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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*

THEME NUM

Activity Report

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# Table of contents

# 1. Team

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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 large sparse linear algebra,
- 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.

# 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*.

**Participants:** Guy Antoine Atenekeng Kahou, Jocelyne Erhel, Frédéric Guyomarc'h, Laura Grigori, Noha Makhoul, Bernard Philippe, Damien Tromeur-Dervout, Petko Yanev, Mohammed Ziani.

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 [49].

More precisely, direct methods involve two steps, first *factoring* the matrix $A$ into the product $A = P_1 L U P_2$ where $P_1$ and $P_2$ are permutation matrices, $L$ is lower triangular, and $U$ is upper triangular, then solving $P_1 L U P_2 x = b$ by solving 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 $P_1 D_1 A D_2$ has a "large diagonal." This helps to assure accuracy of the final solution.
- Choose $P_2$ so that the $L$ and $U$ factors of $P_1 A P_2$ are as sparse as possible.
- Perform *symbolic analysis*, i.e. identify the locations of nonzero entries of $L$ and $U$.
- Factorize $P_1 A P_2$ into $L$ and $U$.

The team works on parallel sparse direct solvers and is involved in the development of SuperLU_DIST [4].

### 3.1.2. *Iterative linear solvers*

The most efficient iterative methods build a Krylov subspace, for example $\{x_0, Ax_0, \cdots, A^k x_0\}$. If the matrix is symmetric positive definite, the 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 [54], [52]. 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 or an approximate inverse [47].

The team studies preconditioners for Krylov methods [1], [7].

### 3.1.3. *Linear least-squares problems*

For linear least-squares problems $\min\limits_x \|Ax - b\|$, direct methods are based on the normal equations $A^T A x = A^T b$, using either a Cholesky factorization of $A^T A$ 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 [51], [46]. 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.

### 3.1.4. Nonlinear problems

Nonlinear methods to solve $F(x) = 0$ include fixed-point methods, nonlinear stationary methods, secant method, Newton method [53], [48]. The team studies stationary and Newton-Krylov methods, where the linearized problem is solved by a Krylov method [2].

Another subject of interest is parallelization in time. 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.

### 3.1.5. 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 $(\lambda, z)$ 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 [3] while the Jacobi-Davidson method is described in [55]. 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 $B^T B$ [3].

### 3.1.6. 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 $\epsilon$-spectrum or equivalently the notion of pseudospectrum was simultaneously introduced by Godunov [50] and Trefethen [56]. Several teams proposed softwares to compute pseudospectra, including the SAGE team with the software PPAT [6], described in Section 5.2.

In some applications which lead to the study of multiple eigenvalues, it is important to characterize their type. For instance, in a standard non symmetric eigenvalue problem, the Jordan structure can be of interest. Unfortunately, computing that structure for a given matrix is an ill-posed problem since the set of diagonalizable matrices is dense in the set of the matrices. Therefore the problem must be recast into: which is the most degenerated Jordan form in a given neighborhood of the initial matrix? When the matrix is large and sparse, the problem is even more difficult since only part of the spectrum can be characterized.

The team works on the determination of partial canonical structures of sparse matrices ; standard eigenproblems (Jordan decomposition of a matrix) as well as generalized eigenvalue problems (Weierstrass decomposition of a pencil) are studied by the team.

## 3.2. High-Performance Computing

**Participants:** Amine Abdelmoula, Jenny Al Khoury, Guy Antoine Atenekeng Kahou, Anthony Beaudoin, Édouard Canot, Caroline de Dieuleveult, Jocelyne Erhel, Frédéric Guyomarc'h, Laura Grigori, Noha Makhoul, Hussein Mustapha, Bernard Philippe, Damien Tromeur-Dervout, Petko Yanev, Samih Zein, Mohammed Ziani.

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 sparse direct solvers ($LU$ factorization), iterative solvers (PCG, GMRES, subdomain method), least-squares solvers ($QR$ factorization). 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. Parallel particle trackers are still an area of research.

### *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. We also investigate the implementation on grid architectures, in collaboration with Paris Inria-team. The challenge is to develop and use a middleware for high-level applications.

### *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

**Participants:** Amine Abdelmoula, Jenny Al Khoury, Édouard Canot, Jocelyne Erhel, Bernard Philippe, Samih Zein.

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 and geological rock formation. 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

**Participants:** Anthony Beaudoin, Édouard Canot, Caroline de Dieuleveult, Jocelyne Erhel, Hussein Mustapha.

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 nonlinear PDAEs. The main objective of the team is to design and to implement an efficient and robust numerical method to solve the systems of nonlinear coupled equations at each time step. The output will be a software running on parallel platforms such as clusters and on experimental computational grids. Simulations of several test cases will assess the performance of the software.

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.

# 5. Software

## 5.1. SCILIN : linear solvers within SCILAB

**Participants:** Édouard Canot, Frédéric Guyomarc'h [corresponding author].

The kernel of SCILAB includes a special format for sparse matrices and some factorizations as well. SCILIN is a SCILAB toolbox for solving large and sparse linear systems. It provides the classical iterative methods (Jacobi, SOR, CG, GMRES, BiCGSTAB, QMR, etc).

The SCILIN toolbox was presented at the Scilab 2004 International Conference, in December 2004, and was then accepted to be part of the Scilab's kernel. Its integration has already started, but because of Software license, we are now implementing a new version of the incomplete factorizations. This new software will be compliant with the Scilab license and will then be included in the main source code.

SCILIN can be downloaded at the address : http://www.irisa.fr/aladin/codes/SCILIN/.

## 5.2. PPAT : pseudo-spectrum

**Participants:** Édouard Canot [corresponding author], Frédéric Guyomarc'h, 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.

