refine the collocation points in this region.

6.3.5. Inverse problems in hydrogeology

Participants: Sinda Khalfallah, Jocelyne Erhel.

This work is done in collaboration with J.-R. de Dreuzy, from Geosciences Rennes, and A. ben Abda, from LAMSIN, Tunisia. It is done in the context of the Hydromed and Co-Advise contracts (7.3.1, 7.2.2).

We study two types of inverse problems in hydrogeology. The direct transient model is governed by classical flow equations and relates transmissivity with hydraulic head. We assume a constant known porosity.

The first type of problem is a so-called data completion problem, whith missing data on some part of the boundary and overdefined data on the other part. In other words, boundary conditions are not defined everywhere, leading to an ill-posed problem. For steady-state problems, we have investigated methods based on an energy norm. Now, we study transient problems and have defined a method based on a fictituous domain decomposition technique.

The second type of problem concerns the identification of the transmissivity in saturated aquifers. Here, we assume that measurements of transmissivity or hydraulic head are done at some points during some time intervals and aim at recovering the transmissivity at any point of the computational domain. Source and sink terms are given, as well as boundary and initial conditions. A first step in such inverse problems is to define the parameters to identify. We did a bibliographic review of two methods, based either on zonation or on pilot points. The transmissivity is then defined by using an interpolation technique, such as a so-called kriging method. A second step is to define the objective function and to apply some regularization. We plan to investigate functions based on an energy norm.

7. Other Grants and Activities

7.1. National grants

7.1.1. GNR MOMAS: reactive transport project

Participant: Jocelyne Erhel.

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 participate in the project entitled “Numerical and mathematical methods for reactive transport in porous media”.

See sections 6.3.1, 4.2.

7.1.2. ANR-CIS: MICAS project

Participants: Édouard Canot, Julia Charrier, Jocelyne Erhel, 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

The project is designed to solve great challenges in hydrogeology and to develop free generic software. Numerical modelling is an important key for the management and remediation of groundwater resources. Natural geological formations are highly heterogeneous, leading to preferential flow paths and stagnant regions. The contaminant migration is strongly affected by these irregular water velocity distributions. In order to account for the limited knowledge of the geological characteristics and for the natural heterogeneity, the project MICAS relies on Uncertainty Quantification methods. In previous and current work, we use a classical Monte-Carlo method, with random permeability fields and random Discrete Fracture Networks. In this stochastic approach, numerical simulations consist in computing the velocity field over large spatial domains and solving solute transport over large temporal scales. This approach must overcome two main difficulties, memory size and runtime, in order to solve very large linear systems and to simulate over a large number of time steps. High performance computing is thus necessary to carry out these large scale simulations. The objectives of MICAS are to get outstanding results in seven well-identified topics: 1. Macro-dispersion in 3D heterogeneous porous media 2. Steady flow in 3D Discrete Fracture Networks (DFN) 3. Well test interpretation in 2D and 3D heterogeneous porous media and in DFN 4. Flow in 2D and 3D fractured porous media 5. Large scale multilevel sparse linear solvers 6. Stochastic models and algorithms for dealing with lack of observation and heterogeneity 7. Deployment of multi-parametric simulations on a computational grid A last topic is devoted to software for integrating all the modules developed in the project. Our commitment is to develop packages available for downloading on the websites of the project and the H2OLAB platform.

See sections 6.1.8, 6.3.2, 6.3.3, 6.3.4, 5.4, 4.2.

7.1.3. competitive cluster LUTB: CINEMAS2 project

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

Contract with Ecole Centrale de Lyon
Time: three years from May 2007.
Title: Conception Interactive par simulation Numérique des Ecoulements couplées à des Méthodes d'optimisation par Algorithmes Spécifiques.

This work is done in the context of the Région Rhône-Alpes initiative called Rhône-Alpes Automotive CLUSTER, and the competitiveness cluster called Lyon Urban Truck and Bus (LUTB). The global objective is to design a new methodology in CFD to reduce drastically computational time in an optimization process. The partners FLUOREM and LMFA have developed the software Turb-Opty based on parametrization. The key part of Sage team is to study sparse linear solvers applied to CFD systems arising in Turb-Opty applications. A first step has been done by using direct multifrontal solvers on systems of moderate size. Another step has been done by using our software implementing parallel GMRES preconditioned by multiplicative Schwarz.

See sections 6.1.4, 6.1.5, 6.1.3,6.1.6.

7.1.4. ANR-RNTL: LIBRAERO project

Participants: Édouard Canot, 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, described above. The main objective for the team Sage is to design efficient algorithms adapted to industrial configurations using the Turb-Opty software developed by Fluorem and LMFA. The challenge is to solve many linear systems of large size.

