

*Project-Team ALADIN**Advanced Algorithms for Scientific
Computing**Rennes*

THEME 4B

The logo features the word "Activity" in a white serif font, with a large, light grey "A" to its left. A horizontal line crosses through the "A" and "Activity". Below this, the word "Report" is written in a white serif font, with a large, light grey "R" to its left.

2003

Table of contents

1. Team	1
2. Overall Objectives	1
2.1. Overall Objectives	1
3. Scientific Foundations	2
3.1. Ordinary and Algebraic Differential Equations	2
3.2. Linear and Nonlinear Problems	4
3.3. Eigenvalue Problems	4
3.3.1. Davidson Methods	4
3.3.2. Pseudospectrum	5
4. Application Domains	5
4.1. Telecommunications	5
4.2. Molecular Dynamics	5
4.3. Environment	6
5. Software	6
5.1. SCILIN : linear solvers within SCILAB	6
5.2. PPAT : pseudo-spectrum	7
6. New Results	7
6.1. Ordinary and Algebraic Differential Equations	7
6.1.1. Long-time averages for molecular simulations	7
6.1.2. Constrained Hamiltonian systems and differential-algebraic systems	8
6.1.3. A Poisson system with boundary conditions	8
6.2. Linear and Nonlinear Problems	9
6.2.1. LDL^T factorization of a symmetric matrix of intervals	9
6.2.2. Rank Revealing QR factorization of sparse matrices	9
6.3. Flow and transport of pollutants	9
6.3.1. 3D network of fractures	9
6.3.2. Saltwater intrusion	10
6.3.3. Transient flow in heterogeneous porous media	11
6.4. Eigenproblems	11
6.4.1. Distance to singularity of operators	11
6.4.2. Partial canonical structure extraction for large matrices	12
6.5. Nonlinear free surface flows	12
6.6. Parallel algorithms for Markov models	13
7. Contracts and Grants with Industry	13
7.1. Industrial Grants	13
7.1.1. ALCATEL CIT - Numerical model for a Raman device	13
8. Other Grants and Activities	15
8.1. National Grants	15
8.1.1. ARC PRESTISSIMO 2003-2004	15
8.1.2. GdR MOMAS - Numerical models for nuclear waste disposal	15
8.1.3. HydroGrid - Multiphysics models in hydrogeology	15
8.1.4. IFREMER contract	15
8.2. European Grants	16
8.2.1. ERCIM Working group - Matrix Computations and Statistics	16
8.2.2. ERCIM Working group - Applications of Numerical Mathematics in Science	16
8.3. International Grants	16
8.3.1. INRIA/NSF Action - Robust and reliable preconditioners	16

8.3.2.	CAMEREAU Action - Hydrogeology in Cameroon	17
8.3.3.	SARIMA - Support to Research Activities in Africa	17
9.	Dissemination	17
9.1.	Programme committees and Editorial Boards	17
9.2.	INRIA and University committees	18
9.3.	Teaching	18
9.4.	Participation in conferences	18
9.5.	International exchanges	19
9.5.1.	Visits	19
9.5.2.	Visitors	19
10.	Bibliography	19

1. Team

Head of project-team

Jocelyne Erhel [DR Inria]

Administrative assistant

Fabienne Cuyollaa [TR Inria]

Staff members (INRIA)

Philippe Chartier [DR]

Erwan Faou [CR]

Bernard Philippe [DR]

Faculty members (university of Rennes 1)

Frédéric Guyomarc'h [MDC]

Staff members (CNRS)

Édouard Canot [CR]

Ph. D. students

Hussein Mustapha [ACI-GRID grant, with CAREN, since October 2002]

Project technical staff

Caroline de Dieuleveult [from October 2003 until July 2005]

Research scientists

Michel Crouzeix [PROF., university of Rennes 1]

Haïscam Abdallah [MDC, university of Rennes 2]

2. Overall Objectives

2.1. Overall Objectives

Key words: *scientific computing, linear algebra, least-squares problems, eigenproblems, sparse matrices, differential equations, Hamiltonians, high-performance computing, grid computing, accuracy, environment, hydrology, molecular dynamics.*

Numerical simulation of physical phenomena can be split into several steps :

- Modeling,
- Mathematical study of the underlying equations,
- Design of the numerical scheme,
- Design of the solver,
- Implementation,
- Visualization and validation.

The research undertaken in Aladin is mainly concerned with the design of numerical schemes, algorithms, solvers and their implementation.

The main objective is to satisfy the two following quality criteria :

- Efficiency: run-time, memory requirements, etc.
- Reliability: convergence proof, bounds on the result, etc.

In order to implement these schemes and algorithms in a complete simulation process, the group implements them on parallel computers and applies them to physical problems, mainly for environment.

The research topics covered are :

- Ordinary and algebro differential equations,
- Nonlinear and linear problems,
- Eigenproblems.

3. Scientific Foundations

3.1. Ordinary and Algebraic Differential Equations

Participants: Philippe Chartier, Erwan Faou.

Key words: *ordinary differential equation, numerical integrator, invariant, Hamiltonian system, reversible system, Lie-group system.*

In many physical situations, the time-evolution of certain quantities may be written as a Cauchy problem for a differential equation of the form

$$\begin{aligned} y'(t) &= f(y(t)), \\ y(0) &= y_0. \end{aligned} \tag{1}$$

For a given y_0 , the solution $y(t)$ at time t is denoted $\varphi_t(y_0)$. For fixed t , φ_t becomes a function of y_0 called the *flow* of (1). From this point of view, a numerical scheme with step size h for solving (1) may be regarded as an approximation Φ_h of φ_h . One of the main questions of *geometric integration* is whether *intrinsic* properties of φ_t may be passed on to Φ_h . This question can be more specifically addressed in the following situations:

Reversible ODEs

The system (1) is said to be ρ -reversible if there exists an involutive linear map ρ such that

$$\rho \circ \varphi_t = \varphi_t^{-1} \circ \rho = \varphi_{-t} \circ \rho. \tag{2}$$

It is then natural to require that Φ_h satisfies the same relation. If this is so, Φ_h is said to be *symmetric*. Symmetric methods for reversible systems of ODEs are just as much important as *symplectic* methods for Hamiltonian systems and offer an interesting alternative to symplectic methods.

