INRIA

INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Team SAGE

Simulations and Algorithms on Grids for Environmental Applications

Rennes

THEME NUM

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1. Team

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2. Overall Objectives

2.1. Overall Objectives

Keywords: *accuracy*, *eigenproblems*, *environment*, *geosciences*, *grid computing*, *grid computing*, *high-performance computing*, *high-performance computing*, *least-squares problems*, *linear algebra*, *parallel 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,
- parallel and grid computing,
- environmental applications, mostly in hydrogeology and geophysics.

3. Scientific Foundations

3.1. Linear and Nonlinear Problems

Keywords: *Krylov subspace*, *LU factorization*, *Newton method*, *iterative method*, *preconditioning*, *sparse matrix*.

Participants: Anthony Beaudoin, Jocelyne Erhel, Frédéric Guyomarc'h, Laura Grigori, Hussein Mustapha, Bernard Philippe.

Linear systems $Ax = b$, where A is a large sparse matrix, arise in many scientific applications.

3.1.1. Direct methods

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, thus memory requirements and floating-point operations [25].

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 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 $P_1D_1AD_2$ 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 works on parallel sparse direct solvers and is involved in the development of SuperLU_DIST [4].

3.1.2. Iterative methods

The most efficient iterative methods build a Krylov subspace, for example $\{x_0, Ax_0, \cdots, A^kx_0\}$. 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 [31][29]. 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 [23].

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

3.1.3. 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 is required [28][22]. 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 [30][24]. The team studies stationary and Newton-Krylov methods, where the linearized problem is solved by a Krylov method [2].

3.2. Eigenvalue Problems

Keywords: *Arnoldi, Davidson, Lanczos, eigenvalue, pseudo-spectrum, singular value.*

Participants: Guy Antoine Atenekeng Kahou, Frédéric Guyomarc'h, Bernard Philippe.

3.2.1. Davidson Methods

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 $H_m = V_m^TAV_m$; then

the Ritz pair $(\lambda, x = V_m z)$ is an approximation of an eigenpair of A. The specificity of the method comes from the way to augment the subspace for the next step. In contrast with the Lanczos method, which is the method to refer to, the subspaces are not Krylov subspaces (see the definition in section 3.1), 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 inexact Newton step ; vector y is sought such that $y \perp x$ and such that $x + y$ is an eigenvector of A ; by neglecting the second order terms with respect to $\|y\|$, the problem to be solved is

$$\begin{aligned} r &= (\lambda I - A)y \\ \text{where } r &= Ax - \lambda x \text{ et } y \perp x \quad . \end{aligned}$$

The Davidson methods consists of solving this system approximately. The Jacobi-Davidson method attempts to solve the equation by applying several steps of the Conjugate Gradient method. The former Davidson methods approximately solve the first equation (relaxing the orthogonality constraint) by replacing A by a preconditioner M. The behaviour of the Davidson method is studied in [3] while the Jacobi-Davidson method is described in [32]. These methods bring a substantial improvement over the Lanczos method when computing the eigenvalues of smallest amplitude. For that reason, the team considered Davidson methods to compute the smallest singular values of a matrix B by applying them to the matrix $B^T B$ [3].

3.2.2. Pseudospectrum

In 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 the given complex domain.

One way to rewrite the problem is to consider a neighborhood $\mathcal{V}$ of matrix A and to characterize the set of the eigenvalues of matrices $B \in \mathcal{V}$. For pseudospectrum, the neighborhood $\mathcal{V}$ is defined by the 2-norm : given $\varepsilon > 0$, the pseudosepctrum $\Lambda_\varepsilon(A)$ is the set of all the eigenvalues of the matrices $A + \Delta$ where $\|\Delta\| \leq \varepsilon \|A\|$. It can also be characterized by :

$$\lambda \in \Lambda_\varepsilon(A) \Leftrightarrow \sigma_{\min}(A - \lambda I) \leq \varepsilon \|A\|$$

where $\sigma_{\min}(A - \lambda I)$ stands for the smallest singular value of matrix $(A - \lambda I)$.

This definition was simultaneously introduced by Godunov [27] and Trefethen [33].

The first direction to draw the pseudospectrum is to compute $\sigma_{\min}(A - \lambda I)$ when λ runs over an a priori given grid over the complex domain under consideration. However, this approach involves too many operations and now the most efficient methods are based on path following procedures. Following that approach, the team designed the reliable and parallel method PPAT [6], described in section 5.2.

4. Application Domains

4.1. Environment

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

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. Geo-chemical processes include, among others, radioactive decay, aqueous speciation and red-ox reactions, interface reactions, precipitation and dissolution of minerals and colloids. Hydrodynamic processes include density-driven groundwater flow, transport of solutes by advection and

diffusion. Reactive transport models are complex non-linear PDEs, coupling the transport engine with the reaction operator. Density-driven flow and transport models are also complex non-linear PDEs, coupling the flow operator with the transport engine. The main objective of the team is to design and to implement an efficient and robust numerical method to solve these 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 corresponding module was developed from the set `templates` of the Netlib site. The initial code, implemented in the MATLAB syntax, was transformed in order to allow a variable number of parameters in the calling sequence, and a user-defined operator.

