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INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Project-Team SAGE

Simulations and Algorithms on Grids for Environmental Applications

Rennes - Bretagne-Atlantique

THEME NUM

Table of contents

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2. Overall Objectives

2.1. Main research areas

Keywords: *accuracy*, *eigenproblems*, *environment*, *geosciences*, *grid computing*, *high-performance computing*, *least-squares problems*, *linear algebra*, *linear systems*, *numerical computing*, *parallel computing*, *scientific computing*, *sparse matrices*.

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

Keywords: *Arnoldi*, *Davidson*, *Krylov subspace*, *LU factorization*, *Lanczos*, *Newton method*, *QR factorization*, *eigenvalues*, *iterative method*, *preconditioning*, *pseudo-spectrum*, *singular values*, *sparse matrices*.

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 [52].

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 [59], [56]. 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 [50].

Multigrid methods can be used as such or as a preconditioner. They can be either geometric or algebraic [56].

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 [56]. 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 [54], [49]. 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 [58], [51], [55]. 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 [60]. 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 [53] and Trefethen [62]. 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 great 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. Recently, the following features have been added or improved:

- ODE and DAE systems can be solved via the SLATEC package; moreover, sparse Jacobian matrices are supported when using the BDF option for ODE or DAE systems;
- sparse QR decomposition is done via the SPQR part of the SuiteSparse-3.2.0 package.

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 1.9.9 (16 october 2008). 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 great 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 collaboration with Carmen GEORGESCU at UPB (University Polytechnica of Bucarest) in Romania.

5.4. H2OLAB: numerical simulations in hydrogeology

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

Website: http://h2olab.inria.fr

This software-platform 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.

Software H2OLab (previously Hydrolab) aims at modeling flow and transport of solute in highly heterogeneous porous or fractured media [30],[38]. 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, Hydrolab 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 registered for the Gforge of Inria; four components are registered for the APP: PARADIS, MP_FRAC, GW_NUM, GW_UTIL.

6. New Results

6.1. Numerical algorithms

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. Unfortunately this second part relies mostly on BLAS1 routines which are known to be unefficient on modern processors. We have introduced BLAS3 operations in this rank-revealing part of the algorithm. We now test the resulting code.

6.1.2. Autoadaptative limited memory Broyden method

Participants: Bernard Philippe, Mohammed Ziani.

This work is done in collaboration with R. Aboulaich, from EMI, Marocco, and with Frédéric Guyomarc'h, from Dart team, at Inria Lille, in the context of the Sarima project, 8.3.2.

Limited memory methods are powerful methods to solve non linear systems. But the difficulty in these methods is to find the right size allocated to the solver for the system. Of course this parameter changes for each system and there is no rule to set it. We propose a new limited memory method that we call autoadaptative because it has the nice ability to find an acceptable parameter for the system. We have then tuned this method so that it is now efficient to solve standard non linear test functions. The most important improvement is a self-adapting threshold to limit the memory during iterations, so that the memory is no more waisted when convergence is fast. We also proved that this algorithm has a super linear convergence under classical assumptions [20]. We have used the new method on a pile problem [13] and on a problem of image processing [29]. The method is presented in the Ph-D thesis which has been defended by M. Ziani in October (coadvised thesis) [11].

6.2. High performance computing

6.2.1. Parallel Schwarz preconditioner for GMRES

Participants: Guy Antoine Atenekeng Kahou, Bernard Philippe.

That work is done in cooperation with E. Kamgnia, from the University of Yaoundé, Cameroon, in the context of the Sarima project, 8.3.2.

We have pursued the work on a parallel version of the GMRES method preconditioned by Multiplicative Schwarz. The scheme consists in building a priori a basis of the Krylov subspace and then in orthogonalizing it. The basis construction involves a double recursion (on the domains of the operator and on the successive vectors of the basis). It is parallelized by pipelining the iterations of the nested loop. It is based on a graph partitioning approach developed in the team [14],[22].

The method has now been improved and tested on a large bunch of matrices [25] and is presented in the thesis defended in December by G.-A. Atenekeng-Kahou(coadvised thesis) [10].

6.2.2. 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, in the context of the Sarima project, 8.3.2.

A rescaling method has been initially designed in [57] for solving evolution problems whose solution was explosive in finite time, in a very efficient way. Its basic idea is to generate, through a change of variables, a sequence of time slices such that the time variable and the solution are restored to zero at the beginning of each slice, and the rescaled solution is controlled by a uniform criterion for ending slices.

During the year 2008, this rescaling technique has been adapted to oscillatory problem, in [17], using a convenient end-of-slice condition allowing having uniform and asymptotic similarity of the rescaled models. More theoretical bases are being devised in order to reach a better control of the rescaled solution.

In non-convergent oscillatory problems, as in some cases of the membrane problem (explosive in infinite time [61]) and in the computation of a satellite trajectory (studied in [2] and [5] using a predictor-corrector multiple shooting scheme based on Newton-type iterations), the ratios are not stabilizing. Therefore, and since the ratios seem strongly related, some statistical techniques are being devised in order to modelize the observed relation between the ratios that are obtained on first slices and predict the following initial values necessary for the starting of the prediction-correction scheme [42].