ODEs with an invariant manifold

The system (1) is said to have an invariant g whenever

$$\mathcal{M} = \{y \in \mathbb{R}^n; g(y) = 0\} \tag{3}$$

is kept *globally* invariant by φ_t . In terms of derivatives and for sufficiently differentiable functions f and g , this means that

$$\forall y \in \mathcal{M}, g'(y)f(y) = 0.$$

As an example, we mention Lie-group equations, for which the manifold has an additional group structure. This could possibly be exploited for the space-discretisation. Numerical methods amenable to this sort of problems are divided into two classes, according to whether they use g explicitly or through a projection step. In both cases, the numerical solution is forced to live on the manifold at the expense of some Newton iterations.

Hamiltonian systems

Hamiltonian problems are ordinary differential equations of the form:

$$\begin{aligned} \dot{p}(t) &= -\nabla_q H(p(t), q(t)) \in \mathbb{R}^d \\ \dot{q}(t) &= \nabla_p H(p(t), q(t)) \in \mathbb{R}^d \end{aligned} \tag{4}$$

with some prescribed initial values $(p(0), q(0)) = (p_0, q_0)$ and for some scalar function H , called the Hamiltonian. In this situation, H is an invariant of the problem. The evolution equation (4) can thus be regarded as a differential equation on the manifold

$$\mathcal{M} = \{(p, q) \in \mathbb{R}^d \times \mathbb{R}^d; H(p, q) = H(p_0, q_0)\}.$$

Besides the Hamiltonian function, there might exist other invariants for such systems: when there exist d invariants in involution, the system (4) is said to be *integrable*. Consider now the parallelogram P originating from the point $(p, q) \in \mathbb{R}^{2d}$ and spanned by the two vectors $\xi \in \mathbb{R}^d$ and $\eta \in \mathbb{R}^d$, and let $\omega(\xi, \eta)$ be the sum of the *oriented* areas of the projections over the planes (p_i, q_i) of P ,

$$\omega(\xi, \eta) = \xi^T J \eta,$$

where J is the *canonical symplectic* matrix

$$J = \begin{bmatrix} 0 & I_d \\ -I_d & 0 \end{bmatrix}.$$

A continuously differentiable map g from \mathbb{R}^{2d} to itself is called *symplectic* if it preserves ω , i.e. if

$$\omega(g'(p, q)\xi, g'(p, q)\eta) = \omega(\xi, \eta).$$

A fundamental property of Hamiltonian systems is that their exact flow is symplectic. Integrable Hamiltonian systems behave in a very remarkable way: as a matter of fact, their invariants persist under small perturbations, as shown in the celebrated theory of Kolmogorov, Arnold and Moser. This behavior motivates the introduction of *symplectic* numerical flows that share most of the properties of the exact flow. For practical simulations of Hamiltonian systems, symplectic methods possess an important advantage: the error-growth as a function of time is indeed linear, whereas it would typically be quadratic for non-symplectic methods.

Differential-algebraic equations

Whenever the number of differential equations is insufficient to determine the solution of the system, it may become necessary to solve the differential part and the constraint part altogether. Systems of this sort are called differential-algebraic systems. They can be classified according to their index, yet for the purpose of this expository document, it is enough to present the so-called index-2 systems

$$\begin{aligned} \dot{y}(t) &= f(y(t), z(t)), \\ 0 &= g(y(t)), \end{aligned} \tag{5}$$

where initial values $(y(0), z(0)) = (y_0, z_0)$ are given and assumed to be consistent with the constraint manifold. By constraint manifold, we imply the intersection of the manifold

$$\mathcal{M}_1 = \{y \in \mathbb{R}^n, g(y) = 0\} \times \mathbb{R}^m$$

and of the so-called hidden manifold

$$\mathcal{M}_2 = \{(y, z) \in \mathbb{R}^n \times \mathbb{R}^m, \frac{\partial g}{\partial y}(y) f(y, z) = 0\}.$$

This manifold $\mathcal{M} = \mathcal{M}_1 \cap \mathcal{M}_2$ is the manifold on which the exact solution $(y(t), z(t))$ of (5) lives.

There exists a whole set of schemes which provide a numerical approximation lying on \mathcal{M}_1 . Furthermore, this solution can be projected on the manifold \mathcal{M} by standard projection techniques. However, it is worth mentioning that a projection destroys the symmetry of the underlying scheme, so that the construction of a symmetric numerical scheme preserving \mathcal{M} requires a more sophisticated approach.

3.2. Linear and Nonlinear Problems

Participants: Jocelyne Erhel, Frédéric Guyomarc'h, Bernard Philippe.

Key words: *sparse matrix, Krylov subspace, iterative method, preconditioning, Newton method.*

Sparse linear systems $Ax = b$, where A is a large sparse matrix, arise in many scientific applications. Direct methods, based on the factorization $A = LU$, induce fill-in in matrices L and U . Renumbering techniques can be used to reduce this fill-in, thus memory requirements and floating-point operations. [39]. The most efficient iterative methods build a Krylov subspace, for example $\{x_0, Ax_0, \dots, A^k x_0\}$. If the matrix is symmetric positive definite, the method of choice is the Conjugate Gradient ; for symmetric indefinite 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 [44][42]. 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 implicitly 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. [37]. The team studies preconditioners for Krylov methods [3][9].

For linear least-squares problems $\min_x \|Ax - b\|$, direct methods are based on the normal equations $A^T Ax = A^T b$, 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 is required [41][36]. The team studies iterative Krylov methods for regularized problems, as well as rank-revealing QR factorizations.

Nonlinear methods to solve $F(x) = 0$ include fixed-point methods, nonlinear stationary methods, secant method, Newton method [43][38]. The team studies Newton-Krylov methods, where the linearized problem is solved by a Krylov method [5].

3.3. Eigenvalue Problems

Participants: Frédéric Guyomarc'h, Bernard Philippe.