It is also included in the free-software CD-ROM of INRIA:
http://www.inria.fr/valorisation/logiciels-libres/cederom.en.html

## 5.3. Viz2D and Gridmesh: visualization and regular mesh generation

**Participant:** Édouard Canot [corresponding author].

Our VIZ2D library allows to visualize scientific results during computation, via appropriate calls of a graphical library. We use the PGPLOT library, a high-level routines package for scientific use, which is free, widely used on Linux machines and available on internet at the following URL: http://www.astro.caltech.edu/~tjp/pgplot/. Our VIZ2D library is a user interface to a slightly modified PGPLOT package : it is a set of Fortran routines intended to make data plot easy via few calls. It is restricted to data spread over a regular rectangular 2D mesh. This library has been tested under Linux and SunOS. It has been used in the Hydrogrid and Ifremer projects, and also in the F90 version of Gridmesh.

Gridmesh is an interactive 2D structured mesh generator. One version has a graphical user interface entirely built with Matlab, and another one uses the above-cited Viz2d library via a F90 program. Gridmesh can create/modify a 2D mesh with associated boundary conditions for both the flow and transport parts. Several numbering schemes can be used, in order to get a more or less banded connectivity matrix. Mesh partition can also be imposed, with an arbitrarily number in subdivisions (but this number must be a power of two). The Matlab version is more friendly than the F90 one, but is practically limited to moderate meshes.

A simple 3D mesh generator has been developed in F90, to use inside the TRACE software (Transport of RadioActive Elements in Subsurface, written by H. Hoteit and Ph. Ackerer from IMFS of Strasbourg).

# 6. New Results

## 6.1. Numerical algorithms

### *6.1.1. Direct linear solvers*

**Participant:** Laura Grigori.

*6.1.1.1. Structure prediction for sparse LU factorization with partial pivoting*

This research considers the structure prediction problem of the Gaussian elimination when used to solve the linear system $Ax = b$, where $A$ is a $n \times n$ nonsingular and unsymmetric matrix and $b$ is a $n$-vector. When $A$ is sparse, during the Gaussian elimination, or equivalently the $A = LU$ factorization, some of the elements that are zero in the original matrix $A$ can become nonzero in the factors $L$ and $U$.

An elimination model based on graph theory was proposed by Rose and Tarjan to describe the creation of nonzero elements, using the directed graph of matrix $A$. In our new results, we propose a model that uses bipartite graphs to characterize the fill-in occurring in the Gaussian elimination of sparse unsymmetric matrices. This model identifies numeric cancellations appearing during Gaussian elimination that are missed by the generally used model based on directed graphs, proposed by Rose and Tarjan. The numeric cancellations are related to submatrices of the input matrix $A$ that are structurally singular, that is, singular due to the arrangements of their nonzeros, and independently of their numerical values.

The theoretical results lead to an algorithm for computing fill-ins using bipartite graphs. Its complexity is bounded by $O(nm)$, where $n$ is the order and $m$ is the number of nonzeros of matrix $A$. This is equivalent to the complexity of the first algorithm proposed by Rose and Tarjan. This work was submitted for publication.

During his internship, J-F. Jamoteau has implemented and tested this algorithm on several matrices from the Harwell-Boeing collection. We have noticed that for the moment the algorithm is more expensive than the existing algorithms. But it can lead to a much smaller number of fill-ins for several matrices. Future work aims at decreasing the runtime of the algorithm.

*6.1.1.2. Performance evaluation of sparse matrix factorization*

A valuable tool in designing a parallel algorithm is to analyze its performance characteristics for various classes of applications and machine configurations. Very often, good performance models reveal communication inefficiency and memory access contention that limit the overall performance. Modeling these aspects in detail can give insights into the performance bottlenecks and help improve the algorithm.

We investigated performance characteristics for the LU factorization of large matrices with various sparsity patterns. We considered supernodal right-looking parallel factorization on a two dimensional grid of processors, making use of static pivoting. We developed a performance model and we validated it using the implementation in SuperLU_DIST, the real matrices and the IBM Power3 machine at NERSC. We used this model to obtain performance bounds on parallel computers, to perform scalability analysis and to identify performance bottlenecks. This work was published in [35]. Currently, we try to improve the performance model by estimating the cost of basic memory operations, such as cache hits and misses.

Our goal is to use this estimation in a scheduling algorithm in a grid environment, for the coupled problems arising in hydrogeology applications, where several systems of equations need to be solved independently (6.2.2). Thus, each system can be solved on a different cluster of processors. A scheduler can thus estimate the workload associated with each resolution and choose an appropriate number of processors for the execution. We aim at performing this work as a collaboration between SAGE and the PARIS group.

### 6.1.2. Iterative linear solvers

**Participants:** Guy Antoine Atenekeng Kahou, Jocelyne Erhel, Laura Grigori, Bernard Philippe, Damien Tromeur-Dervout.

The focus is on the use of iterative methods for solving large sparse linear systems of equations arising in hydrogeology applications. Recent research shows that the direct methods, currently used in this research activity, reached their limits. That is because of the important memory requirements and the computational costs of the large scale problems we deal with in hydrogeology (see 6.2.1).

#### 6.1.2.1. Parallel Preconditioning of Krylov methods using Incomplete LU Factorization

This research is conducted as a collaboration between SAGE team and the group of James Demmel from UC Berkeley (8.3.1, 9.6.1).

The goal of this ongoing research activity is to study and develop efficient parallel algorithms for the incomplete LU (ILU) factorization. The incomplete factorizations are considered to be efficient and simple preconditioners, that in combination with a Krylov subspace iteration (for example GMRES or BICGSTAB for unsymmetric matrices) can provide a robust solver. The ILU factorization we propose is based on a graph partitioning approach that identifies blocks that can be computed independently. Low rank approximations are used in the off-domain blocks. These approximations aim at improving the parallelism, because they allow an efficient application of the preconditioner on the input matrix in a memory distributed environment.

#### 6.1.2.2. Parallel Preconditioning of Krylov methods using Domain Decomposition

This research is done in the context of a collaboration between SAGE team and the University of Yaounde, Cameroon. The first step is the subject of the Ph-D thesis of G. Atenekeng, co-advised by B. Philippe and E. Kamgnia. The second step was the subject of the Master thesis of I. Souopgui, co-advised by B. Philippe and E. Kamgnia (see section 9.6.2).