Also, parallel implementations are being done on clusters of 4 and 8 processors, seeking an optimization of the parallel computations efficiency [43].

6.2.3. Comparison of parallel sparse linear solvers

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

This work is done in the context of the Cinemas2 and the Libraero contracts, 8.1.4 and 8.1.5.

In this work, we are interested in efficient parallel methods (either direct or iterative) for solving large sparse unsymmetric linear systems arising from fluid dynamics. We have studied two parallel direct solvers based on supernodal technique and multifrontal approach. We have found that static pivoting used in the supernodal approach, namely SUPERLU_DIST, does not achieve good accuracy in the final solution for some matrices. Although the multifrontal approach gives best results, it is not suitable for problems under study due to high memory requirements. We have continued our investigation with parallel preconditioners for GMRES. In this way, parallel incomplete LU and parallel approximate inverse preconditioners give valuable results; so, we plan to use GMRES with deflation to achieve better convergence.

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

Participants: Étienne Bresciani, Jocelyne Erhel.

This work is done in the context of the Micas contract, 8.1.3.

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. In our models, we generate the rock fractures or the permeability field randomly from known probabilistic laws. Because a simulation is just one possible realization of the phenomenon, the result is not representative of the reality ; we have to quantify this uncertainty. 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. These parallel deterministic simulations are operational in our software and we investigate scalability issues. The intermediate level is the Uncertainty Quantification non intrusive method, currently Monte-Carlo. We have developed an object-oriented Monte-Carlo module, based on virtual and generic classes. Our objective is to design a facility for running this run of Monte-Carlo by choosing either a parallel approach with MPI or a distributed approach with a grid middleware. We use a specific random number generator in order to guarantee independent simulations. 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 [40].

6.3. Numerical models and simulations in geophysics

6.3.1. 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 Sarima project, 8.3.2.

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). During that year, the Matlab chain of treatments developed in 2006, has been tested and improved.

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 now written: it is expressed as a non-linear least squares problems 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 have considered a first approach based on Slepian basis [28].

6.3.2. Heat transfer in soil and prehistoric fires

Participants: Édouard Canot, Mohamad Muhieddine.

Mohamad Muhhiedine 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.

A first numerical model uses the finite volume method and takes into account the phase change via accumulation of latent heat. The numerical solutions are obtained by using explicit schemes. To reduce physical temperature fluctuations, a classical way is to refine the mesh locally around the phase-change front. We have designed an algorithm to follow the moving front, based on recursive refinement of a fixed, uniform basic cells mesh, via an insert/delete nodes procedure. This work has been presented at the FVCA5 conference ([34]).

In order to do numerical simulation in 2D configurations, a second numerical model has been designed. It is based on a Finite Volume Method and the Apparent Capacity Method; we have successfully included coupling with the water-steam gas flow inside the soil. First applied to a 1D test-problem (fig. 1), the method of lines leads to a DAE system, which is solved via a BDF automatic solver. This second work has been presented to the ECCOMAS Conference ([33]).

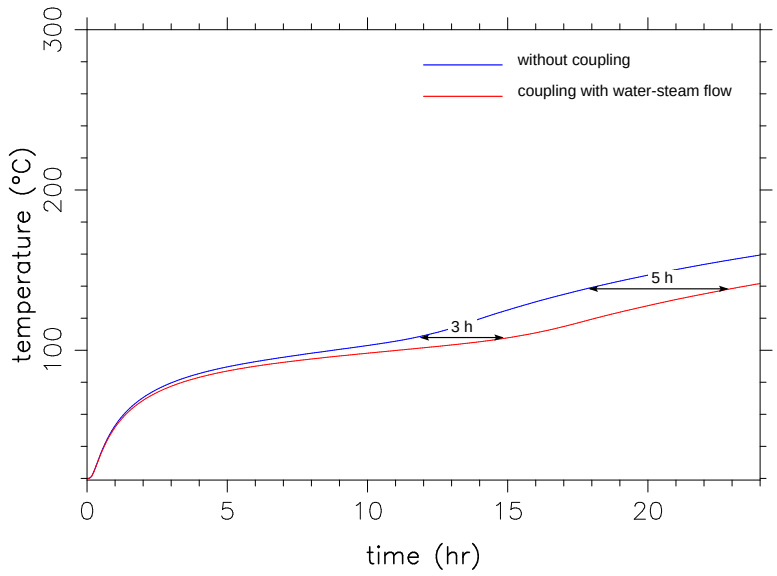

Figure 1. Effects of coupling heat diffusion with water steam flow. Curves represent temperature histories at $5\ cm$ *in the soil. 1D test-problem.*

Recently, 2D and 3D-axisymmetric configurations of the same physical problem have been solved. 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 (see fig. 2). All these modifications are done inside MUESLI, giving an easy-to-use programming interface for the user.