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

3.3.1. 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 which builds a sequence of subspaces which the initial problem is projected onto. At every step, approximations of the sought eigenpairs are computed : let V_m be an orthonormal basis of the subspace at step m and let (λ, z) be an eigenpair of the matrix $H_m = V_m^T A V_m$; then the Ritz pair $(\lambda, x = V_m z)$ is an approximation of an eigenpair of A . The specificity of the method comes from 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 3.2), 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

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

The Davidson methods consist of solving approximately this system. The Jacobi-Davidson method attempts to solve the equation by applying several steps of the Conjugate Gradient method. The former Davidson methods solve approximately the first equation (relaxing the orthogonality constraint) by replacing A by

a preconditioner M . The behaviour of the Davidson method is studied in [6] while the Jacobi-Davidson method is described in [45]. These methods bring a substantial improvement over the Lanczos method when computing the eigenvalues of smallest amplitude. For that reason, the Aladin team considered them to compute the smallest singular values of a matrix B by applying them to the matrix $B^T B$.

3.3.2. Pseudospectrum

In applications, the eigenvalues of a non symmetric matrix are often needed to decide whether they belong to a given part of the complex plane (eg. 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 precisely the eigenvalues but to characterize whenever 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 the matrices $B \in \mathcal{V}$. For pseudospectrum, the neighborhood \mathcal{V} is defined by the 2-norm : given $\epsilon > 0$, the pseudospectrum $\Lambda_\epsilon(A)$ is the set of all the eigenvalues of the matrices $A + \Delta$ where $\|\Delta\| \leq \epsilon\|A\|$. It can also be characterized by :

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

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

This definition was simultaneously introduced by Godunov [40] and Trefethen [46].

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 Aladin team designed the reliable and parallel method PPAT [8].

4. Application Domains

4.1. Telecommunications

Participants: Philippe Chartier, Erwan Faou.

Laser physics considers the propagation over long space (or time) scales of high frequency waves. Typically, one has to deal with the propagation of a wave having a wavelength of the order of $10^{-6}m$, over distances of the order $10^{-2}m$ to 10^3m . In these situations, the propagation produces both a short-scale oscillation and exhibits a long term trend (drift, dispersion, nonlinear interaction with the medium, or so), which contains the physically important feature. For this reason, one needs to develop ways of filtering the irrelevant high-oscillations, and to build up models and/or numerical schemes that do give information on the long-term behavior. In other terms, one needs to develop high-frequency models and/or high-frequency schemes.

This task has been partially performed in the context of a contract with Alcatel, in that we developed a new numerical scheme to discretize directly the high-frequency model derived from physical laws.

Generally speaking, the demand in developing such models or schemes in the context of laser physics, or laser/matter interaction, is large. It involves both modeling and numerics (description of oscillations, structure preserving algorithms to capture the long-time behaviour, etc).

4.2. Molecular Dynamics

Participants: Philippe Chartier, Erwan Faou.

In classical molecular dynamics, the equations describe the evolution of atoms or molecules under the action of forces deriving from several interaction potentials. These potentials may be short-range or long-range and are treated differently in most molecular simulation codes. In fact, long-range potentials are computed at only a

fraction of the number of steps. By doing so, one replaces the vector field by an approximate one and alternates steps with the exact field and steps with the approximate one. Although such methods have been known and used with success for years, very little is known on how the “space” approximation (of the vector field) and the time discretization should be combined in order to optimize the convergence. Also, the fraction of steps where the exact field is used for the computation is mainly determined by heuristic reasons and a more precise analysis seems necessary. Finally, let us mention that similar questions arise when dealing with constrained differential equations, which are a by-product of many simplified models in molecular dynamics (this is the case for instance if one replaces the highly-oscillatory components by constraints).

4.3. Environment

Participants: 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. 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 [correspondant], Bernard Philippe.

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, coded 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.

The code was developed by Emeric Martin, during his one-year contract at INRIA in 2001.

SCILIN can be retrieved at the address : <http://www.irisa.fr/aladin/codes/SCILIN/>.

It will be included in a future lease of SCILAB.

5.2. PPAT : pseudo-spectrum

Participants: Edouard Canot [correspondant], 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 everywhere a derivative. 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 retrieved from: <http://www.irisa.fr/aladin/codes/PAT/>.

It is also included in the CD of the free softwares of INRIA:

<http://www.inria.fr/valorisation/logiciels/cederom.fr.html>

6. New Results

6.1. Ordinary and Algebraic Differential Equations

6.1.1. Long-time averages for molecular simulations

Participants: Philippe Chartier, Erwan Faou.

Given a Hamiltonian dynamics of the form (4), it is a common problem (for instance in molecular dynamics simulations) to estimate the *space* average of an observable A over a manifold S (say a surface of constant energy for instance)

$$\langle A \rangle := \int_S A(q, p) d\sigma(q, p), \quad (6)$$

through the limit of the *time* average

$$\langle A \rangle(T) := \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T A(q(t), p(t)) dt. \quad (7)$$

The conditions under which the two quantities coincide are not known in general and this is a difficult and largely open question linked to the *ergodicity* of the system. In contrast, if the Hamiltonian system is assumed to be *integrable*, a well-known result of Arnold states that, under a *diophantine* condition, the time-average converges to its space-counterpart with a rate of $1/T$.

In a first step, in collaboration with CERMICS, we have shown that the convergence of the *time* average (7) toward the *space* average (6) can be accelerated through the use of weighted integrals of the form

$$\int_0^T \varphi\left(\frac{t}{T}\right) A(q(t), p(t)) dt, \quad (8)$$

where φ is a *filter* function. This has led us to the definition of a close-to-optimal filter which brings a significant speed-up. To become of practical use, the integrals involved in the averages need to be discretized and evaluated not along the exact trajectory, which is obviously not available, but along a numerical approximation of it. In this context, symplectic integrators naturally come into play, since the length T of the interval of integration is allowed to become “as large as necessary” for the convergence to occur. The use of some basic symplectic schemes in combination with filtered averages define a practical method, which, in some physically relevant situations, has proven to be a real improvement over the usual averaging technique, as demonstrated by numerical experiments.

6.1.2. Constrained Hamiltonian systems and differential-algebraic systems

Participants: Philippe Chartier, Erwan Faou.

Constrained Hamiltonian systems with holonomic constraints (i.e. constraints involving only the positions) appear typically when dissipative forces (such as *friction*) may be neglected. In this situation, a Lagrange-type principle allows to write the equations of the dynamics as

$$\begin{aligned} p' &= -\nabla_q H - \lambda^T C(q) \\ q' &= \nabla_p H, \\ 0 &= c(q) \end{aligned} \quad (9)$$

where, when compared to (4), the additional terms λ , $c(q)$ and $C(q)$ denote respectively the Lagrange multipliers, the function of constraints and its first derivative. As in (4), the exact flow is symplectic and preserves the Hamiltonian¹. Notice eventually, that as a DAE, problem (9) is usually of index 3.