We consider algebraic preconditioners for accelerating iterative methods when solving large sparse linear systems. In the previous paragraph, we have studied $ILU$ preconditioners. Here, the idea is to build a class of preconditioners from domain decomposition methods. We consider techniques which are only defined from the matrix, where the block partition is obtained from the pattern of the non-zero structure of the matrix. When overlapping between subdomains is allowed, two methods are usually considered : the Multiplicative Schwarz (MS) and the Additive Schwarz (AS) iterations. The later one is easy to parallelize but its quality as preconditionner is lower than the quality of the former one. Therefore, the challenge is to define parallel versions of Krylov methods preconditionned by (MS). We are currently working on a parallel version of the GMRES method preconditionned (on left or right side) by (MS). The code is developped into the PETSc standard using MPI for communication primitives. Experiments are run on the Grid platform at Irisa.

In that direction, the first step was to define a new explicit expression of the (MS) preconditionner [18] and a first analysis of its parallel implementation [38]. In order to obtain better parallelism in the computation, the second step was to define a parallel construction of an a priori basis of the Krylov subspace. It is now included in our GMRES procedure.

During M. Sosonkina's visit (see 9.6.2), it has been decided that our preconditioner will be compared to hers, by defining a common set of experiments.

#### 6.1.2.3. Aitken-Schwarz Domain Decomposition for flow transport on Grid architecture

This work is done in collaboration with J-R. de Dreuzy, from CAREN and with A. Frullone, from University of Lyon 1, in the context of his Ph-D thesis advised by D. Tromeur-Dervout.

Here, the Domain Decomposition method is used rather as a semi-iterative solver, which is not combined with a Krylov solver. The objective of this study is to introduce generalized Schwarz domain decomposition in an oriented object code for Flow transport in porous media, using a finite volume framework (see 6.2.1). The software architecture is slightly modified to handle the domain decomposition with no overlap and Robin conditions at artificial interfaces. The Aitken acceleration of convergence technique will be applied in order to obtain the converged solution at artificial interfaces generated by the generalized Schwarz as shown in [22]. Some numerical studies to approximate the matrix error at interfaces are under investigation by A. Frullone. Then the computation will be performed on grid'5000, each subdomain running on a multi-processors system (see 8.1.4).

### 6.1.3. Linear least-squares problems

**Participants:** Laura Grigori, Frédéric Guyomarc'h, Bernard Philippe, Petko Yanev.

#### 6.1.3.1. Parallel sparse $QR$ factorization using a block angular structure

One of the applications of the sparse QR factorization we worked on this year is a problem issued from a collaboration with RTE (see Section 7.1). This was the subject of the Master thesis of Antoine Elie Daou (4 months, from June to September). One of the problems RTE works on is a state estimator problem in Energy Management Systems. This problem can be solved using a weighted least squares approach. It involves the QR factorization of a very large sparse matrix. Some row permutations and column pivoting can be performed during the factorization to improve numerical robustness (see below). For this work, we have restricted our attention to a factorization that does not perform pivoting.

To be able to solve the large matrices arising in this application, a parallel algorithm for distributed memory machines was developed for the sparse $QR$ factorization. The algorithm exploits the structure of the input matrix, that consists of several large diagonal blocks followed by a number of columns at the end coupling all the previous blocks (block angular structure). The algorithm was tested using the clusters at IRISA (see 8.1.4) and the matrices provided by RTE. It showed a good scalability behaviour up to 64 processors.

#### 6.1.3.2. Rank-Revealing $QR$ factorization

This work was undertaken in collaboration with D. Mezher, from the University Saint-Joseph, Beirut, Lebanon (see section 9.6.2).

To improve numerical robustness, it may be necessary to use a rank-revealing $QR$ factorization. It is still challenging when dealing with large sparse unstructured matrices. There exist now efficient procedures to compute the $QR$ factorization of matrices. They adress the difficulty of maintaining the level of fill-ins at a feasable level during the procedure by considering appropriate orderings of the columns. But for rank-revealing procedures, other orderings must be considered which lead to unfeasable level of fill-ins, except for small matrices. Therefore, we have designed a new approach, where we consider the rank-revealing procedure as a post treatment applied to the sparse triangular factor obtained by the best QR factorizers. Two strategies were considered and compared on dense matrices [37]. Ongoing work addresses the sparse situation.

### 6.1.4. Eigenvalue problems

**Participants:** Frédéric Guyomarc'h, Bernard Philippe.

#### 6.1.4.1. Eigenvalue solvers using Domain Decomposition

This work was done in collaboration with Y. Saad, from University of Minnesota (see 9.6.2). By combining two directions of our research, namely the eigenvalue solvers developped with the Jacobi-Davidson and Davidson algorithms and the Domain decomposition techniques, eigensolvers adapted to a domain partitions are considered. Block corrections of basis of approximate invariant subspaces are defined and compared [45]. This approach allows the computation of the smallest or even intermediate eigenvalues of large sparse symmetric matrices.

#### 6.1.4.2. Krylov-Schur methods for generalized eigenvalue problems

The work on Partial canonical structure extraction for large matrices is the follow up of the collaboration with Bo Kågström from the Umeå University (Sweden), in the context of the swedish project entitled *Matrix Pencil Computations in Computer-Aided Control System Design: Theory, Algorithms and Software Tools*.

When $A$ and $E$ are very large, computing the Schur decomposition of a matrix pencil $A - \lambda E$ is far too expensive if we use the dense linear algebra algorithms, and if we use the classical routines for sparse matrices, they do not treat the case of multiple eigenvalues.

B. Kågström and P. Wiberg have a method to compute a partial Weierstrass decomposition for the biggest eigenvalue of the spectrum. It is based on D. Sorensen's algorithm, IRAM (*Implicitly Restarted Arnoldi Method*). Unfortunately this later does not deal intrinsically with multiple eigenvalues. So we have to compute very precisely information for the first multiplicity of the eigenvalue and then deflate it explicitely (*lock and purge*). Then we can compute information about the next multiplicity.