Application to archeology was presented in a panel on prehistoric fires [41].

6.3.3. Reactive transport

Participants: Caroline de Dieuleveult, Jocelyne Erhel.

This work is done in the context of the MOMAS GdR (8.1.2) and in the context of the Andra contract (8.1.1).

Reactive transport models are complex nonlinear PDEs, 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 PDAE (Partial Differential Algebraic Equations) framework, 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. The code is based on a method of lines in combination with a global approach in order to solve

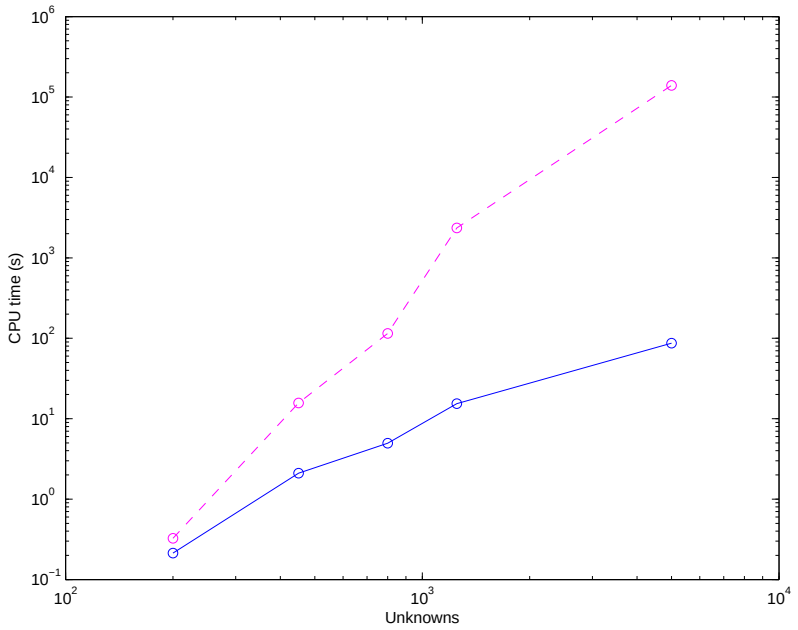

Figure 2. CPU time versus the number of unknowns in the simulation with sparse matrix (blue curve) and dense matrix (dashed magenta curve) structures. Used grids are: 10×10, 15×15, 20×20, 25×25 *et* 50×50.

the Partial Differential Algebraic Equations involving transport and chemistry. In the current version, spatial discretization is achieved by interfacing software MT3DMS, using a classical finite difference method, upwind for advection, centered for dispersion. The resulting differential algebraic equations (DAE) are solved by an external, robust and efficient DAE solver. The time scheme is an elaborated multistep implicit scheme: a Backward Differentiation Formula (BDF) with variable order and variable timestep. BDF is used in connection with a modified Newton method in order to deal with the non linearity; the sparse linear systems are solved by a direct method, a multifrontal gaussian elimination with pivoting. Symbolic factorization and renumbering for fill-in reduction are done once by using the matrix structure. Thanks to the connection between BDF and Newton, the jacobian matrix is updated only when necessary and the timestep is controlled in order to ensure both convergence of Newton and accuracy of the scheme. Since chemistry is linearized here, the main cost is to factorize the jacobian matrix and to solve the triangular systems. For large computational domains, it is thus 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 validate our approach and to show its efficiency and robustness. We could compare our results to analytical solutions with some test cases in 1D and 2D. We have also pursued our work on the benchmark proposed by Momas. We have extended the results obtained on the 1D domain and got new results on the 2D domain.

Publications related to this work are [36], [45], [32], [24]. The work is presented in the thesis defended in December by C. de Dieuleveult [12].

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

Participant: Jocelyne Erhel.

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 (8.1.3).

We have pursued our work for simulating flow and solute transport in 2D domains, where the permeability field is highly heterogeneous [21]. We have extended the method to 3D domains and developed a fully parallel package, called Paradis, which is embedded in the scientific platform H2Olab, described in section 5.4. The challenge is to design efficient parallel and grid algorithms in order to increase the computational size by several orders of magnitude.

6.3.5. 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 (8.1.3).

We have pursued our work for simulating flow in a 3D network of interconnected plane fractures. We have developed a package, which is embedded in the scientific platform H2Olab, described in section 5.4). We have run Monte-Carlo simulations (see section 6.3.6), for various parameters, in order to validate thoroughly our algorithms. The challenge is to design efficient parallel and grid algorithms in order to increase the computational size by several orders of magnitude. We also aim at developing a new method for non conforming discrete fractures. The objective is to mesh fractures independently and to use Mortar-like elements at the intersections. We have done several experiments with some networks [44]. The challenge is to get a generic method for any type of network.

6.3.6. Uncertainty Quantification methods

Participants: Julia Charrier, Jocelyne Erhel.

This work is done in collaboration with A. Debussche and E. Faou, from ENS-Cachan-Rennes and Ipso INRIA team. It is done in the context of the Micas contract (8.1.3).