An ideal numerical method for (9) would preserve the constraints, the two hidden constraints obtained by differentiation, the Hamiltonian function and the symplecticity of the flow. The Lobatto IIIA-III B pair is very appealing, since it is both symplectic and preserves the constraints. However, it has some limitations regarding stability for stiff systems.

An alternative approach consists in differentiating once the constraints c and solving the resulting index-2 system. This technique is usually dismissed, in particular for long-term integration, for there are no symplectic methods for the index-2 formulation, but the situation is completely changed if the system is *reversible*, i.e. if there exist isomorphisms ρ and $\tilde{\rho}$ such that the functions f and g of (5) satisfy

$$\rho f(y, z) = -f(\rho y, z) \quad \text{and} \quad g(\rho y) = \tilde{\rho} g(y). \quad (10)$$

It has been shown in [16] that symmetric Runge-Kutta together with a suitable *symmetric projection* procedure mimic the qualitative behavior of Hamiltonian systems with holonomic constraints.

6.1.3. A Poisson system with boundary conditions

Participants: Philippe Chartier, Erwan Faou.

This work is related to the contract with Alcatel and is devoted to the mathematical and numerical aspects of a model for a n -th order cascaded Raman device. In their discretized version, the equations involve waves traveling backward and forward in the cavity, and interacting together via the Raman gain. Let us briefly present the most significant aspects of the Alcatel model with geometric integration in view: denote by L the length of the cavity, and suppose that n rays at given frequencies $\nu_1, \nu_2, \dots, \nu_n$ are represented by $2n$ functions $F_i(x)$ and $B_i(x)$ for $x \in (0, L)$ denoting the powers of the *forward* and *backward* waves respectively.

The model equations can now be written as follows, where the index i runs from 0 to n :

$$\begin{aligned} \dot{F}_i &= -\alpha_i F_i - \sum_{j < i} g_{ij} (F_j + B_j) F_i + \sum_{j > i} g_{ij} (F_j + B_j) F_i, \\ \dot{B}_i &= \alpha_i B_i + \sum_{j < i} g_{ij} (F_j + B_j) B_i - \sum_{j > i} g_{ij} (F_j + B_j) B_i. \end{aligned} \quad (11)$$

The coefficients g_{ij} are non-negative and represent the Raman gain between the wave length of the level i and j . The coefficients $\alpha_i > 0$ are attenuation coefficients.

It is interesting to notice that the system has several mathematical invariants. A simple calculation shows indeed that

$$\forall i = 1, \dots, n, \quad \forall x \in (0, L), \quad (F_i B_i)(x) = (F_i B_i)(0) = (F_i B_i)(L).$$

¹A prominent example (as a toy-problem) of such systems is the *double-pendulum* (a system composed of two connected arms moving below its fixed point without friction in the field of gravity). However, this is just one of the numerous more complex systems encountered in robotics.

If we make the further assumption that the exchange of energy is symmetric through the Raman process, and that there is no loss of energy within the fiber, then we can further notice that $\sum_j (F_j - B_j)$ is kept constant along the fiber. This quantity can be interpreted as the energy of the system and its preservation in absence of attenuation is physically sounded.

The existence of these two invariants becomes natural if one notices that the ODE system (11) has a Poisson structure (i.e. a Hamiltonian-type structure where the canonical matrix J in (4) is replaced by a suitable matrix B depending on the point (p, q)). It is a well-know fact that such systems can be brought back to canonical form, through a local change of variables. In the context of the present study, it is in fact possible to exhibit a *global* change of variables, whose existence is of main importance to devise the algorithm implemented for Alcatel [15].

6.2. Linear and Nonlinear Problems

6.2.1. LDL^T factorization of a symmetric matrix of intervals

Participant: Bernard Philippe.

In a cooperation with E. Kamgnia, from the University of Yaoundé I, we have designed an $O(n^3)$ algorithm which provides an enclosure of the LDL^T Bunch-Kaufman factorization of an interval matrix. The algorithm is based on the so-called *Krawczyk operator* defined from a Newton step of the update of a given LDL^T factorization. We used the factorization to determine the inertia of a symmetric interval matrix. We also derived a bound of the condition number of the factorization. Numerical results show that the algorithm is robust; however it can suffer from an ill-conditioned factorization or from the failure of the Krawczyk operator to contract in a sufficiently large neighborhood of the origin. This work has been submitted to a journal.

6.2.2. 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. In this code, several strategies for dropping fill-ins were considered for obtaining efficient preconditioners to solve linear systems through the normal equations. A preliminary report on the behaviour of the obtained preconditioner was presented [29].

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. The next step will be to consider dropping strategies for building new preconditioners.

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 Ph-D thesis and is done in collaboration with J-R. de Dreuzy, from CAREN, University of Rennes 1, in the context of the Hydrogrid project.

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. We have investigated a subdomain method, where each fracture is a subdomain and where interfaces are the intersections of the fractures. It can be seen as a multiscale method, working at the scale of the network and the scale of the fractures. The challenge here is to deal with a very large number of subdomains. 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 project, 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 build several meshes for a network of a few fractures and plan to get an automatic tool for larger networks. Then, we use a Mixed Finite Element method to build the matrix and the right-hand side. We use the TRACE software (developed by H. Hoteit at IMFS, Strasbourg) but we have to modify it in order to assemble the contributions from all the fractures and their intersections. We will compare a global direct solver with a subdomain solver on various small networks.

This work has been presented at the SIAM conference on Geosciences [25]. Previous work on 2D networks of fractures has been published [17].

6.3.2. Saltwater intrusion

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

This work was done in collaboration with M. Kern and M. Mancip, from the Estime INRIA-team, in the context of the Hydrogrid project. It was partly undertaken as a project from S. Zein, student at DEA of Beyrouth.