We now have adapted the Krylov-Schur method to treat generalized problems. This method does not need to preserve the Hessenberg form of the Rayleigh quotient, thus it offers a better flexibility. We are now working on a block version of the algorithm, which is essential for canonical structure computations, because we can then deal with multiple eigenvalues without explicite deflation. That means that convergence towards many eigenvalues can occur at the same time. During his internship, B. Poirriez has studied the convergence of this block version of our algorithms. Experiments indicate that our algorithm can run faster than the well-known ARPACK solver in the case of multiple eigenvalues [36].

We will also test our solver with an application coming from EDF, dealing with nonlinear dynamic simulation and modal analysis for the control of large-scale power systems.

### *6.1.5. Nonlinear problems*

**Participants:** Jocelyne Erhel, Frédéric Guyomarch, Noha Makhoul, Mohammed Ziani.

#### *6.1.5.1. Newton-Krylov methods*

Mohammed Ziani has started a Ph. D. under the direction of R. Aboulaïch (EMI, Morocco) and F. Guyomarc'h, in the context of the Sarima project (8.3.3,9.6.2). The topic is the study of Krylov methods to solve non linear equations. It will focus on two particular problems: a pillar problem and Navier-Stokes equations.

The first part of our work this year was to develop a numerical model of the pillar and to solve it with the classical Newton algorithm. A pillar is embedded in the ground and is subject to a force at the surface, and the objective is to compute the displacement of the pillar. We studied two different cases: the ground structure is piecewise constant and it is a non linear function.

The second part was the implementation of the nonlinear solver in Scilab.

#### *6.1.5.2. Parallelization in time*

This subject concerns N. Makhoul's PhD thesis, co-advised with N. Nassif, from the American University of Beirut, Lebanon, in the context of the Sarima project (8.3.3,9.6.2). The objective is to design a parallel algorithm for time discretization in PDEs. The work this year was essentially devoted to bibliographic search.

## 6.2. Applications

### *6.2.1. Large-scale linear problems in hydrogeology*

**Participants:** Anthony Beaudoin, Jocelyne Erhel, Hussein Mustapha.

This work is related to H. Mustapha's PhD thesis and to A. Beaudoin's post-doc work and is done in collaboration with J.-R. de Dreuzy, from CAREN, University of Rennes 1, in the context of the Hydrogrid project(8.1.3) and the Grid'5000 project (8.1.4).

The first objective is to compute the steady-state flow either in a highly heterogeneous porous medium or in a large network of fractures; after spatial discretization, it amounts to a huge sparse symmetric positive definite linear system. The second objective is to simulate the transport of solutes by advection-diffusion, where the advection operator uses the velocity field computed by the flow step.

#### *6.2.1.1. Flow and transport in highly heterogeneous porous medium*

The domain of computation is a 2D rectangle, where the permeability field is highly heterogeneous. We have developed a parallel software for both flow and transport. The flow module includes problem generation, spatial discretization by a finite volume method using a structured mesh, linear solving, flux computation and visualization. The transport module includes a parallel particle tracker for advection-dispersion. All algorithms are parallelized using a message-passing approach. For spatial discretization, we define a subdomain distribution. Currently, we use parallel sparse linear solvers from the public domain; we have tested two direct solvers (MUMPS from INRIA and PSPASES from the University of Minnesota and IBM) and one iterative solver using a Structured Multigrid method (SMG/HYPRE from Lawrence Livermore National Laboratory).

Our results show that we are able to deal with very large 2D highly heterogeneous porous media [23]. We have obtained very good performances and a good scalability using the parallel clusters of the Grid platform at Irisa [25]. In collaboration with UC Berkeley, we plan to develop a software for 3D porous media and to study parallel iterative solvers (6.1.2).

#### *6.2.1.2. Flow in 3D networks of fractures*

The domain of computation is a 3D network of interconnected plane fractures; we assume that the matrix (the rock) surrounding the fractures is impervious and that the fractures have a constant thickness. We have developed a software for flow computation, which includes problem generation, mesh generation, spatial discretization by a mixed finite element method, linear solving, flux computation and visualization. All algorithms are parallelized using a message-passing approach. We define a distribution of the fractures. Currently, we use parallel direct sparse linear solvers from the public domain (MUMPS from INRIA and PSPASES from the University of Minnesota and IBM).

Our results show that we are able to deal with large 3D networks of fractures [8], [39]. We have obtained good performances using the parallel clusters of the platform Grid at Irisa. However, scalability is not so good [25], [40]. In collaboration with UC Berkeley, we plan to investigate a block angular structure (see 6.1.3) and to develop a computational model.

### *6.2.2. Coupled nonlinear problems in hydrogeology*

**Participants:** Jenny Al Khoury, Édouard Canot, Caroline de Dieuleveult, Jocelyne Erhel.

The first objective is to design parallel methods for solving coupled nonlinear PDEs or PDAEs. The second objective is to design parallel software components, guided by the coupling algorithm. We study two applications, saltwater intrusion and reactive transport.

#### *6.2.2.1. Parallel software components for saltwater intrusion*

This work is done in the context of the Hydrogrid project (8.1.3), in collaboration with C. Perez (Paris Inria team at Rennes).

Saltwater intrusion is modelled by coupled nonlinear PDEs, taking into account the flow generated by the density contrast and the convection of salt induced by the flow. We started from an original sequential version, provided by IMFS, to develop a parallel numerical software for density-driven flow and transport in porous media. We define a subdomain decomposition for spatial discretization, using the public domain software METIS, from the University of Minnesota. Linear systems arising in both flow and transport models are either symmetric positive definite or unsymmetric. We use the parallel linear solver MUMPS from INRIA to solve them [44], [26], [28].

We have designed software components to couple flow and transport models. Each model is implemented as a component, with a component which controls the time step and the numerical coupling. These components are written in Paco++, the middleware developed by the Paris team.