See section 6.1.4, 6.1.5, 6.1.3,6.1.6.

7.2. European Grants

7.2.1. ERCIM Working group: Computing and statistics

Participants: Jocelyne Erhel, Bernard Philippe.

Webpage: http://www.dcs.bbk.ac.uk/ercim/index.html

This ERCIM Working Group was created in 2007 and follows the past ERCIM WG entitled "Matrix Computations and Statistics", created in 2001. The Sage team is involved in the specialized group named "Matrix computations and Statistics" and Bernard Philippe is co-chair of this track. It deals with topics of research emerging from statistical applications which involve the use of linear algebra methods, optimization and parallel computing. The track is especially concerned by the very large problems which necessitate the design of reliable and fast numerical procedures. The solution of large-scale linear system of equations using High Performance Computing is addressed.

7.2.2. Marie Curie program: Co-Advise project

Participants: Amine Abdelmoula, Julia Charrier, Jocelyne Erhel, Sinda Khalfallah, Mestapha Oumouni, Bernard Philippe.

COADVISE Project supported by the European Commission [Seventh Framework Programme - Marie Curie Actions 'People' International Research Staff Exchange Scheme (IRSES)] 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 2009, three PhD students visited the Sage team during 3 months each: Amine Abdelmoula, Tunisia; Sinda Khalfallah, Tunisia; Mestapha Oumouni, Morocco.

7.2.3. PECO-NEI program: project with Romania and Slovakia

Participant: Bernard Philippe.

PECO-NEI Network for Education-Research with Eastern Europe Countries,
Title: Efficient sparse rank revealing QR factorization for solving least squares problems.
Time: 2006 - 2009
Coordination: INRIA-Saclay team Grand Large (Laura Grigori),
Partners: Politechnica University of Bucarest (Bogdan Dumitrescu), Slovakia Academy of Sciences (Gabriel Oksa).

This project aims at developing efficient algorithms for performing the QR factorization with rank revealing of sparse and dense matrices. In particular target matrices are those arising in geodesy applications. See section 6.1.1.

7.3. International Grants

7.3.1. INRIA Euro-Mediterranean Program: HYDROMED project

Participants: Édouard Canot, Julia Charrier, Jocelyne Erhel, Sinda Khalfallah, Mestapha Oumouni, Bernard Philippe.

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.

8. Dissemination

8.1. Program committees, organizing committees, Editorial Boards

- É. Canot and J. Erhel were co-organizers with E. Kamgnia of the conference NUMCOOP'09, in honor of B. Philippe, Yaounde, Cameroon, March.
- É. Canot and J. Erhel were co-organizers of the kick-off meeting of the HYDROMED project, Rennes, May.
- J. Erhel organized with J. Roberts a mini-symposium on "fractured media", at SIAM conference on Geosciences, Leipzig, Germany, June.
- 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).
- B. Philippe is reviewer of the AMS Mathematical Reviews.

8.2. INRIA and University committees

- É. Canot is member of the CUMI (Commission des Utilisateurs de Moyens Informatiques), of INRIA-Rennes, from September 2007.
- J. Erhel is member and secretary of the Comité de Gestion Local of AGOS at INRIA-Rennes.
- J. Erhel is member of Comité Technique Paritaire and Comité de Concertation of INRIA.
- J. Erhel is member of Conseil d'Administration of INRIA.
- In the International Affairs Department of INRIA, B. Philippe was in charge of the cooperating programmes with scientific teams in Africa and Middle-East countries, until June 2009.

8.3. Teaching and internship supervision

- A. Abdelmoula is teaching assistant (permanent position) in computer science at the University of Tunis, Tunisia.
- N. Makhoul-Karam is teaching assistant (temporary position) in mathematics at the american University of Beirut.
- J. Charrier is teaching assistant (monitrice) in mathematics at ENS-Cachan-Rennes.
- D. Nuentsa Wakam is teaching assistant (moniteur) in computer science at faculty of law, University of Rennes 1.
- B. Poirriez is teaching assistant (moniteur) in computer science at IFSIC, University of Rennes 1.
- É. Canot, J. Erhel and M. Muhieddine taught about Applied Mathematics (MAP) for DIIC, IFSIC, Rennes 1 (second year).

  Lecture notes on http://www.irisa.fr/sage/jocelyne
- Hélène Philippe has completed a two months summer internship in team Sage, under supervision of J. Charrier and J. Erhel.
- Frédéric Wang has completed a two months summer internship in team Sage, under supervision of N. Soualemn and J. Erhel.

- Ibrahim Zangré has completed a two months summer internship in team Sage and team LOMC at University of Le Havre, under supervision of A. Beaudoin, N. Soualemn and J. Erhel.