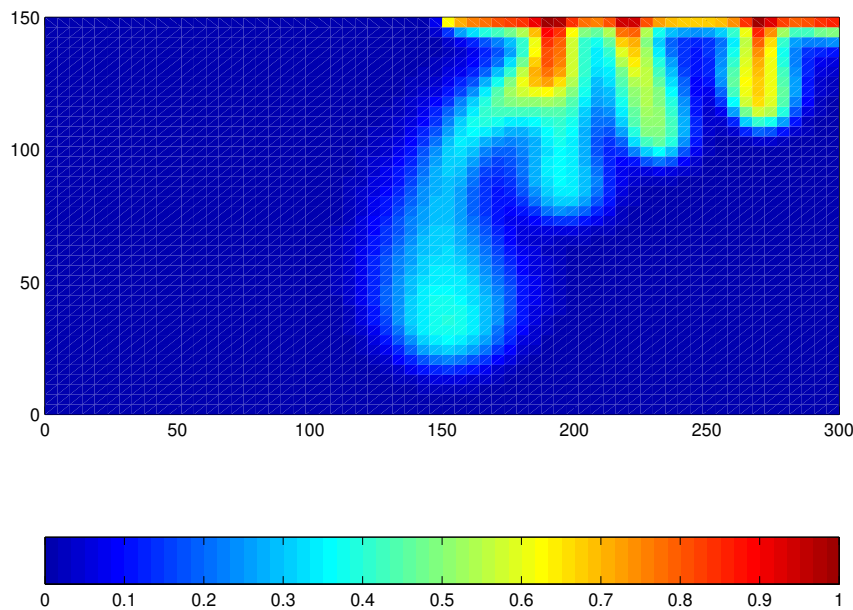


Figure 1. Elder test case - Salt Concentration

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 use the same discretizations as in the TRACE software, with a splitting of the convection and diffusion operators in the transport of solutes. The first objective was to reduce the CPU requirements of the software developed at IMFS. We have defined a new coupling method, with a fully explicit convection term and an explicit dispersion factor, which allows to compute first the transport then the flow at each time step, with no iteration, thus with a gain factor of about 12. We have modified the matrix computations in the flow model and reduced again the CPU time, at the price of increased storage. We have changed the linear solver in the flow computation, using a direct solver (MUMPS, from the INRIA-team ReMap) instead of an iterative solver (preconditioned BICGSTAB). The most CPU time expensive part, solving the flow linear system, is thus parallel thanks to the parallel MUMPS software. The same work must be done in the diffusion computation.

We have also started to change the hybrid approach, in order to compute directly the fluxed instead of the hydraulic charges. This will allow to reduce memory requirements as well as CPU requirements, with an

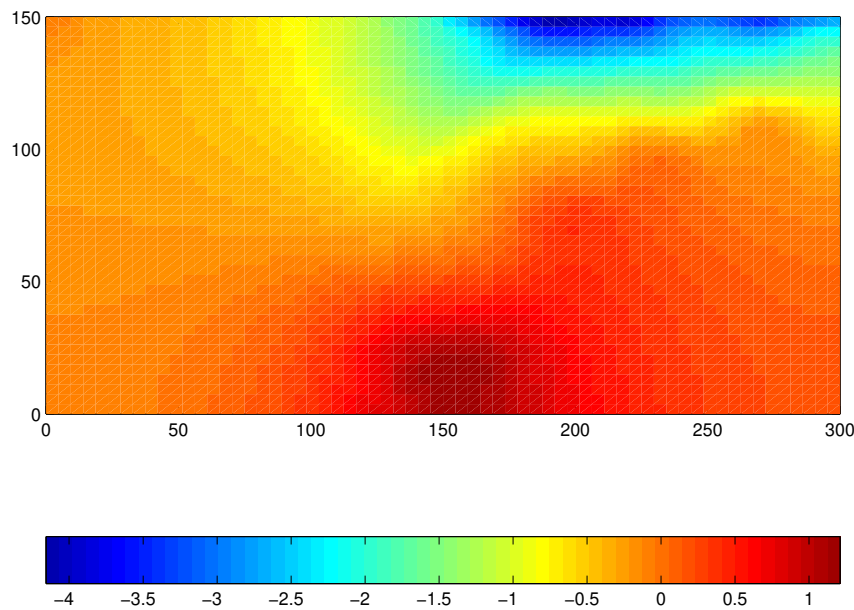


Figure 2. Elder test case - Pressure

improved accuracy. On the other hand, the linear system will be indefinite and the use of MUMPS will not be as straightforward as in the hybrid approach.

Figures 1 and 2 show numerical results for Elder test case. A paper on this work is in preparation.

6.3.3. Transient flow in heterogeneous porous media

Participant: Jocelyne Erhel.

This work is done in collaboration with J-R. de Dreuzy, from CAREN, University of Rennes 1.

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.

This work has been presented at the ICIAM conference [24] and at the european SALTRANS workshop [22].

6.4. Eigenproblems

6.4.1. 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 [32].

6.4.2. Partial canonical structure extraction for large matrices

Participant: Frédéric Guyomarc’h.

This work is a collaboration with Bo Kågström from the Umeå University (Sweden), in the context of the swedish entitled project *Matrix Pencil Computations in Computer-Aided Control System Design: Theory, Algorithms and Software Tools*.

When A et 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 don’t 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 explicitly (*lock and purge*). Then we can compute information about the next multiplicity.

Our work is to adapt this method to treat the multiple eigenvalues (essential for canonical structure computations) with block strategies and also with a new algorithm based, not on the Arnoldi decomposition, but on a more general form called Krylov-Schur which does not need to preserve the Hessenberg form of the Rayleigh quotient.

This work has been presented at the GAMNI-PSMN day at Lyon [28].

6.5. Nonlinear free surface flows

Participant: Édouard Canot.

When dealing with non-linear free-surface flows, mixed Eulerian-Lagrangian methods have numerous advantages, because we can follow marker particles distributed on the free-surface and then compute with accuracy the surface position without the need of interpolation over a grid. Besides, if the liquid velocity is great enough, Navier-Stokes equations can be reduced to a Laplace equation, which is numerically solved by a Boundary Element Method (BEM); this latter method is very fast and efficient because computing occur only on the fluid boundary. This method is applied to the spreading of a liquid drop impacting on a solid wall. We have applied this numerical model to ink-jet printing processes.