#### *6.2.2.2. Nonlinear solvers for reactive transport*

This work was done in the context of the Hydrogrid project (8.1.3) and the MOMAS GdR (8.1.2), in collaboration with M. Kern (Estime Inria team at Rocquencourt). The subject concerns J. Al Khoury's Ph-D thesis, co-advised with M. Al Ghoul, from the American University of Beirut, Lebanon, in the context of the Sarima project (8.3.3,9.6.2). It is also the subject of C. de Dieuleveult's Ph-D thesis, 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 and kinetic chemical equations. After spatial and temporal discretisation, the problem to solve at each time step is a huge system of nonlinear equations. We use a PDAE (Partial Differential Algebraic Equations) framework to design an algorithm based on the Newton method [27], [28], [29]. During his master thesis, R. Vietor has tested various algorithms on a Momas benchmark.

### 6.2.3. Inverse problems in submarine acoustics

**Participants:** Édouard Canot, Jocelyne Erhel, Samih Zein.

This work is the subject of S. Zein's Ph-D thesis, co-advised with N. Nassif, from American University of Beirut, Lebanon (9.6.2) and is done in the framework of the Ifremer contract (8.1.5).

Our work this year was devoted to the inverse problem: to find the mechanical properties of the sub-marine soil (eventually many sub-layers) from pressure measurements in the sea due to the propagation/transmission of a seismic wave. The reflection of the wave at each interface allows us to collect information in the fluid and, via appropriate numerical methods (described below), to determine the density and the elasticity of each layer constituting the solid sub-marine soil.

Two stochastic methods, Markov Chain Monte Carlo (MCMC) with an accelerated version, and Stochastic Perturbation Simultaneous Approximation (SPSA) have been implemented and compared together with respect to cost and accuracy. Both are based on forward simulations, which were developed during previous years by adapting the FLUSOL code developed by Ondes team from Inria Rocquencourt.

Validation is made on synthetic data: first, the physical properties (parameters lambda, mu and rho) of the soil are chosen; then an acoustic wave (with appropriate shape and frequency) is generated in the sea and the time dependent pressure value at some fixed locations are recorded. Finally, some Gaussian noise (5% in relative error) is added to these measures, and the MCMC method is applied (it requires a very great number of forward computations of the FLUSOL code) and stopped when the three parameters have converged to stable values. For example, the convergence of these parameters is shown in Figure 1.

Moreover, the histograms shown in Figure 2 ensure that the parameters have converged to acceptable and unique values (no oscillation between two states, for example) :

Many tests show that 6000 realizations (i.e. 6000 computations of the forward code FLUSOL) are required to obtain convergence of the MCMC method. Confidence interval was estimated to be of the order of few percents. The other method, SPSA, gives the same level of accurary as MCMC when compared for a one layer solid but it has the advantage to be much less expensive in computations. These latter method is also able to solve the case of a three layers solid with the same cost [42].

# 7. Contracts and Grants with Industry

## 7.1. Industrial Grant with RTE

**Participants:** Laura Grigori, Bernard Philippe.

RTE contract
partners: Irisa, RTE
time: from May 25 2005 until September 25 2005.

This project deals with the power system parameter estimation problem occuring in energy management systems. Due to its statistical properties, the weighted least squares approach is used to solve this problem. This involves the QR factorization of a very large sparse matrix.

The goal of this collaboration was twofold. First, we showed the robustness of the QR factorization compared to the method of normal equations for this problem. The normal equations can also be used to solve this problem and are less expensive from a computational point of view. Second, a parallel implementation of