SCILIN includes a module for the construction of preconditioners from incomplete factorizations. The module interfaces the SPARSKIT library (a FORTRAN coded library developed by Y. Saad at the University of Minneapolis).

SCILIN includes a third module for generating test cases of sparse matrices. For that purpose, the module includes procedures for loading and saving matrices under the format of the library MatrixMarket which provides a very large set of sparse matrices. It includes some SPARSKIT procedures as well.

SCILIN is now compliant with SCILAB 3.0 and will be included in a future release of SCILAB. It can be downloaded at the address : http://www.irisa.fr/aladin/codes/SCILIN/.

5.2. PPAT : pseudo-spectrum

Participants: Edouard Canot [corresponding author], Frédéric Guyomarc'h, Bernard Philippe.

PPAT (Parallel PATh following software) is a parallel code for following 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 from: http://www.irisa.fr/aladin/codes/PAT/.

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

6. New Results

6.1. Linear and Nonlinear Problems

6.1.1. LU factorization of large unsymmetric matrices

Participant: Laura Grigori.

During Laura Grigori's postdoctoral position at UC Berkeley and Lawrence Berkeley National Laboratory, together with Professor James Demmel and Xiaoye S. Li, we worked on the development of parts of SuperLU_DIST, a widely used software to solve large sparse systems of linear equations on supercomputers. SuperLU_DIST had been previously developed at UCB and LBNL with NSF and DOE funding, and has been used to solve problems from accelerator design to quantum mechanics. We have identified several algorithmic improvements to SuperLU to improve its *scalability*, i.e. ability to run efficiently on the growing numbers of parallel processors available in modern supercomputers, and improve its *applicability*, i.e. ability to solve more general classes of large sparse linear systems for which its current "complete factorization" approach is inappropriate. During this year, we continued our collaboration to make these improvements to SuperLU_DIST [17][16].

A goal of this collaboration is also to apply SuperLU_DIST to challenging problems in hydrogeology that the team works on, namely saltwater intrusion and reactive transport of contaminant in groundwater flows.

6.1.2. Parallel symbolic factorization algorithm

Participant: Laura Grigori.

In the last several years, there has been significant research effort in the development of fully parallel direct solvers for computing the solution of large unsymmetric sparse linear system of equations. Earlier work has adressed the parallelization of the numerical factorization, because its complexity is generally of higher order compared to the other steps. This is now a well understood problem and for example the algorithm implemented in SuperLU_DIST solver proved to be highly parallel and efficient. Then techniques were proposed for computing fill-reducing ordering in parallel and more recent research focused on the development of efficient parallel algorithms for permuting large entries on the diagonal. All these algorithms use distributed data structures, and in particular the input matrix A is distributed over the processors. They offer an overall good scalability. This includes memory scalability, i.e. if both the problem size and the number of processors are increased by the same factor, then the same amount of memory is used per processor.

The symbolic factorization is the only step that is sequential and that needs the structure of the input matrix and of the factors to reside on one processor. Thus it is currently the memory bottleneck in the SuperLU_DIST solver. It is critical to decrease the memory requirements of this step.

We designed and implemented a memory scalable parallel symbolic factorization algorithm, which is suitable for general sparse unsymmetric matrices. This algorithm exploits the parallelism exposed by the sparsity of the matrix. The parallel fill-reducing ordering step partitions the matrix in a suitable way for parallel factorization and also provides a tree structure representing the dependencies among computations. All this information is exploited in our algorithm. Issues of memory balance, as well as load balance and communication are well addressed in this development.

This work is presented at the International Workshop on Parallel Matrix Algorithms and Applications, Marseille, France, in October 2004 [15].

6.1.3. Structure prediction for sparse LU factorization with partial pivoting

Participant: Laura Grigori.

This research considers the problem of structure prediction when solving the linear system $Ax = b$ by Gaussian elimination, where A is a $n \times n$ nonsingular and nonsymmetric matrix and b is an n-vector. In this context, new results were obtained this year, in a continued collaboration with John Gilbert from the University of California at Santa Barbara.

When A is sparse and pivoting is necessary, the structure of L and U depends on the structure of A and on the row interchanges. As the row interchanges are determined while doing the numerical factorization, only upper bounds of the structures of L and U can be determined prior to the numerical factorization. Many researches aim to predict the structures of L and U as tight as possible, and the existing results in the litterature assume a combinatorial assumption on the structure of A, which is the strong Hall property.

Our primary purpose is to predict bounds for the nonzero structure of the factors L and U under a weaker combinatorial assumption, which is the Hall property. For this, we study the interplay between the

combinatorial properties of the nonzero structure of the matrix A and the algebra associated with the LU factorization.