Ink-jet printing processes are characterized by small geometrical scales (50 to 100 μm) and high velocities (5 to 15 $m s^{-1}$). 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 : $Fr = \frac{U^2}{gD}$, Weber number : $We = \frac{\rho U^2 D}{\sigma} \simeq 150$, Reynolds number : $Re = \frac{\rho U D}{\mu} \simeq 750$.

Due to high Reynolds value, the liquid flow can be approximated by a scalar potential which verifies a Laplace equation. The dynamic boundary condition on the free-surface is derived from the classical transient Bernoulli equation. In comparison with usual BEM codes which can be found in litterature and/or internet, for example :

- http://stokes.ucsd.edu/c_pozrikidis/BEMLIB/,
- <http://www.boundary-element-method.com/>,

our version has the following 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 large matrix);
- the potential model, which is not valid near solid boundaries, is corrected via a simple drainage model between two parallel plane plates;

Figure 3 shows the time evolution of a water drop of diameter 2.4 mm at 1 m/s , spreading on a hydrophilic substrate with an equilibrium angle of 70° . Oscillations of the droplet are due to concurrent forces : inertia and surface tension; viscous forces make that the phenomenon tends quickly (few ms) to an equilibrium state.

Figure 3 shows the numerical simulation of the same case, using the described BEM method. Parameters are : $Fr = 1260$, $We = 5$, $Re = 250$

This work was the subject of a DEA training stage (D. Vadillo), and has been made during a collaboration with PIM research team in Grenoble (common project between LEGI laboratory and LETI-CEA Grenoble). It has been published in [31].

6.6. Parallel algorithms for Markov models

Participant: Haïscam Abdallah.

Markov models are used for studying the behaviour of computer systems and networks. Some differential systems are solved on an interval $[0, t]$ to get performance measures and to evaluate their sensitivity to some given parameter. However, this study is faced to a complexity which increases with the order M of the generator and with the time t .

We have chosen stochastic automata networks for modelling and solving such large problems. We have designed parallel algorithms for the uniformisation method and obtained results for a ATM network with about one million of states. [11], [19], [18].

7. Contracts and Grants with Industry

7.1. Industrial Grants

7.1.1. ALCATEL CIT - Numerical model for a Raman device

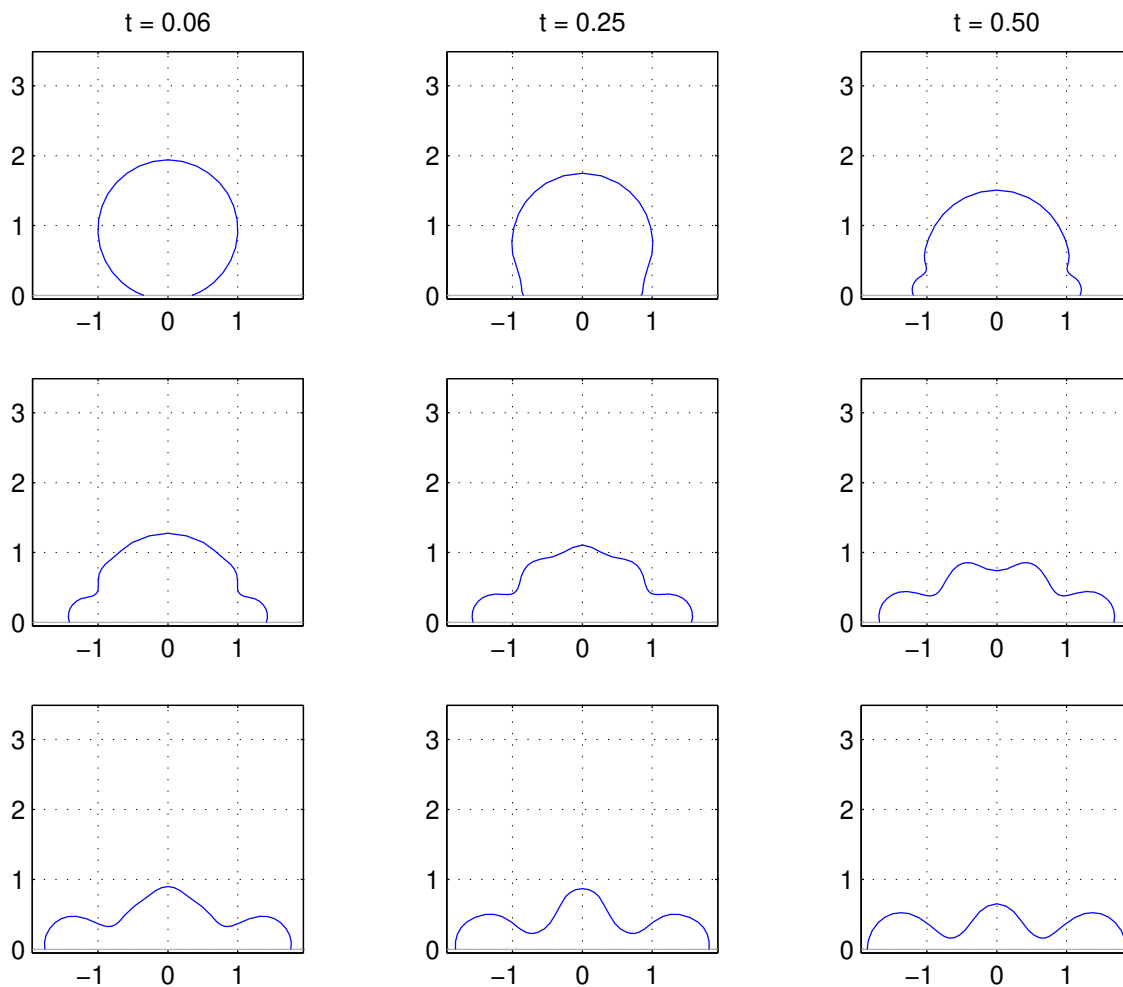
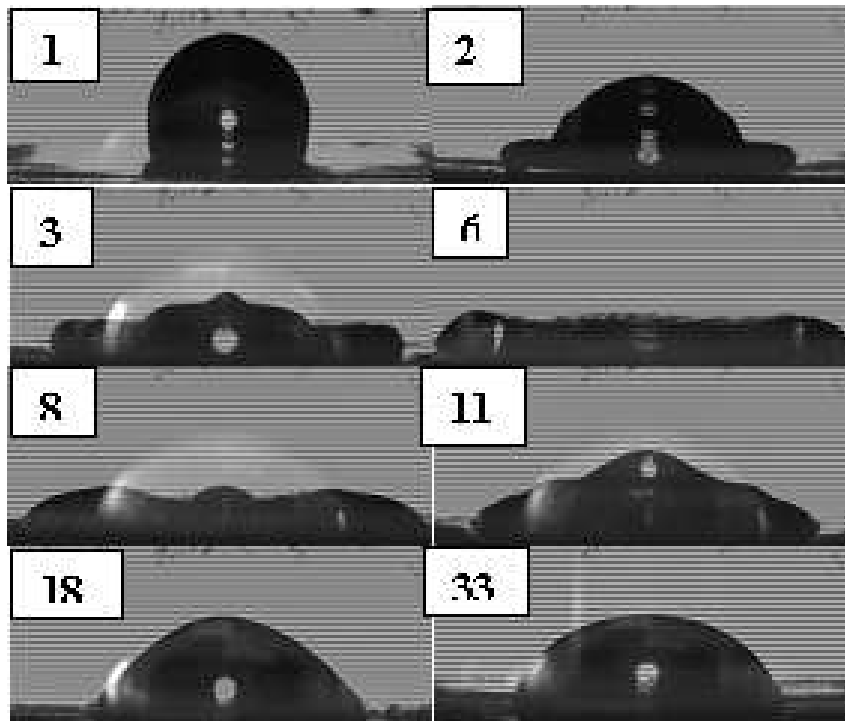
Participants: Philippe Chartier, Erwan Faou.