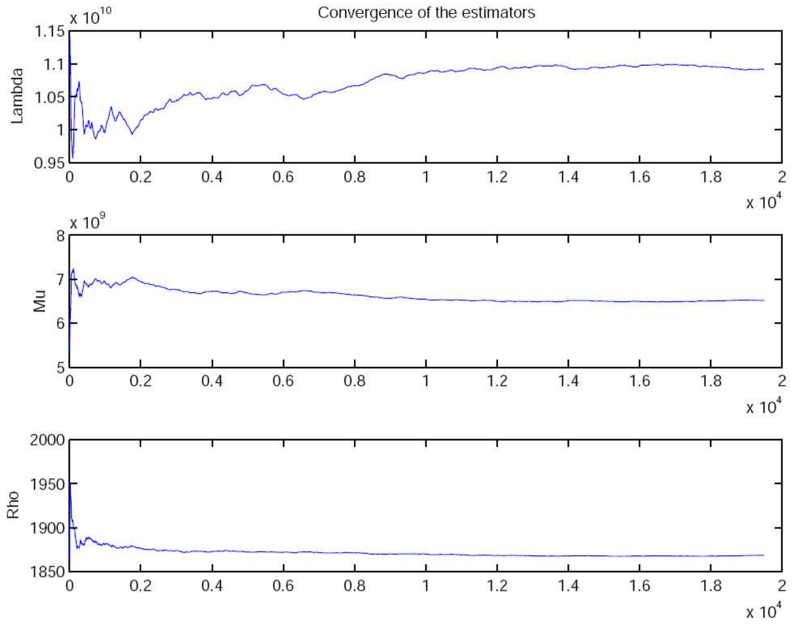

*Figure 1. Convergence of the estimators*

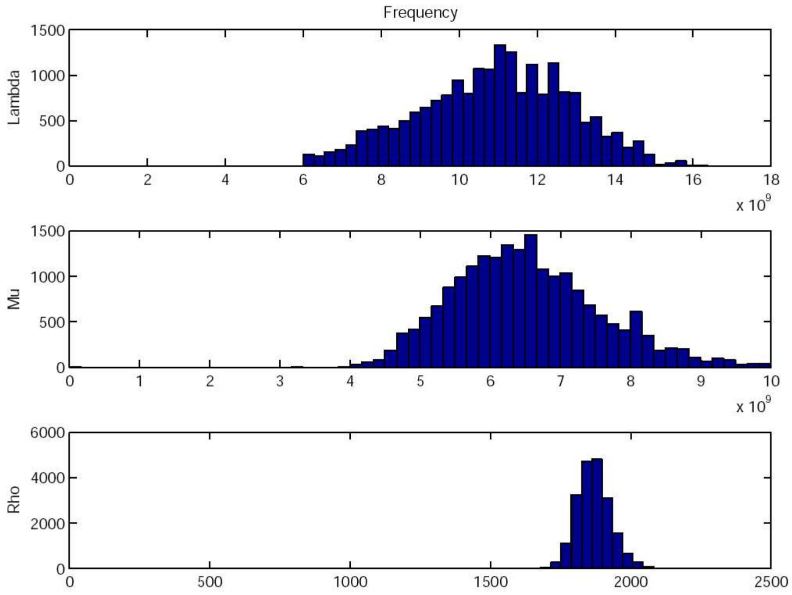

*Figure 2. Histograms of the posterior distribution*

the sparse QR factorization was proposed that takes into account the specific sparse structure of the matrix. For more details, see Section 6.1.3.

# 8. Other Grants and Activities

## 8.1. National Grants

### *8.1.1. ANDRA*

**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. For more details, see Sections 6.2.2, 4.1.

### *8.1.2. GdR MOMAS - Numerical models for nuclear waste disposal*

**Participant:** Jocelyne Erhel.

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

The working group MOMAS is led by A. Bourgeat from the university of Lyon and includes many partners from CNRS, INRIA, universities, CEA, ANDRA, EDF, BRGM. It covers many subjects related to mathematical modeling and numerical simulations for nuclear waste disposal problems. We participate in the subject devoted to multiphysics models and collaborate with Estime team, Inria-Rocquencourt, in the project entitled "Numerical schemes and coupling algorithms for reactive transport problems" [29]. See section 6.2.2.

### *8.1.3. HydroGrid - Multiphysics models in hydrogeology*

**Participants:** Édouard Canot, Caroline de Dieuleveult, Jocelyne Erhel, Hussein Mustapha.

HydroGrid: Coupling codes for flow and solute transport in geological media: a software component approach.
ACI GRID grant, No. 102C07270021319
time: from October 2002 until October 2005
Coordinator: M. Kern, Estime Inria team
Participants: Paris Irisa team, Estime Inria team, Sage Irisa team, IMFS (U. of Strasbourg), CAREN (U. of Rennes 1).

See http://www-rocq.inria.fr/~kern/HydroGrid/HydroGrid.html

We have worked on three applications described above : saltwater intrusion, reactive transport and network of fractures. In collaboration with Paris team, Inria-Rennes, we have developed parallel software components, for density-driven flow and for transport, and applied them to the saltwater intrusion problem. Experiments were done on the Grid at Irisa. In collaboration with Estime team, Inria-Rocquencourt, we have designed numerical methods and specified software components for reactive transport. In collaboration with CAREN, we have developed a parallel software for flow in 3D networks of fractures. Experiments were done on the Grid at Irisa. See Sections 6.2.2,6.2.1.

A poster has been presented at Paristic, Bordeaux, November.

### *8.1.4. Grid'5000-Rennes*

**Participants:** Anthony Beaudoin, Édouard Canot, Caroline de Dieuleveult, Jocelyne Erhel, Laura Grigori, Hussein Mustapha.

ACI GRID program GRID'5000
Coordinator : Y. Jégou, Paris team, INRIA-Rennes.

Our parallel algorithms for iterative linear solvers and $QR$ factorizations were tested on the clusters of the Grid at Rennes. See Sections 6.1.3 and 6.1.2.

Our different projects on hydrogeology involve very large sparse linear systems. We have used the clusters and the grid built at INRIA-Rennes to deal with large 2D and 3D domains. Our objective is now to run multi-parametric simulations. See sections 6.2.1 and 6.2.2.

### 8.1.5. *IFREMER contract*

**Participants:** Édouard Canot, Jocelyne Erhel, Samih Zein.

IFREMER contracts, No 03/2 210 413
Partners : Irisa, IFREMER
Title : Numerical model for the propagation of elastic waves
time : from June 2004 until January 2005 and from February 2005 until December 2005.

This work is done in the context of the “Contrat de Plan Etat Région Bretagne 2000-2006” (signed in October 2002), for the development of new geophysical exploration means.

The first objective of this study was to develop a software simulating the propagation of elastic waves in the seawater and in the underwater geophysical layers. We have used the code FLUSOL from the INRIA-team ONDES.

The second objective is to study inverse methods to find layer properties in the ground, only from acoustic measurements recorded near the sea surface by a ship. The reflection of the wave at each interface allows us to collect information in the fluid and, via appropriate numerical methods, to determine the density and the elasticity of each layer constituting the solid sub-marine soil. See 6.2.3.

Comparison with experimental measures, from many oceanographical campaign of IFREMER institute, have not been done yet but are planned for the upcoming year.

## 8.2. European Grants

### 8.2.1. *ERCIM Working group - Matrix Computations and Statistics*

**Participants:** Jocelyne Erhel, Laura Grigori, Frédéric Guyomarc’h, Bernard Philippe.

ERCIM Working Group, started in 2001.
**Title :** Matrix Computations and Statistics
**Chairmen :** B. Philippe and E. Kontoghiorghes (U. Cyprus)
**Members :** 45 researchers from 13 European countries.
http://www.irisa.fr/sage/wg-statlin/

This working group aims to find new topics of research emerging from some statistical applications which involve the use of linear algebra methods. The members are especially concerned by very large problems that need the design of reliable and fast procedures. High Performance Computing including parallel computing is addressed.

In 2005, the WG met in Copenhagen in April and in Lemassol (Cyprus) during the CSDA’05 conference. In CSDA, the WG organized two sessions; among them, the team Sage organized the session devoted to sparse matrix factorization.