In [26], George and Ng predict an upper bound of the nonzero structure of L and U (called the row merge graph) that contains the nonzeros in L and U for all possible row permutations which can later appear in the numerical factorization due to pivoting. Motivated by its usage, in our previous work we have studied the properties of the row merge graph when used to predict the structure of the factors L and U when the matrix A satisfies only the Hall property. First, we considered a symbolic analysis, that is we ignored the possibility of numerical cancellation during the factorization. With this assumption, we showed that the row merge graph is a lower bound for the factors L and U. In other words, for every edge of the row merge graph of a Hall matrix, there is a permutation such that this edge corresponds to a symbolic nonzero in the factors $L + U$.

In the research conducted this year, we consider an exact analysis, that is we assume only that the nonzero values in A are algebraically independent from each other. By a simple counterexample, we show that the row merge graph is not a tight bound for the factors L and U in the exact sense. This means that the row merge graph predicts as nonzero elements of L and U, that during the actual factorization are zeroed, and that for any valid rows permutations and regardless the nonzero values of A.

We determine tight exact bounds for the nonzero structure of L and U, under the assumption that the matrix A satisfies the Hall property. That is, we identify necessary and sufficient conditions, in terms of paths in the bipartite graph of A, for an element of L and U to become nonzero during the factorization with row interchanges. In the future, we plan to determine efficient algorithms for the computation of this upper bound.

This work was submitted to the SIAM Conference on Computational Science and Engineering, February 2005.

6.1.4. *Incomplete LU factorization of a large sparse matrix*

Participants: Laura Grigori, Jocelyne Erhel.

This work was partly undertaken as a project by J. S. Tchaptchet, student at DEA of Yaounde, Cameroon.

The incomplete factorization is a popular preconditioning technique, and it consists of dropping some filled-in entries of the factors L and U during the factorization. There are several criteria to decide which entries to drop. The goal of our reasearch is to investigate a combination of these criteria and consider new ones, that will allow the development of a robust preconditioner, which in adition has good scalability properties. These include, but are not limited to, methods that consider dropping entries that break up the problem in a set of independent problems.

A longer term research goal of this research is the development of a parallel incomplete factorization for a distributed memory environment.

6.1.5. *Rank Revealing QR factorization of sparse matrices*

Participant: Bernard Philippe.

Through a cooperation with D. Mezher from the University St Joseph in Beyrouth, we first designed a code which computes the QR factorization of a sparse matrix based on a multifrontal scheme using Householder transformations.

The previous work is now extended to Rank Revealing QR factorization (RRQR) of sparse matrices. The new code includes column pivoting. Consequently, at step k, a precise estimation of the condition number of the corresponding set of k columns of the matrix is given. This procedure provides a way to replace at a lower cost a Truncated Singular Value Decomposition of the matrix, for pseudo-inverse. A special care is put on the computer management of the matrix storage.

A first version of the code is now available. The experiments on a test suite exhibit the high cost of the procedure due to an important amount of fill-in when compared to the existing codes which do not address the rank-revealing issue [20].

Two directions are now considered to solve this problem. The first one is to make more flexible the criterion on the column order selection in order to introduce a measure of the future fill-ins in the selection. Such a technique would imply a post-treatment to address situations where the new criterion fails. The second

direction is to consider dropping strategies for building new preconditioners. The study for comparing a given dropping procedure with or without a column pivoting monitored by a rank reavealing strategy has to be done.

6.1.6. Supernodal QR factorization

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

This work is done in collaboration with B. Canet, from the Ascii team at INRIA-Rennes.

To achieve high performance, we start to develop a framework for QR factorization which heavily uses the supernode paradigm. With this strategy we can guaranty that all operations call the BLAS3 subroutines. This framework has to be highly configurable so that we can test the classical algorithms (right-looking and multifrontal) for the factorization.

This supernodal approach unfortunately has a major drawback for the rank revealing goal : it cannot handle any permutation on the columns, because of the block scheme. Therefore we consider to develop a post processing step to obtain a full rank revealing procedure.

6.2. Eigenproblems

6.2.1. Computing eigenvalues and Domain Decomposition

Participants: Guy Antoine Atenekeng Kahou, Bernard Philippe.

This work has been done in cooperation with E. Kamgnia, from the University of Yaoundé I and is related to G. Atenekeng's PhD thesis.

The advantage of the Domain Decomposition is to break an initial huge problem into a sequence of coupled problems of much smaller size. Such an approach has been thoroughly studied during the two last decades but almost only for solving linear and nonlinear equations. We consider the situation where eigenvalues of an operator based on Domain Decomposition must be computed.

When internal eigenvalues are to be computed, a necessary shift-and-invert technique implies to solve a linear system at each iteration of the eigenvalue solver. For solving linear systems, the class of methods which constitutes the main reference in Domain Decomposition is the Schwarz method under its different versions. It has been proved in the literature that these methods can be viewed as relaxation methods corresponding to some splittings of the matrix. We have given an explicit expression of the splitting in the case of the so-called Multiplicative Schwarz method. This expression is more effective when the splitting is used as a preconditioner of an iterative method. We also proved that, with a Krylov method, this preconditioner implies an early termination of the process [19].