8.4. Participation in training

- D. Nuentsa Wakam: participation in training for teaching assistants, March.
- D. Nuentsa Wakam: participation in training for the first aid services (Premiers secours civiques de niveau 1), November.
- B. Poirriez: participation in training for teaching assistants.

8.5. Seminars and dissemination for the general public

- M. Muhieddine contributed to the one-day seminar of Ph-D students, at Caren, Rennes, June.
- J. Erhel participated in the operation "à la découverte de la recherche", organized in the area of Rennes in March-April. She visited a high school in Rennes where she gave a talk entitled *Le calcul scientifique et la modélisation. Exemple : les eaux souterraines*. She also discussed with the scholars about research profession.
- J. Erhel visited a high school in Rennes, where she gave a presentation with P. Hellier, in November.
- J. Erhel contributed to Inedit, No 69, about saltwater intrusion in aquifers.
- J.-R. de Dreuzy and J. Erhel wrote a paper in the journal La Recherche, about pollution in aquifers, May [38].
- A. Beaudoin presented a poster designed with J.-R. de Dreuzy and J. Erhel at the forum Ter@tec, Paris, July.

8.6. Conferences, scientific visits

- É. Canot: participation with contribution in the conference NUMCOOP'09, Yaounde, Cameroon, March.
- É. Canot: participation with contribution in the school on advanced numerical methods, Annaba, Algeria, December.
- J. Charrier: participation with contribution in the workshop on uncertainty and evolution systems organized by the GDR MASCOTNUM, Paris, France, May.
- J. Charrier: participation with contribution in the workshop on uncertainty organized by members of the INRIA team project TOSCA, Nancy, France, December.
- J. Erhel: participation with contribution in the conference NUMCOOP'09, Yaounde, Cameroon, March.
- J. Erhel: invited speaker at MAMERN'09, Pau, June.
- J. Erhel: invited in a mini-symposium at the SIAM conference on Geosciences, Leipzig, Germany, June.
- J. Erhel: participation with contribution in the Momas scientific days, Marseille, France, December.
- M. Muhieddine: participation with contribution in the conference NASCA'09, Agadir, Morocco, May.
- M. Muhieddine: participation with contribution in the conference MAMERN'09, Pau, France, June.
- M. Muhieddine: participation with contribution in the conference Virtual retrospect, Bordeaux, France, November.
- D. Nuentsa Wakam: participation with contribution in the conference NUMCOOP'09, Yaounde, Cameroon, March.

- D. Nuentsa Wakam: participation with contribution in Sparse Days 2009, Toulouse, France, May.
- D. Nuentsa Wakam: participation with contribution in PARCO'09, Lyon, France, September.
- D. Nuentsa Wakam: participation with contribution in the second workshop of the Joint Laboratory (INRIA-NCSA) for Petascale Computing, Urbana-Champaign, USA, December.
- B. Philippe: participation in the conference NUMCOOP'09, Yaounde, Cameroon, March.
- B. Philippe: invited speaker at the conference NASCA'09, Agadir, Morocco, May.
- B. Philippe: invited speaker at the LinkSceem Beirut Meeting, Beirut, Lebanon, June.
- B. Poirriez: invited in a mini-symposium at the SIAM conference on Geosciences, Leipzig, Germany, June.

8.7. International exchanges

8.7.1. Visits

- N. Soualem: scientific visit at University of Barcelona, Spain, one week, July.
- B. Philippe: scientific visit and collaboration with Ahmed Sameh [26], at the CS Department of Purdue University, USA , 3 months, September-October-November.
- B. Philippe: scientific visit and collaboration with L. Reichel, at Kent State University, USA, one week, October.

8.7.2. Visitors

The team has invited the following persons:

- M. El Fatini, Rabat, Morocco, two weeks in May.
- L. Reichel, Kent University, USA, two weeks in July.
- J-C. Ferreri, Argentina, one week in October.

9. Bibliography

Major publications by the team in recent years

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

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

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

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

[6] L. GRIGORI, X. LI. *A New Scheduling Algorithm for Parallel Sparse LU Factorization with Static Pivoting*, in "Proceedings of IEEE/ACM Supercomputing Conference", 2002.

[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", vol. 6, 2002, p. 161-194.

[8] D. MEZHER, B. PHILIPPE. *Parallel computation of pseudospectra of large sparse matrices*, in "Parallel Computing", vol. 28, n° 2, 2002, p. 199-221.

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

Year Publications

Doctoral Dissertations and Habilitation Theses

[10] M. MUHIEDDINE. *Simulation numérique des structures de combustion préhistoriques*, University of Rennes 1, October 2009, Ph. D. Thesis.