### 8.2.2. *ERCIM Working group - Applications of Numerical Mathematics in Science*

**Participants:** Jocelyne Erhel, Bernard Philippe.

ERCIM Working Group, started in 2001.
**Title :** Applications of Numerical Mathematics in Science
**Chairman :** Mario Arioli, RAL.
**Members :** 27 european research teams.
http://www.numerical.rl.ac.uk/ercim/WGanms.html

The Working Group wants to create a forum within ERCIM Institutional Organizations in which a cross fertilization between numerical techniques used in different fields of scientific computing might take place.

Thus, the Working Group intends to focus on this underpinning theme of computational and numerical mathematics. In this way, the intention is that any resulting numerical algorithm will achieve wider applicability, greater robustness, and better accuracy.

### *8.2.3. DOD ECONET project*

**Participant:** Édouard Canot.

ECONET project.
**Title:** Drop-On-Demand (DOD, 08163RD).
**Participants:** France, Romania and Poland.
**Time:** 2004 and 2005.

ECONET is a European program, supported by the french foreign office. The topics of the DOD project are the following:

- experimental studies of drops formation by piezo-electric or thermal processes;
- exhaustive measurements by use of cameras and laser velocimetry;
- modelization and numerical computations via specific methods.

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 flow is due to impulsive external conditions, 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 occurs only on the fluid boundary. This method is applied to the spreading of a liquid drop impacting on a solid wall; applications take place, among others, in ink-jet printing processes.

Ink-jet printing processes are characterized by small geometrical scales (50 to 100 $\mu m$) and high velocities (5 to 15 $ms^{-1}$). This leads to competition between inertia, viscous and capillary forces. Using a numerical method has the advantage of getting rid of any assumption about the shape of the spreading drop. Dimensionless parameters are Froude, Weber and Reynolds number.

Many simulations have been carried out to analyse a large spectrum of droplets size, velocity, frequency, and also to derive conditions for non-satellite formation; results have been presented in the Euromech 472 colloquium ([31]).

This work is related to the following recent publications [19], [15], [13], [11], [30], [20].

## 8.3. International Grants

### *8.3.1. Mini-Call INRIA for USA*

**Participants:** Jocelyne Erhel, Laura Grigori.

The goal was to join the expertise of Sage team and of J. Demmel's group from UC Berkeley in a research effort into the parallel preconditioning of large sparse linear systems of equations arising in hydrogeology applications. See Sections 6.1.2,6.2.1,9.6.1.

### *8.3.2. STIC INRIA/Tunisia*

**Participants:** Amine Abdelmoula, Bernard Philippe, Jocelyne Erhel.

The team SAGE collaborates with the laboratory LAMSIN at ENIT, Tunis. The collaboration is funded by an agreement between INRIA and the Ministry of University and Research in Tunisia. The title of the activity is “Generalized Least Squares Problems - Application to the determination of the Geoid of Tunisia”. In that framework, Maher Moakher (ENIT) and B. Philippe co-advise A. Abdelmoula's PhD research.

In a collaboration with OTC (Office de Topographie et Cartographie), the Tunisian Department of Topography and Cartography, the goal is to compute the geoid (the level surface of the earth attraction at the sea level) for Tunisia. The problem ends up with a large structured generalized least squares problem. Therefore, we plan to apply our algorithms on $QR$ factorizations (6.1.3). In order to gain insight into geodesy, we have contacted the French institute IGN (Institut Géographique National).

### *8.3.3. SARIMA - Support to Research Activities in Africa*

**Participant:** Bernard Philippe.

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** : 2004-2007.

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

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, a team in Tunisia acting for the whole Maghreb and one 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 2005, more than 60 researchers (PhD students and researchers) were funded to visit France for one to six months long visits.

As far as Sage team is concerned by Sarima, see Sections 9.6.1,9.6.2.

# 9. Dissemination

## 9.1. Program committees and Editorial Boards

- J. Erhel was member of the program committee of Renpar'16, April, Le Croisic, France.
- B. Philippe and the SAGE team are the organizers of the PMAA'06 (Third edition of the Parallel Matrix Algorithms and Applications workshop) which will be held in Rennes (September 7-9, 2006).
- B. Philippe is member of the following program committees : CSDA'05 (Lemassol, Cyprus, October 28-31, 2005), A.A. Markov Anniversary Meeting (Charleston, June 12-14, 2006) and COMPSTAT'06 (Rome, August 28 - September 1st, 2006).
- B. Philippe is editor of the electronic journal ARIMA.
- B. Philippe is member of the editorial board of the journal International Journal on High Speed Computing (Word Scientific Publishing)

## 9.2. INRIA and University committees

- 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 of INRIA.
- J. Erhel was member of the Evaluation Board of INRIA until July 2005.
- J. Erhel is member of commission de spécialistes, section 27, of the University of Rennes 1.
- F. Guyomarc'h is member of the CUMI (Commission des Utilisateurs de Moyens Informatiques), of INRIA-Rennes.
- F. Guyomarc'h is member of commission de spécialistes, section 27, of the University of Rennes 1.
- F. Guyomarc'h is responsible for the first year of the DIIC (Diplôme d'Ingénieur en Informatique et Communication) and is a member of the working group for updating the academic plans.
- B. Philippe is the INRIA coordinator for the SARIMA project.
- B. Philippe is correspondent for the agreement between the University of Rennes 1, the Lebanese University and AUF (Agence Universitaire Francophone) which supports a Master.

## 9.3. Teaching

- J. Erhel gave a one-week course in February on Methods for Solving Large Systems, in Beirut, Lebanon (DEA de mathématiques appliquées, co-organized by the Lebanese University, EPFL of Lausanne, IRISA and University of Reims). Lecture notes on http://www.irisa.fr/sage/jocelyne
- F. Guyomarc'h gave lectures on algorithms (ALG2) for Master (M2-CCI), IFSIC, University of Rennes 1.
- F. Guyomarc'h gave lectures on object oriented programmation (PROG2) for Master (M2-CCI), IFSIC, University of Rennes 1 and also in the first year of DIIC.
- 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".
- B. Philippe gave two one-week courses, in April and in November, on Parallel Algorithms in Linear Algebra, in Yaounde (DEA d'informatique).
- B. Philippe gave a two hours tutorial on parallel eigenvalue solvers at the CSDA'05 conference.