In our applications described above, we use stochastic models and rely on uncertainty quantification methods. We use Monte-Carlo methods (see section 6.2.4) and study other UQ methods based on stochastic finite element methods. We have analyzed their application to flow computations in heterogeneous porous media. This was the subject of the master's thesis of Julia Charrier. We are now investigating error estimation of our method applied to flow and transport in heterogeneous porous media.

6.3.7. Database and web portal

Participants: Étienne Bresciani, Jocelyne Erhel, Nadir Soualem.

This work is done in the context of the Micas contract (8.1.3).

Because we are doing a huge number of simulations, we have a huge amount of results. In addition, some simulations are very costly in terms of computational time : several hours on a cluster. Therefore, there is a need for an efficient storage or these results. We have designed and implemented a generic MySQL relational database, in which we can store simulations (parameters, results and metadata) for all our applications. The web portal H2OLab is designed to interface this database, to access documentation, to generate parameter files and to launch remote computing. See section 5.4.

7. Contracts and Grants with Industry

7.1. Industrial contracts

No industrial contract this year.

8. Other Grants and Activities

8.1. National grants

8.1.1. ANDRA contract

Participants: Caroline de Dieuleveult, Jocelyne Erhel.

Contract with Andra
time: three years from October 2005.

This contract is related to C. de Dieuleveult's PhD thesis. The subject is reactive transport, with application to nuclear waste disposal [48].

See sections 6.3.3, 4.2.

8.1.2. GdR MOMAS - Numerical models for nuclear waste disposal

Participants: Caroline de Dieuleveult, 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 6.3.3, 4.2.

8.1.3. MICAS contract

Participants: Édouard Canot, 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 6.2.4, 6.3.4, 6.3.5, 6.3.6, 6.3.7, 5.4, 4.2.

8.1.4. CINEMAS2 contract

Participants: Guy Atenekeng Kahou, Jocelyne Erhel, Désiré Nuentsa Wakam.

Contract with Ecole Centrale de Lyon
Time: three years from May 2006 (actually started in 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 section 6.2.3.

8.1.5. LIBRAERO contract

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

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 6.2.3.

8.2. European Grants

8.2.1. 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 concerns 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.

8.2.2. PECO-NEI 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 the algorithms target matrices arising in geodesy applications. Funding is provided for visits and a student in co-direction between INRIA Futurs and Politechnica of Romania.

8.3. International Grants

8.3.1. INRIA Euro-Mediterranean Program 3+3

Participants: Édouard Canot, Caroline de Dieuleveult, Bernard Philippe, Jocelyne Erhel, Mohamed Ziani.

Title: Numerical simulations in hydrogeology
This 3-year project includes six partners from Rabat (Morroco), Annaba (Algeria), Tunis (Tunisia), Naples (Italy), Barcelona (Spain) and Rennes. R. Aboulaïch (LERMA, Rabat) chairs the activity with B. Philippe.
Webpage: http://www.emi.ac.ma/hydro3p3/hydro1.html

The project deals with the numerical simulation of the groundwater flows and the transport of pollutants. The goal consists in organizing a network of teams which gathers expertise for the whole spectrum of the domain from the physical models, the mathematical methods, the numerical algorithms, the codes. The activity will be organized through a list of cooperative actions which will be defined during the first year. The network will be a training tool for each involved team. The success of the approach should be materialized after three years, by the availability of some common codes, by publications and by the ability to access and use computing grids.

In 2008, a workshop dedicated to water treatment and hydrology was co-organised with another project of the same EuroMediterranee programme. The workshop was set in the core of a summer school in Tlemcen. See http://www.cimpa-icpam.org/Anglais/2008Prog/Algeria08.html.

A follow-up of the project has been accepted at the last call for tenders of the same programme. It will start in 2009.

8.3.2. SARIMA - Support to Research Activities in Africa

Participants: Guy Antoine Atenekeng Kahou, Amine Abdelmoula, Jocelyne Erhel, Noha Makhoul, Bernard Philippe, Mohamed Ziani.

SARIMA project Inria/Ministry of Foreign Affairs
Support to Research Activities in Mathematics and Computer Science in Africa
Partner : CIMPA (International Center for Pure and Applied Mathematics)
Duration : 2004-2008,
Website : http://www.sarima.org/.

The project SARIMA is managed by the ministry of Foreign Affairs. It involves INRIA and CIMPA as financial operators.

The aim of the project is to reinforce the cooperation between French research teams and African and Middle-East ones in mathematics and computer science. The strategy consists in reinforcing existing research teams so that they become true poles of excellence for their topic and their region. A network based organization should strengthen the individual situation of the groups. From the CARI experience (African Conference on Research in Computer Science) and the CIMPA's experience (International Center for Pure and Applied Mathematics), the initial network includes seven teams (five teams in French speaking sub-Saharan countries, two teams acting for the whole Maghreba, one in Tunisia in Applied maths and one in Algeria in Computer Science, and one team in Lebanon).