Alcatel contract, No. 102C40200331319012

partners : Irisa, Alcatel CIT

time : from June 2002 until October 2003

The results presented in this section have been obtained jointly with the engineers from the laboratory of optronics from Alcatel Marcoussis. This project with Alcatel is devoted to the mathematical and numerical aspects of a model for a n -th order cascaded Raman device. In their discretized version, the equations involve waves traveling backward and forward in the cavity, and interacting together via the Raman gain. In its most general form, a n -th order cascaded Raman fiber laser is described by a set of partial differential equations. However, it has become common, based on the experience that only a few frequencies contribute significantly to the phenomenon, to discretize the full spectrum and to simulate the resulting system of ordinary differential equations. Using a change of variable, the questions of existence and uniqueness of a solution have been solved and a more efficient and more stable algorithm has been proposed and implemented [34]. However, this initial work has emphasized some limitations, and it now appears necessary to consider a more elaborated model, including the whole spectrum of frequencies.



Numerical simulation of Figure 3 test case. $Fr = 1260$, $We = 5$, $Re = 250$

Figure 3. Experimental spreading of a 2.4 mm water drop, impacting a solid wall at 1 m/s

8. Other Grants and Activities

8.1. National Grants

8.1.1. *ARC PRESTISSIMO 2003-2004*

Participants: Philippe Chartier, Erwan Faou.

The PRESTISSIMO group associates E. Faou and P. Chartier from the Aladin team, F. Castella from the university of Rennes 1, E. Cancès, C. Le Bris, F. Legoll and G. Turinici, 4 members of the INRIA team MICMAC (Laboratoire CERMICS, Ecole Nationale des Ponts et Chaussées, Marne-La-Vallée), Gilles Zerah from the CEA and Olivier Coulaud from the INRIA-team ScAIApplix (INRIA Bordeaux). It is funded for two years onward from January 2003. Erwan Faou is the manager of PRESTISSIMO. The main objective of the group is to share knowledge on time integrators for molecular dynamics simulation and to solve some of the theoretical and practical questions raised by long-time integration. First results have been obtained and are about to be published [33].

A workshop was held in Paris in December :

<http://www.irisa.fr/aladin/perso/faou/prestissimo/workshop03.html>

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

Participant: Jocelyne Erhel.

The working group MOMAS is led by A. Bourgeat from the university of Lyon and include many partners from universities, CEA, ANDRA, EDF. 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 “development of numerical methods for reactive transport”. In the case of chemistry at equilibrium, the model is a set of coupled partial differential equations (transport) and algebraic equations (chemistry) and becomes a set of Differential Algebraic Equations (DAEs) after spatial discretization. We have reviewed the different numerical methods used in the literature and proposed some variants to improve the efficiency [26].

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

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

We have worked on two applications described above : saltwater intrusion 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 [20].

8.1.4. *IFREMER contract*

Participants: Édouard Canot, Jocelyne Erhel.

IFREMER contract, No. 03/2 210 412

Partners : Irisa, IFREMER

Title : Mise au point d’un modèle numérique pour la propagation d’ondes élastiques

time : from July 2003 until March 2004

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 use the code FLUSOL from the INRIA-team ONDES.

In a first step, we will design several test cases relevant for Ifremer applications. Then we will analyze the code in order to improve performances.

8.2. European Grants

8.2.1. *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 Aladin) and E. Kontoghiorghes (U. Neuchatel)

Members : 45 researchers from 13 European countries.

<http://www.irisa.fr/aladin/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 the very large problems which necessitate the design of reliable and fast procedures. High Performance Computing including parallel computing is addressed.

In 2003, the WG met in Bari (September 22-24) within the framework of the seminar Numerical Linear Algebra and its Applications. The next meeting is scheduled to happen during the COMPSTAT 2004 conference in Prague.

In 2003, a handbook on Parallel Matrix Algorithms was completed in a joint activity between the Working Group and the PMAA'02 conference [10].

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.

8.3. International Grants

8.3.1. *INRIA/NSF Action - Robust and reliable preconditioners*

Participants: Jocelyne Erhel, Bernard Philippe.

INRIA/NSF action , started in 2001

Titre : Robust Parallel Preconditioning methods: Bridging the Gap between Direct and Iterative Solvers

Members :

USA : Y. Saad (coordinator, U. Minneapolis), R. Bramley (U. Indiana), G. Golub (Stanford U.), E. Ng (Laurence Berkeley Lab.), A. Sameh (U. Purdue),

France : B. Philippe (coordinator, team Aladin), F. Desprez (team Remap), P. Amestoy (ENSEEIH/ team Scalapplx, Toulouse), J. Roman (Labri/team Scalapplx, U. Bordeaux 1).