The present research develops eigenvalue solvers using the previous preconditioners. The goal of the work is to obtain a set of parallel programs which can compute some eigenvalues and eigenvectors of very large matrices. The test matrices are selected in quantum chemistry and in structural mechanics.

6.2.2. Distance to singularity of operators

Participant: Bernard Philippe.

The distance of a matrix to the set of the singular matrices, when expressed with the Frobenius norm, is equal to the smallest singular value of the matrix. Since several years, the team has been spending effort on the computation of this element. For very large matrices, the situation is still under research. A whole review on the computation of singular values on parallel computers will appear in a handbook [9].

6.2.3. Partial canonical structure extraction for large matrices

Participant: Frédéric Guyomarc'h.

This work 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 we can have convergence towards many eigenvalues at the same time.

6.3. Flow and transport of pollutants

6.3.1. 3D network of fractures

Participants: Jocelyne Erhel, Hussein Mustapha.

This work is related to H. Mustapha's PhD thesis and is done in collaboration with J.-R. de Dreuzy, from CAREN, University of Rennes 1, in the context of the Hydrogrid project (7.1.2).

The objective is to compute the steady-state flow in a large network of fractures ; after spatial discretization, it amounts to a huge sparse linear system.

Several steps are required to build the matrix of the system. The mesh generation is not a trivial task, since the network is not a classical 3D domain. Our choice is to use a 2D mesh generator in each fracture (EMC2, from the Gamma Inria team, with MEDIT for visualization) and to develop a software for matching all the intersections. Several problems arise due to the heterogeneous scales of the fractures. We have designed an automatic mesh generator for large general networks of fractures.

Then, we use a Mixed Finite Element method to discretize the flow equation. We have modified procedures of the TRACE software (developed by H. Hoteit and P. Ackerer at IMFS, Strasbourg) in order to take into account the contributions from all the fractures and their intersections. Finally, we use a global sparse direct solver (currently UMFPACK).

Preliminary results show that we are able to deal with large general fracture networks. It has been submitted to SIAM conference on Geosciences, June 2005.

6.3.2. Saltwater intrusion

Participants: Édouard Canot, Caroline de Dieuleveult, Jocelyne Erhel.

This work is done in the context of the Hydrogrid project (7.1.2), in collaboration with C. Perez, from 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 develop a numerical software for density-driven flow and transport in porous media. The original version was provided by IMFS.

We have developed several test cases, including Henry and Elder test cases, along with different meshes. Figure 1 shows numerical results for Henry test case.

One objective is to reduce the CPU requirements of the sequential code. In both flow and dispersion modules, we have modified the matrix computations and we use a sparse linear direct solver (MUMPS, from the INRIA-team Graal), which is in this case more performant than an iterative solver.

The most CPU time expensive parts, solving the flow and dispersion linear systems, are thus parallel thanks to the parallel MUMPS software, using MPI. We have run experiments on a cluster at IRISA and a cluster in Grenoble. Because the matrix is small and very sparse, good speed-ups are obtained only if the cluster network is very fast.

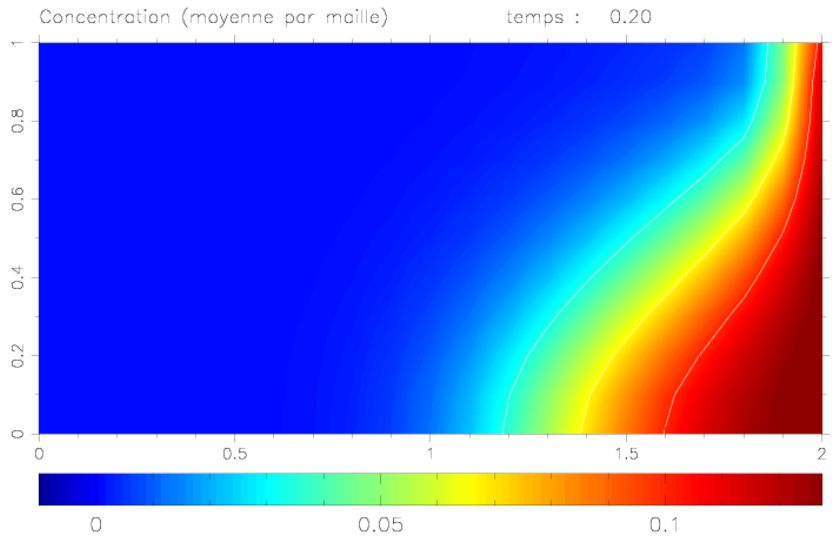

Figure 1. Henry test case

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 CORBA.

Currently, a fixed-point scheme iterates between flow and transport at each time step. We are working on a new coupling method, with a fully explicit convection term, which allows to compute first the transport then the flow at each time step.