The activity of the network is managed by the SARIMA GIS (Groupe d'Intérêt Scientifique). In this project, INRIA is responsible for all the visits of African researchers to research groups in France. In 2006, more than 120 researchers (PhD students and researchers) were funded to visit France for one to six months long visits.

B. Philippe is the coordinator of the project for INRIA and the president of the Goupement d'Intérêt Scientifique which manages the project.

Four Ph-D students are entirely or partially supported by the project :

Amine Abdelmoula : co-advised by Maher Moakher (ENIT, Tunisia) and B. Philippe. Signed agreement between the universities of Tunis El Manar and Rennes 1 (see section 6.3.1).

Guy-Antoine Atenekeng Kahou : co-advised by Emmanuel Kamgnia (University of Yaounde I, Cameroon) and B. Philippe. Signed agreement between the universities of Yaounde I and Rennes 1 (see section 6.2.1). The thesis was defended in December 2008.

Mohamed Ziani : co-advised by Rajae Aboulaïch (LERMA, Morroco) and F. Guyomarc'h (under B. Philippe's signature) (see sections 6.1.2 and 8.3.1). The thesis was defended in October 2008.

Noha Makhoul : co-advised by Nabil Nassif (American University of Beirut, Lebanon) and J. Erhel (see section 6.2.2).

E. Kamgnia visited the Sage team in the context of Sarima, see 9.7 and 6.2.1.

9. Dissemination

9.1. Program committees, organizing committees, Editorial Boards

- J. Erhel organized with L. Giraud a mini-symposium on "Preconditioning techniques in domain decomposition", at IMACS conference, Lille, March.
- B. Philippe was in charge of the track "'Scientific Computing and Parallelism"' in the programme committee of the conference CARI'08.
- B. Philippe was co-organizer of a summer school on hydrology and water treatment in Algeria (Tlemcen, May).
- B. Philippe was co-organizer of a workshop on free scientific software in Algeria (Setif, October).
- 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.

9.2. 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 organized the evaluation seminar of INRIA theme NumB, Paris, March.
- 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 commission de spécialistes, section 27, of the University of Rennes 1.
- In the International Affairs Department of INRIA, B. Philippe is in charge of the cooperating programmes with scientific teams in Africa and Middle-East countries.
- B. Philippe is the INRIA coordinator for the SARIMA project (see 8.3.2).
- B. Philippe is the corresponding person for the agreement between the University of Rennes 1, The University of Reims, the Lebanese University (Lebanon) and AUF (Agence Universitaire Francophone) which supports a Master.

9.3. Teaching and internship supervision

- A. Abdelmoula was hired as teaching assistant (permanent position) in computer science at the University of Tunis, Tunisia.
- G. Atenekeng-Kahou is teaching assistant (permanent position) at the University of Yaoundé, Cameroon.
- 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 gave a lecture about "Floating-Point Arithmetic and Roundoff errors" during the CIMPA-INRIA-UNESCO school in Tlemcen, Algeria; 16 may 2008.
- É. Canot, C. de Dieuleveult, 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
- B. Philippe taught a one-week course in Beirut for the common master. The topics was "'Iterative linear solvers for large systems"'.

  Lecture notes on http://www.irisa.fr/sage/jocelyne
- B. Philippe gave a 3 hours tutorial on eigenvalue solvers at the Collège Polytechnique in Paris (March) during the session "Méthodes performantes en algèbre linéaire pour la résolution de systèmes linéaires et le calcul de valeurs propres".
- Jessy Haikal has completed a two months summer internship in team Sage, in collaboration with American University of Beirut, Lebanon, under supervision of J. Erhel, N. Makhoul and N. Nassif.

9.4. Participation in training

- C. de Dieuleveult : participation in training on professional integration, MATISSE, February.
- D. Nuentsa-Wakam: participation in training on scientific writing and on public talks, Inria-Rennes, October.
- B. Poirriez: participation in training for teaching assistants.

9.5. Seminars and dissemination for the general public

- É. Bresciani and J. Erhel contributed to the one-day seminar with Veolia, at Caren, Rennes, January.
- M. Muhieddine contributed to the one-day seminar of Ph-D students, at Caren, Rennes, June.
- M. Muhieddine participated in an archeological campaign at the site of Pincevent, Montereau, France; one week in july 2008.
- J. Erhel participated in the meeting INRIA-Andra, Paris, september.
- J. Erhel participated in the two meetings INRIA-EDF, Paris, October and November.
- J. Erhel contributed to the one-day seminar of Momas group on numerical methods, Paris, November.
- J. Erhel participated in the operation "à la découverte de la recherche", organized in the area of Rennes. She visited three high schools in Rennes and Vitré 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 participated in the operation "100 femmes, 100 métiers", organized in Rennes. She answered to questions of the general public about computer science and applied mathematics.
- C. de Dieuleveult and J. Erhel contributed to Inedit, No 65, July, special release about Computer science for environment.