## 9.4. Participation in scientific review

- The work on software components for saltwater intrusion (6.2.2) is briefly described in Inedit 50 (Special issue - Grid challenges), July 2005 and in Interstices (La programmation des grilles informatiques), October 2005.
- The team Sage participated in Portes Ouvertes de l'Irisa, Rennes, October. A software demonstration entitled "Mais où passe donc le désherbant du jardinier ?" was prepared by É. Canot and a talk for the general public entitled "Les eaux souterraines mises sur ordinateur" was given by J. Erhel. Also, with the help of B. Poirriez during his internship, we made a poster entitled "30 ans d'algèbre linéaire".

## 9.5. Participation in conferences

- L. Grigori : participation in SIAM Conference on Computational Science and Engineering, Orlando, Florida, February. Communication co-authored with J.R. Gilbert.
- G.A. Atenekeng Kahou and B. Philippe: participation in École sur les Méthodes performantes en algèbre linéaire pour la résolution de systèmes linéaires et le calcul de valeurs propres, École Polytechnique, Paris, March. Tutorial by B. Philippe.
- A. Beaudoin: participation in workshop of Réseau Génie Civil et Urbain (RGCU), Paris, March.
- J. Erhel: participation in 16ème Rencontres Francophones du Parallélisme, Le Croisic, April.
- B. Philippe: participation in the 6th Workhop of the Working Group Matrix Computations and Statistics, Copenhagen, Denmark, April.
- É. Canot: participation in École thématique du CNRS sur la Visualisation Scientifique: Modèles physiques, méthodes numériques et évolutions informatiques associées, Aussois, May.
- A. Beaudoin: participation in XXIIIèmes Rencontres Universitaires de Génie Civil, Grenoble, May. Communication co-authored with J.-R. de Dreuzy and J. Erhel.
- A. Beaudoin, É. Canot, C. de Dieuleveult, J. Erhel and H. Mustapha: participation in SIAM Conference on Mathematical and Computational Issues in the Geosciences, Avignon, June. Three communications.
- L. Grigori : participation in Second International Workshop on Combinatorial Scientific Computing (CSC05) , CERFACS, Toulouse, June. Communication co-authored with J. Demmel and X. Li.
- N. Makhoul: participation in colloque Auto-similarité et applications, Toulouse, June.
- G.-A. Atenekeng Kahou and B. Philippe : participation in the IMACS congress, Paris, July. Communication.
- A. Beaudoin: participation in 17e congrès français de mécanique, Troyes, September. Communication.
- É. Canot, C. de Dieuleveult and H. Mustapha: participation in Parallel Computing 2005, Malaga, Spain, September. Two communications co-authored with J. Erhel.
- J. Erhel: participation in workshop on Model order reduction, coupled problems and optimization, Leiden, The Netherlands, September. Invited presentation.
- É. Canot, F. Guyomarc'h, L. Grigori, B. Philippe, S. Zein : participation in Computational Statistics and Data Analysis and 7th Workshop of the ERCIM working group “Matrix Computations and Statistics”, Limassol, Cyprus, October. Three communications and one tutorial.
- É. Canot: participation in Journées Panorama des Recherches Incitatives en STIC (PARISTIC), Bordeaux, November. Poster presentation.
- J. Erhel: participation in Journées scientifiques MOMAS, Marseille, November. Communication co-authored with M. Kern.
- F. Guyomarc'h and B. Philippe: participation in 8èmes Journées d'Analyse Numérique et Optimisation, Rabat, Morocco, December. Communication and invited presentation.
- S. Zein: participation in Workshop on Inverse Problems (WIP2005), Marseille, December. Communication.

## 9.6. International exchanges

### *9.6.1. Visits*

- B. Philippe visited the Purdue University, Indiana, USA, during two weeks in January.
- B. Philippe visited ENIT/LAMSIN in Tunis, during two weeks, one in June and the second in September.
- For SARIMA purposes, B. Philippe travelled to Beyrouth (August) and to East Algeria (May).
- L. Grigori has visited for 5 weeks, from July 20 to August 30, the University of California at Berkeley, to work with Professor James Demmel and his group. This visit was funded by the INRIA International Program “Actions 2005 avec les Etats-Unis, la Scandinavie et Taiwan”.
- J. Erhel has visited the same group, with the same fund, for 1 week, in October. She gave a talk entitled "Parallel Simulation of Underground Flow in Porous and Fractured Media" at the Matrix Computations and Scientific Computing" seminar (organizers B. Parlett and J. Demmel).

### *9.6.2. Visitors*

The team has invited the following persons:

- Y. Saad, University of Minnesota, USA, 3 days, February.
- N. Tlatli-Hariga and A. Ben Abda, University of Tunis, Tunisia, 3 days, February.
- M. Sosonkina, University of Iowa, USA, 2 weeks, May.
- N. Nassif, American University of Beirut, Lebanon, 1 week, June.
- M. Al Ghoul, American University of Beirut, Lebanon, 2 weeks, June.
- S. Georgescu, Romania, 3 days, June.
- M. Moakher, University of Tunis, Tunisia, 2 weeks, July.
- D. Mezher, University of Saint-Joseph in Beirut, Lebanon, 1.5 month, July-August.
- R. Aboulaich, EMI, Rabat, Morroco, one week in September.
- E. Kamgnia, University of Yaounde, Cameroon, 2 months, September-October.

# 10. Bibliography

## Major publications by the team in recent years

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[2] 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.

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

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

[5] 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.

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

[7] 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.

## Doctoral dissertations and Habilitation theses

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[9] A. BEAUDOIN, S. HUBERSON, E. RIVOALEN. *From Navier-Stokes to Stokes by means of particle methods*, in "Journal of Computational Physics", to appear.

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