6.3.3. Reactive transport in porous media

Participant: Jocelyne Erhel.

This work is done in the context of the Hydrogrid project (7.1.2) and the MOMAS GdR (7.1.1), in collaboration with M. Kern (Estime Inria team at Rocquencourt). It was partly undertaken as a project from A. Haidar, student at DEA of Beyrouth, Lebanon.

Reactive transport models are complex nonlinear PDEs, coupling the transport engine with the reaction operator. We consider here chemical reactions at equilibrium. After spatial and temporal discretisation, the problem to solve at each time step is a huge system of non-linear equations. Different numerical methods have been considered. Most approaches use the so-called sequential iterative method, which is indeed a block Gauss-Seidel non-linear iterative method. Another method is the so-called Global Implicit or Direct Substitution approach, based on the Newton method.

We have developed a 1D model in Matlab, in order to compare both methods. In both approaches, we have used the Matlab function ode15s, a DAE solver which controls the order of the method and the time step. Preliminary results seems to show that the Newton method outperforms the Gauss-Seidel method, because it converges faster and delivers more accurate solutions.

This work has been submitted to SIAM conference on Geosciences, June 2005.

6.3.4. Transient and permanent flow in heterogeneous porous media

Participants: Anthony Beaudoin, Jocelyne Erhel.

This work is done in collaboration with J.-R. de Dreuzy, from CAREN, University of Rennes 1, in the context of Grid'5000 project (7.1.3).

Prediction of natural underground flow circulation and solute transport have brought up the concern of medium heterogeneity. This broad-ranged heterogeneity induces high flow localization and channeling at virtually all scales of the medium and thus prevents the use of any homogenization approach. The heterogeneity is not completely random but has found to be nested and well-modeled by fractals. Mathematically expressed, finding a new flow equation consists in relating the time evolution to the spatial heterogeneity in a consistent way at different scales. To answer this question, we use both theoretical physical arguments and a numerical model. Numerical simulations are computationally intensive since they have to handle a large number of spatially extended domains on a wide range of time scales.

For transient models, we have used the LSODES package, which is adapted to stiff ODE problems. One objective is to replace the included sparse linear solver by a more efficient one. The work has been published in [13].

For stationary models, we currently use either PETSC or UMFPACK to solve the linear systems. We plan to use PSPACES or parallel preconditioned iterative solvers and to run experiments on clusters and experimental grids to increase performances.

6.4. Graphical tools

6.4.1. Visualization Library

Participant: Édouard Canot.

In order to visualize scientific results, two options are available :

- results are stored in files and are visualized by a post-processing software;
- results are visualized during computation via appropriate calls of a graphical library.

The second possibility is generally preferred during development because of the need to quickly validate updates. Our choice is to use the PGPLOT library, which is free, available on Internet at the following URL : http://www.astro.caltech.edu/~tjp/pgplot/, and widely spread on Linux machines.

PGPLOT is a high-level routines package for scientific use. It includes many drivers, such as X11, GIF, PostScript, etc. All routines have a Fortran interface. The X11 driver is a good choice for visualizing data across a TCP/IP network. It is very efficient because it calls only low-level X11 routines, without using any toolkit (Xt or Motif). All sources of PGPLOT are also available. Besides PGPLOT, other graphical libraries exist but they do not have all the advantages of PGPLOT : e.g. DISLIN is free for Linux boxes but only binaries versions are provided; on the other hand, PSPLOT is source-free but produces only PS files.

We have developed a library, called Viz2D, which is a user interface to a slightly modified PGPLOT package : it is a set of Fortran routines intended to make data plot easy via a few calls. It is currently restricted to data spread over a regular rectangular 2D mesh. It can draw array data, contours and arrow fields and has the following characteristics :

- each can be created in a X11, GIF and/or color EPS device. Color are compressed via the ZLIB library in the EPS files;
- each graphic window can be subdivided in up to 6 sub-panels;
- 5 colormaps are predefined (4 colors and one in grey shades) and personal colormaps can be defined by the user. These colormaps can be stretched by any analytical functions in order to emphasize some sub-range of the colormap;
- Arrow color is automatically chosen to be visible on the background;
- array data can be viewed by a 'pcolor' routine (pseudo-color) which can use 'flat' or 'bi-linear' shading. Arrays can be flipped and/or rotated.

Our library Viz2D has been tested under Linux and SunOS. It has been used in the Hydrogrid (7.1.2) and IFREMER (7.1.4) projects, and also in the F90 version of Gridmesh (6.4.2).

6.4.2. Structured mesh generator

Participants: Édouard Canot, Frédéric Guyomarc'h, Caroline De Dieuleveult.

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 (6.4.1) via a Fortran 90 program. Primarily, it has been designed to generate a 2D mesh and connectivity relationships, via an easy and quick process, for the Hydrogrid project (7.1.2).