9.6. Conferences, scientific visits

- M. Muhieddine: participation with contribution in a round-table organized at CEPAM about archeology, Valbonne, May.
- É. Canot and M. Muhieddine: participation with contribution in FVCA 2008, Aussois, June.
- É. Canot and M. Muhieddine: participation with contribution in WCCM8-ECCOMAS 2008, Venice, July.
- É. Canot: presentation of the H2OLAB software platform during the final colloquium Hydro 3+3 in Tlemcen, Algeria; 10-13 may 2008.
- C. de Dieuleveult: participation with contribution in the international workshop on modelling reactive transport in porous media, Strasbourg, January.
- C. de Dieuleveult: participation with contribution in WCCM8-ECCOMAS 2008, Venice,July.
- J. Erhel: invited in a mini-symposium at the first conference of SM2A, Rabat, Marocco, February.
- J. Erhel: participation with contribution in ParCFD conference, Lyon, May.
- B. Philippe: CARI'08, Rabat, October.
- B. Philippe: invited speaker at IMACS'08, Lille, March.
- B. Philippe: invited speaker at the Parallel Matrix Algorithms and Application (PMAA'08), Neuchatel, June 20-22.
- B. Philippe: participation as panelist in a round-table on "Mathematics and Development", organized at the European Congress of Mathematics, Amsterdam, July 17.

9.7. International exchanges

The team has invited the following persons:

- L. Reichel, Kent University, USA, one month in July-August.
- G. Oksa, Slovakian Academy of Sciences, Bratislava, Slovakia, two weeks in August.
- R. Ramlau, University of Linz, Austria, one week in August.
- E. Kamgnia, University of Yaounde, Cameroon, two months in September-October.

10. Bibliography

Major publications by the team in recent years

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

[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^{o} 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^{o} 5, 2000, p. 1909-1926.

Year Publications

Doctoral Dissertations and Habilitation Theses

[10] G.-A. ATENEKENG-KAHOU. *Parallélisation de GMRES préconditionné par une itération de Schwarz multiplicatif*, Ph. D. Thesis, University of Rennes 1 and University of Yaounde I, December 2008.

[11] M. ZIANI. *Accélération de la convergence des méthodes de type Newton pour la résolution des systèmes non-linéaires*, Ph. D. Thesis, Univ. Rennes 1 and Univ. Mohamed V Rabat-Agdal, October 2008.

[12] C. DE DIEULEVEULT. *An efficient and robust global method for reactive transport*, Ph. D. Thesis, University of Rennes 1, December 2008.

Articles in International Peer-Reviewed Journal

[13] R. ABOULAICH, F. GUYOMARC'H, M. ZIANI. *Numerical solution of a Pile problem*, in "International Journal of Appl. Math.", to appear.

[14] G.-A. ATENEKENG-KAHOU, L. GRIGORI, M. SOSONKINA. *A Partitioning Algorithm for Block-Diagonal Matrices with Overlap*, in "Parallel Computing", vol. 34, n^{o} 6-8, 2008, p. 332-344.

[15] I. T. DIMOV, B. PHILIPPE, A. KARAIVANOVA, C. WEIHRAUCH. *Robustness and applicability of Markov chain Monte Carlo algorithms for eigenvalues problems*, in "Applied Mathematical Modelling", vol. 32, n^{o} 8, 2008, p. 1511–1529.

[16] L. GRIGORI, J. R. GILBERT, M. COSNARD. *Symbolic and Exact Structure Prediction for Sparse Gaussian Elimination with Partial Pivoting*, in "SIAM Journal on Matrix Analysis and its Applications", vol. 30, n^{o} 4, 2008, 15201545.

[17] 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", 2008.

[18] S. ZEIN, É. CANOT, J. ERHEL, N. NASSIF. *Determination and Sensitivity Analysis of the Seismic Velocity of a Shallow Layer from Refraction Traveltimes Measures*, in "International Journal of Multiphysics", to appear.

[19] S. ZEIN, É. CANOT, J. ERHEL, N. NASSIF. *Determination of the Mechanical Properties of a Solid Elastic Medium from a Seismic Wave Propagation Using Two Statistical Estimators*, in "Mathematics and Mechanics of Solids", vol. 13, 2008, p. 388 - 407.

[20] M. ZIANI, F. GUYOMARC'H. *An autoadaptative limited memory Broydens method to solve systems of nonlinear equations*, in "Appl. Math. Comput", vol. 205, 2008, p. 202-211.

[21] J.-R. DE DREUZY, A. BEAUDOIN, J. ERHEL. *Reply to comment by A. Fiori et al. on "Asymptotic dispersion in 2D heterogeneous porous media determined by parallel numerical simulations"*, in "Water Resources Research", vol. 44, W06604, 2008.

Invited Conferences

[22] G.-A. ATENEKENG-KAHOU, E. KAMGNIA, B. PHILIPPE. *A fully automatic parallel GMRES solver preconditionned by a Multiplicative Schwarz iteration*, in "9th IMACS International Symposium on Iterative Methods in Scientific Computing, Lille", invited in a mini-symposium, March 2008.