Articles in International Peer-Reviewed Journal

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

[12] M. MUHIEDDINE, É. CANOT, R. MARCH. *Various Approaches for Solving Problems in Heat Conduction with Phase Change*, in "International Journal on Finite Volumes", vol. 6, n° 1, 2009, 20 pages.

[13] N. NASSIF, N. MAKHOUL-KARAM, Y. SOUKIASSIAN. *Computation of blowing-up solutions for second-order differential equations using re-scaling techniques*, in "Journal of Computational and Applied Mathematics", vol. 227, n° 1, 2009, p. 185-195 (doi:10.1016/j.cam.2008.07.020) LB .

[14] C. DE DIEULEVEULT, J. ERHEL. *A global approach to reactive transport: application to the MoMas benchmark*, in "Computational Geosciences", 2009, http://dx.doi.org/10.1007/s10596-009-9163-9, published online first.

[15] C. DE DIEULEVEULT, J. ERHEL, M. KERN. *A global strategy for solving reactive transport equations*, in "Journal of Computational Physics", vol. 228, 2009, p. 6395-6410, http://www.sciencedirect.com/science/article/B6WHY-4WGDR6C-1/2/ada7965dcd60969843658 76b64411966.

Invited Conferences

[16] A. BEAUDOIN, J.-R. D. DREUZY, J. ERHEL. *Impact de la dispersion locale sur la macro dispersion*, in "workshop on uncertainty, Nancy", December 2009, invited contribution.

[17] J. CHARRIER. *Méthodes numériques pour le transport et la diffusion en milieu poreux aléatoire*, in "workshop on uncertainty and evolution systems, Paris", May 2009, invited contribution.

[18] J. CHARRIER. *Méthodes numériques pour le transport et la diffusion en milieu poreux aléatoire*, in "workshop on uncertainty, Nancy", December 2009, invited contribution.

[19] J. ERHEL, J. CARRAYROU, M. KERN, A. YOUNES. *Méthodes numériques pour le transport réactif*, in "Journées scientifiques du GNR Momas", 2009, invited contribution.

[20] J. ERHEL, C. DE DIEULEVEULT. *Analysis of Numerical Methods for Coupling Transport Andgeochemistry Equations*, in "SIAM Conference on mathematical and computational issues in the Geosciences, Leipzig, Germany", 2009, Invited talk in a mini-symposium.

[21] J. ERHEL, B. POIRRIEZ, G. PICHOT, J.-R. DE DREUZY. *How to compute flow in three-dimensional fracture networks*, in "Numerical methods and North-South Cooperation NUMCOOP'09, Yaounde, Cameroon", 2009, Invited contribution. International conference organized by J. Erhel and É. Canot and E. Kamgnia.

[22] D. NUENTSA-WAKAM, É. CANOT, J. ERHEL. *Comparison of some linear solvers on systems arising from fluid dynamics*, in "Numerical methods and North-South Cooperation NUMCOOP'09, Yaounde, Cameroon", 2009, Invited contribution. International conference organized by J. Erhel and É. Canot and E. Kamgnia.

[23] D. NUENTSA-WAKAM, É. CANOT, J. ERHEL. *Mixing Direct and Iterative methods for the solution of large linear systems*, in "CERFACS Sparse days, Toulouse, France", May 2009, invited contribution.

[24] D. NUENTSA-WAKAM, É. CANOT, J. ERHEL. *Two-level parallelism in GMRES with multiplicative Schwarz preconditioner*, in "Second Workshop of the Joint Laboratory INRIA/NCSA for Petascale Computing, Urbana-Champaign, USA", 2009, Invited contribution.

[25] B. PHILIPPE. *A Parallel Solver for Large Linear Systems*, in "LinkSCEEM", June 2009, invited plenary talk.

[26] B. PHILIPPE, A. SAMEH. *The Parallel Lanczos method for computing many eigenvalues of large symmetric matrices*, in "Numerical Analysis and Scientific Computing with Applications (NASCA)", May 2009, invited plenary talk US .

[27] B. POIRRIEZ, J. ERHEL, J.-R. DE DREUZY. *Flow simulation in 3D Discrete Fracture Networks*, in "SIAM Conference on mathematical and computational issues in the Geosciences, Leipzig, Germany", 2009, organization of a mini-symposium by J. Roberts and J. Erhel.

[28] C. DE DIEULEVEULT, J. ERHEL. *Numerical Results with a Global Method for 2D Reactive Transport Problems*, in "SIAM Conference on mathematical and computational issues in the Geosciences, Leipzig, Germany", 2009, Invited talk in a mini-symposium.

International Peer-Reviewed Conference/Proceedings

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