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 arbitrary number of 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 (200 by 200) due to internal management of graphical objects by Matlab. The F90 version can generate and/or modify big meshes (up to 4000 by 4000), but requires at least 2.2 Gb of RAM.

The main drawback of Gridmesh is that the created mesh file is very big (e.g. 350 Mb for a 1000 by 1000 mesh) because data are currently written under the ASCII format. Work is in progress to write directly compressed binary data by using the zlib.

7. Other Grants and Activities

7.1. National Grants

7.1.1. GdR MOMAS - Numerical models for nuclear waste disposal

Participant: Jocelyne Erhel.

See https://mcs.univ-lyon1.fr/MOMAS/

The working group MOMAS is led by A. Bourgeat from the university of Lyon and include many partners from CNRS, INRIA, universities, CEA, ANDRA, EDF, BRGM. It covers many subjects related to mathematical modelling and numerical simulations for nuclear waste disposal problems. We participate in the subject devoted to multiphysics models and collaborate with M. Kern, from the INRIA-team Estime, in the project entitled "Numerical schemes and coupling algorithms for reactive transport problems". See section 6.3.3.

7.1.2. 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. We have specified the software components along with their interfaces and the scheme of communications. We have also specified the parallel algorithms used in each component. See sections 6.3.2,6.3.1, 6.3.3.

7.1.3. 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 different projects on hydrogeology involve very large sparse linear systems. Our objective is to use the clusters and the grid built at INRIA-Rennes to deal with large 3D domains and to run multi-parametric simulations.

7.1.4. IFREMER contract

Participants: Édouard Canot, Jocelyne Erhel, Samih Zein.

IFREMER contracts, Nos. 03/2 210 412 and 03/2 210 413
Partners : Irisa, IFREMER
Title : Numerical model for the propagation of elastic waves
time : from July 2003 until March 2004 and from June 2004 until January 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 objective of this study is 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.

In a first step, we have designed several test cases relevant for IFREMER applications. Then we have improved performances and developed visualisation tools based on our Viz2D graphic library (6.4.1). For example, small linear systems solving has been improved by removing the Cramer method originally used and making calls to appropriate routines of the LAPACK library.

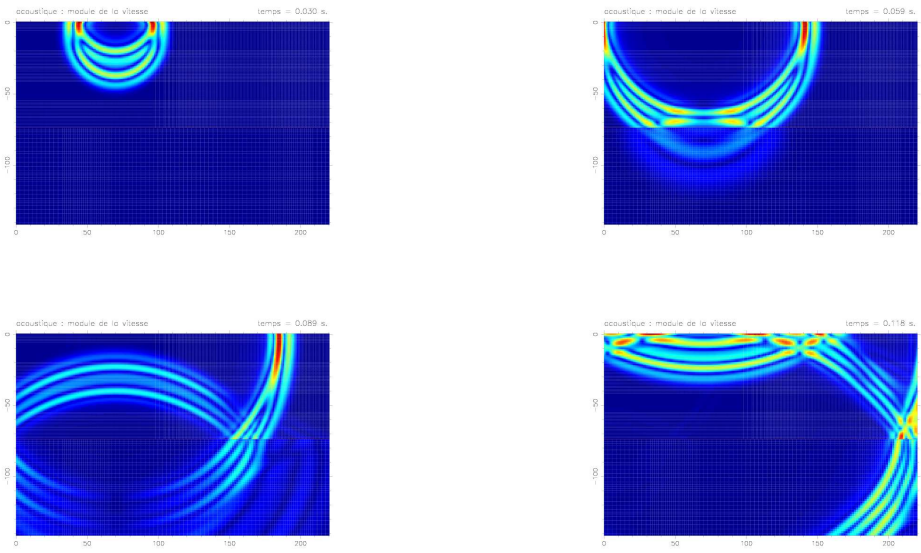

Figure 2. Numerical simulation of acoustic wave propagation in sea-water and under-sea ground (red line is the sea floor).

In a second step, we have designed a numerical scheme to consider general water-soil interfaces. Our approach uses a stairway discretisation of the interface. Preliminary results show consistency with previous results.

The next part of this study will use inverse methods to try to find layer properties in the ground, only from acoustic measurements recorded near the sea surface by a ship. Comparison will be possible due to a lot of results from a recent oceanographical campaign.

7.2. European Grants

7.2.1. ERCIM Working group - Matrix Computations and Statistics

Participants: Jocelyne Erhel, Bernard Philippe.

ERCIM Working Group, started in 2001.
Title : Matrix Computations and Statistics
Chairmen : B. Philippe (team Sage) and E. Kontoghiorghes (U. Neuchatel)
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 2004, the WG met in Prague (August 27-29) in parallel with COMPSTAT 2004 conference.

7.2.2. 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.

7.2.3. DOD ECONET project

Participant: Edouard Canot.