[23] É. CANOT. *Roundoff Errors and Floating-Point Arithmetic*, in "CIMPA-INRIA-UNESCO-ALGERIA School: Mathematical models for water flows and water refining, Tlemcen, Algeria", invited lecture at the school, May 2008.

[24] J. ERHEL, C. DE DIEULEVEULT. *A global strategy for solving reactive transport equations*, in "First conference of SM2A. Porous media and scientific computing, Marocco", invited in a mini-symposium, February 2008.

[25] B. PHILIPPE. *A parallel GMRES method preconditioned by a Multiplicative Schwarz iteration*, in "5th International Workshop on Parallel Matrix Algorithms and Applications (PMAA'08), Neuchatel", invited plenary talk, June 2008.

[26] B. PHILIPPE. *Numerical accuracy in scientific software*, in "Workshop on free scientific software, Setif", organizer, October 2008.

[27] B. PHILIPPE, Y. SAAD, A. SAMEH. *Domain Decomposition and Symmetric Eigenvalue problems*, in "9th IMACS International Symposium on Iterative Methods in Scientific Computing, Lille", invited plenary talk, March 2008.

International Peer-Reviewed Conference/Proceedings

[28] A. ABDELMOULA, M. MOAKHER, B. PHILIPPE. *Localized spectral analysis for an inverse problem in geodesy*, in "CARI'08", 2008, p. 369-376.

[29] R. ABOULAICH, F. GUYOMARC'H, M. ZIANI. *Nonlinear solvers in image processing*, in "CARI 08", 2008, p. 273-279.

[30] J. ERHEL, J.-R. DE DREUZY, A. BEAUDOIN, E. BRESCIANI, D. TROMEUR-DERVOUT. *A parallel scientific software for heterogeneous hydrogeology*, in "PARCFD'2007 conference proceedings", I. H. TUNCER, U. GULCAT, D. R. EMERSON, K. MATSUNO (editors), to appear, Springer.

[31] D. GUIBERT, D. TROMEUR-DERVOUT. *A Schur Complement Method for DAE/ODE Systems in Multi-Domain Mechanical Design*, in "Domain Decomposition Methods in Science and Engineering XVII", U. LANGER, M. DISCACCIATI, D. KEYES, O. WIDLUND, W. ZULEHNER (editors), Lecture Notes in Computational Science and Engineering, vol. 60, 2008, p. 535-541.

[32] N. HARIGA, J. ERHEL. *Different misfit functionals for recovering data in ElectroCardioGraphy problems.*, in "proceedings of IACM-ECCOMAS 2008 Congress, Venice, Italy", B. A. SCHREFLER, U. PEREGO (editors), July 2008, 2.

[33] M. MUHIEDDINE, É. CANOT, R. MARCH. *Numerical solution of a 1-D time-dependent phase change problem*, in "Proc. of the Fifth ECCOMAS, Venice, Italy", B. A. SCHREFLER, U. PEREGO (editors), July 2008, 2.

[34] M. MUHIEDDINE, É. CANOT. *Recursive mesh refinement for vertex centered FVM applied to a 1-D phase-change problem*, in "5th International Symposium on Finite Volumes for Complex Applications, Aussois, France, June 9-13", R. EYMARD, J.-M. HÉRARD (editors), Wiley, June 2008, p. 601–608.

[35] J. TAILLARD, F. GUYOMARC'H, J.-L. DEKEYSER. *A Graphical Framework For High Performance Computing using An MDE Approach*, in "Proceedings of 16th Euromicro Conference on Parallel Distributed and network-based Processing (PDP'2008), Toulouse, France", IEEE computer society, February 2008, p. 165 - 173.

[36] C. DE DIEULEVEULT, J. ERHEL. *Global method for coupling reactive transport*, in "Proceedings of IACM-ECCOMAS 2008 Congress, Venice, Italy", B. A. SCHREFLER, U. PEREGO (editors), July 2008, 2.

Workshops without Proceedings

[37] A. BEAUDOIN, J.-R. DE DREUZY, J. ERHEL. *Dispersion dans des milieux hétérogènes*, in "XXIV Rencontres Universitaires de Génie Civil AUGC, Nancy, France", june 2008.

[38] É. CANOT. *La plate-forme Hydrolab*, in "Workshop Hydro 3+3, Tlemcen, Algeria", contribution to workshop, May 2008.

[39] É. CANOT, S. ZEIN, J. ERHEL, N. NASSIF. *Application des méthodes d'optimisation stochastiques à deux problèmes d'inversion sismique*, in "International marine science and technology week (Sea Tech): Appraisal of the Undersea Acoustics and Geophysics Elements of the Regional Strategic Development Plan, Brest", contribution to CPER "Acoustique et Sismique sous-marine" final meeting, See Tech week, october 2008.

[40] J. ERHEL, J.-R. DE DREUZY, E. BRESCIANI. *Multi-parametric intensive stochastic simulations for hydrogeology on a computational grid*, in "Parallel CFD conference, Lyon", contribution, May 2008.