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

ECONET is a European program which monitors joint projects between EU countries. Its main objectives are firstly, to help to build a reserch framework in EU and secondly, to promote links between old EU countries and Balkan countries or other new, emergent countries. ECONET is 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;
- exhautive measurements by use of cameras and laser velocimetry;
- modelization and numerical computations via specific methods.

The aim of this project is a good comprehension of mechanical and/or physico-chemical phenomena which drive ink-jet drop formation. Today, ink-jet setup produces micro-drops of the order of 10 picoliters. We hope to go down to only few picoliters.

Ink-jet printing processes are characterized by small geometrical scales (50 to 100 μm) 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 involved are :

Froude number : $Fr = \dfrac{U^2}{gD}$

Weber number : $We = \dfrac{\rho U^2 D}{\sigma}$

Reynolds number : $Re = \dfrac{\rho U D}{\mu}$

Due to high Reynolds value, the liquid flow can be approximated by a scalar potential that verifies a Laplace equation. The dynamic boundary condition on the free-surface is derived from the classical transient Bernoulli equation. When dealing with nonlinear 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. The Laplace equation is numerically solved by a Boundary Element Method (BEM), which is very fast and efficient because computing occurs only on the fluid boundary. In comparison with usual BEM codes that can be found in literature and/or internet [1], our version has the following general features :

- axisymmetric geometry (the computation is not fully 3D);
- high-order BEM (cubic splines for geometry, Hermite cubic basis functions for the unknowns);
- semi-implicit scheme for the ODE system (dynamic and kinematic parts) coupled with a stability criterion which is derived from linear analysis via symbolic calculus only (this feature avoids to compute, at each time step, eigenvalues of a big matrix);

Figure 3 shows a numerical simulation, using the described BEM method. Parameters are : $Fr = \infty$ (no gravity influence), $We = 1, Re = 50$. Drop interface position is drawn by the blue curve.

Our software is related to the following recent publications [14][10]. [2].

7.3. International Grants

7.3.1. 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 African and middle-East research in applied 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), the initial network includes seven teams (five teams in French speaking sub-Saharan countries, a team in Tunisia and one in Lebanon).

In this project, INRIA is responsible for all the visits of African researchers to research groups in France.

[1] *e.g.* http://dehesa.freeshell.org/BEMLIB/ or http://www.boundary-element-method.com/
[2] See also : http://test.interface.free.fr/ (test cases 21 & 22)

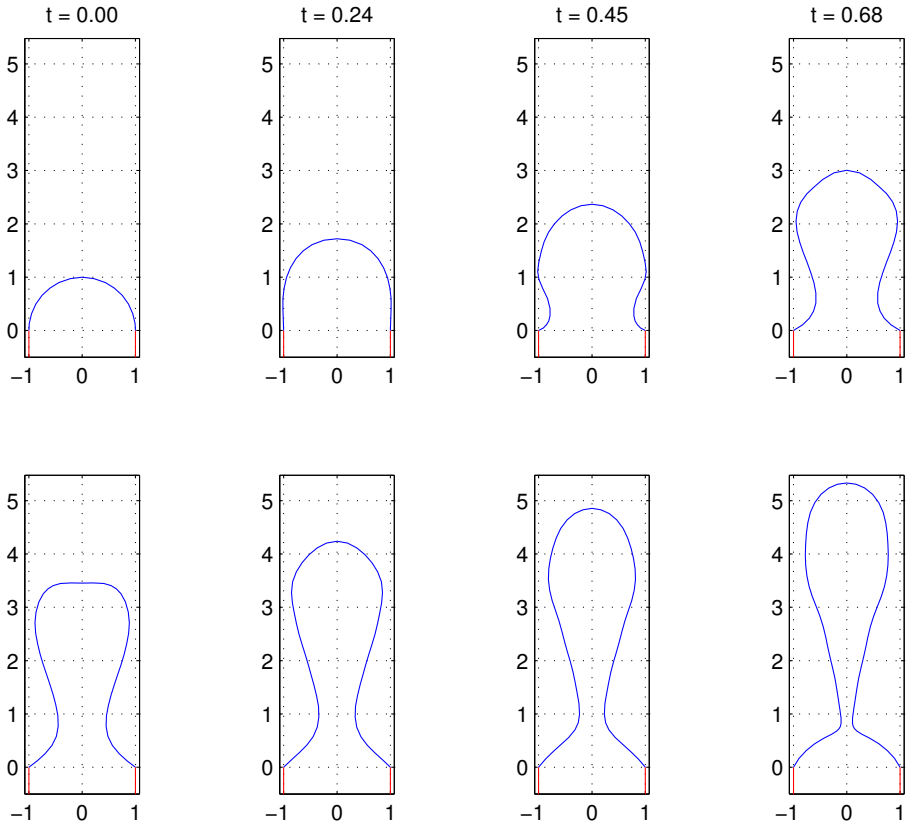

Figure 3. Numerical simulation of ink-jet drop formation

8. Dissemination

8.1. Program committees and Editorial Boards

- J. Erhel was member of the program committee of ICS'2004, Saint-Malo, France.

- B. Philippe was member of the following program committees :

- PMAA'04 and MSO, October 18-22, Luminy, France.
- CARI'04, November 22-25, 2004, Hammamet, Tunisia.

- 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)

8.2. 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 is member of the Evaluation Board of INRIA.

- 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, since November 2002.

- 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 also for the recruiting.

- B. Philippe is involved in the relations between INRIA and research teams in Africa : he is the INRIA coordinator for the SARIMA project and the secretary of the CARI permanent committee.

- B. Philippe is correspondent for the agreement between the University of Rennes 1, the Lebanese University and AUF (Agence Universitaire Francophone) which supports the DEA.

8.3. Teaching

- É. Canot, J. Erhel and H. Mustapha taught about Applied Mathematics (MAP) for DIIC, IFSIC, Rennes 1 (first year). Lecture notes on http://www.irisa.fr/aladin/perso/erhel/

- J. Erhel gave a one-week course in February on Methods for Solving Large Systems, in Beyrouth (DEA de mathématiques appliquées, co-organized by the Lebanese University, EPFL of Lausanne, IRISA and University of Reims).

- J. Erhel gave a one-week course in March on Numerical models and grid computing applied to hydrogeology problems, in Tunis (First semester of the UNESCO Chair at LAMSIN - High Performance Computing, coordinator Bernard Philippe). See http://www.tn.refer.org/unesco/semestre1/semestre1-eng.htm. Lecture notes on http://www.tn.refer.org/unesco/semestre1/Cours-sem1/course_documents.html

- 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.

- F. Guyomarc'h has supervised projects in C for magistère de mathématiques, ENS Cachan Rennes (second year).

- F. Guyomarc'h gave lectures on graph theory (ALG) for the DIIC (second year), IFSIC, University of Rennes 1

- B. Philippe gave a one-week course, in June, on Parallel Algorithms in Linear Algebra, in Yaounde (DEA d'informatique).

- B. Philippe taught three courses in Tunis, on the following topics : methods for solving very large systems, parallelism in numerical linear algebra, eigenvalue problem solvers.

8.4. Participation in conferences

- E. Canot and F. Guyomarc'h : communication to Scilab-2004 International Conference, Paris, December.

- J. Erhel : communication to France-Korea Joint Workshop on Grid Computing - Application and Middleware system, Irisa, Rennes, July.

- J. Erhel : communication to RedGrid workshop, Bordeaux, March.

- J. Erhel : participation in International Conference on Supercomputing, Saint-Malo, France, June.

- J. Erhel : participation in Irisa School on Signal Processing, Cesson-Sévigné, France, October.

- L. Grigori : communication to SIAM Conference on Parallel Processing for Scientific Computing and participation in Workshop on Combinatorial Scientific Computing, San Francisco, USA, February.

- L. Grigori : communication to PARA'04 Workshop on State-of-the-Art in Scientific Computing, Copenhagen, Denmark, June.

- L. Grigori : communication to International Workshop on Parallel Matrix Algorithms and Applications, Marseille, France, October.

- F. Guyomarc'h organized "Les journées pédagogiques de l'Ifsic" (June, 21st to 23rd at Vannes) about software components.

- B. Philippe : communication to COMPSTAT Conference and 5th Workshop of the ERCIM working group "Matrix Computations and Statistics", Vienna, Austria, August.

- B. Philippe and G. Ateneke : communication to International Workshop on Parallel Matrix Algorithms and Applications, Marseille, France, October.

- B. Philippe : participation in CARI'04, Hammamet, Tunisia, November.

- S. Zein : participation in CEA-INRIA-EDF Summer School on Numerical Analysis, Numerical and computing methods for coupling physical models.

8.5. International exchanges

8.5.1. Visits

- E. Canot has visited for 4 days, November 25-28, the University of Poytechnics of Bucarest, Romania, to work on the DOD-ECONET project.

- F. Guyomarc'h has been invited for two weeks in July at HPC2N, University of Umeå, Sweden.

- L. Grigori has visited for 2 days, February 23 and 24, the Lawrence Berkeley National Laboratory, to work with Esmond Ng and Xiaoye S. Li.

- L. Grigori has visited for two months, from July 1st to September 3rd, the University of California at Berkeley, to work with Professor James Demmel and his group.

- B. Philippe was invited professor at ENIT, Tunis, Tunisia, during one year, from September 2003 until August 2004. During that time, he organized the first semester of the UNESCO Chair "Mathematics and Development", which is granted to the LAMSIN (Laboratoire de Modélisation et de Simulation Numérique dans les Sciences de l'Ingénieur). This semester, "High Performance Computing", included 8 one-week courses on Parallelism, Linear Algebra and Applications.

8.5.2. Visitors

The team has invited the following persons :

- M. Maboub, University of Tlemcen, Algeria, one month, December 2003.

- E. Kamgnia, University of Yaounde, Cameroon, three months, from August until October 2004.

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