[41] R. MARCH, A. LUQUIN, D. JOLY, G. DUMARCAY, Q. DONG, M. MUHIEDDINE. *Processus de formation et transformation des structures de combustion archéologiques: regards sur la complexité*, in "Table ronde Taphonomy of organic burned residues and combustion structures in archaeological context, Valbonne, Cépam (UMR 6130)", contribution, May 2008.

[42] N. NASSIF, J. ERHEL, N. MAKHOUL-KARAM. *Ratio-Based Parallel Time Integration (RaPTI) for Satellite Trajectories*, in "SIAM conference on Parallel Processing for Scientific Computing, Atlanta, USA", contribution, March 2008.

[43] N. NASSIF, N. MAKHOUL-KARAM, Y. SOUKIASSIAN. *Ratio based time parallel integration (RaPTI) for a second order differential equation*, in "CONFERENCE IN NUMERICAL ANALYSIS (NumAn 2008); RECENT APPROACHES TO NUMERICAL ANALYSIS: THEORY, METHODS AND APPLICATIONS, Kalamata, Greece", contribution, September 2008.

[44] G. PICHOT, J. ERHEL, J.-R. DE DREUZY. *A Mixed-Hybrid Mortar Method for Domain Decomposition with non matching grids applied to solve flow in Discrete Fracture Networks*, in "Scaling Up and Modeling for Transport and Flow in Porous Media, Dubrovnik, Croatia", contribution, october 2008.

[45] C. DE DIEULEVEULT, J. ERHEL. *A global approach for coupling chemistry and transport*, in "International Workshop on Modelling reactive transport in porous media, Strasbourg", contribution, January 2008.

[46] J.-R. DE DREUZY, A. BEAUDOIN, J. ERHEL. *Asymptotic dispersion in 2D heterogeneous porous media*, in "EGU General Assembly", vol. 10, n^{o} EGU2008-A-00000, 2008.

Scientific Books (or Scientific Book chapters)

[47] B. PHILIPPE, Y. SAAD. *Calcul des valeurs propres*, in "Méthodes numériques de base - Algèbre numérique", C. BREZINSKI (editor), vol. AF1224, Editions-TI (Techniques de l'Ingénieur), 2008, 24 pages.

Research Reports

[48] C. DE DIEULEVEULT, J. ERHEL. *Résultats numériques avec la méthode globale appliquée à des problèmes de transport réactif*, Rapport de contrat Andra, INRIA, March 2008.

References in notes

[49] A. BJÖRCK. *Numerical methods for least-squares problems*, SIAM, 1996.

[50] A. BRUASET. *A survey of preconditioned iterative methods*, Pitman Research Notes in Mathematics Series, Longman Scientific and Technical, 1995.

[51] J. E. DENNIS, R. B. SCHNABEL. *Numerical Methods for Unconstrained Optimization and Nonlinear Equations*, Prentice-Hall series in Computational Mathematics, 1983.

[52] I. DUFF, A. ERISMAN, J. REID. *Direct Methods for Sparse Matrices*, Oxford Science Publications, 1986.

[53] S. K. GODUNOV, O. P. KIRILJUK, V. I. KOSTIN. *Spectral portrait of matrices and criteria of spectrum dichotomy*, in "Computer arithmetic and enclosure methods", J. HERZBERGER, L. ATHANASSOVA (editors), 1991.

[54] P. C. HANSEN. *Rank-deficient and discrete ill-posed problems*, SIAM, 1997.

[55] C. T. KELLEY. *Solving nonlinear equations with Newton's method*, Fundamentals of Algorithms, Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2003.

[56] G. MEURANT. *Computer solution of large linear systems*, North Holland, Amsterdam, 1999.

[57] N. NASSIF, D. FAYAD, M. CORTAS. *Sliced-Time Computations with Re-scaling for Blowing-Up Solutions to Initial Value Differential Equations*, in "ICCS 2005", Lecture Notes on Computational Sciences, vol. 3514, Springer-Verlag, 2005, p. 58-65.

[58] J. ORTEGA, W. RHEINBOLDT. *Iterative Solution of Nonlinear Equations in Several Variables*, Computer science and applied mathematics, Academic Press, 1970.

[59] Y. SAAD. *Iterative methods for sparse linear systems*, PWS publishing, 1995.

[60] G. L. G. SLEIJPEN, H. A. VAN DER VORST. *A Jacobi-Davidson iteration method for linear eigenvalue problems*, in "SIAM J. Matrix Anal. Appl.", vol. 17, 1996.

[61] P. SOUPLET, M. JAZAR, M. BALABANE. *Oscillatory blow-up in nonlinear second order ode's: The critical case*, in "Discrete And Continuous dynamical systems", vol. 9, n^{o} 3, 2003.

[62] L. N. TREFETHEN. *Pseudospectra of matrices*, in "Numerical Analysis", D. F. GRIFFITHS, G. A. WATSON (editors), Longman Scientific and Technical, 1991.