The main objective is to define efficient preconditioners which accelerate the convergence of iterative methods for solving linear systems. For ill-posed least squares problems, the research focuses on procedures of regularization.

The second direction for research is the definition of software for the QR factorization of sparse matrices. One of the goals is to obtain the rank of a matrix and possibly, a basis of the null space. Another objective is to include a dropping strategy for defining new preconditioners which should be well adapted to the solution of normal equations.

The Aladin team is mostly involved in the latter direction.

8.3.2. *CAMEREAU Action - Hydrogeology in Cameroon*

Participant: Bernard Philippe.

CORUS Action (formally CAMPUS action) accepted in 2000 by the French ministry of Foreign Affairs, extended up to the end of 2003.

Title: Une action de recherche et de formation universitaire en hydrologie au Cameroun.

Partners : University of Yaoundé I, Office of the Weather Forecast in Douala, Aladin project.

The action is structured upon three topics. The first two consist of data acquisition and modelling underground water flows in the region of Yaounde. On this topic, the researcher A. Njifenjou visited our group. During the stay, he made himself acquainted with the code TRACES which has been developed by H. Hoteit, former PhD researcher in Aladin and in the institute IMF in Strasbourg. One goal is to transfer this code in Yaounde.

The last research axis was dedicated to smoothing and interpolation for data in pluviometry. That work ended one year ago.

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 : 2004-2006.

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.

9. Dissemination

9.1. Programme committees and Editorial Boards

- E. Faou organized the workshop Prestissimo, in December, in Paris.

<http://www.irisa.fr/aladin/perso/faou/prestissimo/workshop03.html>

- B. Philippe is member of the following programme committees :

- Sparse Days'03, May 15-16, 2003, Calais, France.
- NSMC '03 (International Conference on the Numerical Solution of Markov Chains), September 3-5, 2003, Urbana, Illinois, USA
- RenPar'15, October 14-17, 2003, La Colle sur Loup, France.
- CARI'04, November 22-25, 2004, Hammamet, Tunisia.

- B. Philippe is editor of the new electronic journal ARIMA.
- B. Philippe is member of the editorial board of the journal International Journal on High Speed Computing (Word Scientific Publishing)
- B. Philippe is guest editor for the special issue of Parallel Computing dedicated to the conference Parallel Matrix Algorithms and Applications (PMAA '02).

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 is member of Commission d'Évaluation 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.
- B. Philippe is the correspondent for INRIA for the relations with African teams. He is secretary of the CARI permanent committee.
- B. Philippe is member, on behalf of INRIA, of the board of directors of Cimpa.

9.3. Teaching

- É. Canot and J. Erhel taught about applied mathematics (MAP) for DIIC, IFSIC, Rennes 1 (first year).
Lecture notes on <http://www.irisa.fr/aladin/perso/erhel/>
- P. Chartier and J. Erhel taught about elliptic and hyperbolic equations (MODL), for maîtrise de mathématiques et de mécanique, UFR Mathématiques, Rennes 1.
- P. Chartier and E. Faou gave a course, in June, entitled "Intégration symplectique des systèmes hamiltoniens intégrables : comportement en temps long", for DEA NIVEAU II, UFR Mathématiques, Rennes 1.
- J. Erhel gave a one-week course in January on Numerical Schemes for hyperbolic equations, in Beyrouth (DEA de mathématiques appliquées, co-organized by the Lebanese University, EPFL of Lausanne, Irisa and University of Reims).
- F. Guyomarc'h gave lectures (cours and TD) on algorithms (ALG2) for DESS CCI, IFSIC, Rennes 1.
- F. Guyomarc'h has supervised projects in C for magistère de mathématiques, ENS Cachan Rennes (second year).
- F. Guyomarc'h gave lectures (TD and TP) on algorithms (ALG and AC) for DIIC, IFSIC, Rennes 1 (second year).
- F. Guyomarc'h taught at IFSIC (DEUG MIAS) and IRMAR (Maths master).
- B. Philippe gave a course, in cooperation with K. Bouatouch, member of the team Siames, on Linear Systems and Radiosity (option (SYRA) of DEA d'informatique at IFSIC).
- B. Philippe gave a one-week course, in January, on Parallel Algorithms in Linear Algebra, in Yaounde (DEA d'informatique).
- B. Philippe 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).
- B. Philippe is invited professor at ENIT (University of Tunis) for the academic year 2003-2004.

9.4. Participation in conferences

- H. Abdallah : communication to CIMNA, Beyrouth, Lebanon, November.
- É. Canot : demo of PPAT software at IPDPS, Nice, April. Flyer presentation on Hydrogrid and participation to ACI-GRID days, Nice, April.
- É. Canot : invited speaker at RENPAR, La Colle-sur-Loup, October.
- P. Chartier : communication to SCICADE, Trondheim, Norway, July.

- J. Erhel : communication to SIAM GS03, Austin, USA, March.
- J. Erhel : two communications to ICIAM, Sydney, Australia, July.
- J. Erhel : communication to GDR MOMAS workshop, Marseille, November.
- E. Faou : communication to SCICADE, Trondheim, Norway, July.
- F. Guyomarc'h : participation in the Sparse Days and Grid Computing, St Girons, June.
- F. Guyomarc'h : invited talk on eigensubspace computations at the GAMNI-PSMN day on eigenvalue problems, ENS Lyon, December.
- B. Philippe : invited speaker at the conference TamTam'03 (North African conference, Tendances pour les Applications des Mathématiques), Rabat, Morocco, April.
- B. Philippe : participation in the "Journées Universitaires de la Science et de la Technologie (JUST 2003)", Yaoundé, Cameroon, February-March. The minister of higher education, Maurice Tchente, presented him the medal of "croix de Chevalier de l'ordre de la valeur", by way of thanks for numerous cooperation actions between INRIA and the University of Yaoundé I.
- B. Philippe : participation in the 4th workshop on algorithms applied to industrial problems, Calais, April.

9.5. International exchanges

9.5.1. Visits

- P. Chartier and E. Faou visited the University of Pays Basque, San Sebastian, Spain, during one week, in November 2003.
- J. Erhel visited the University of Queensland, Australia, during 2 weeks, in July 2003.
- E. Faou visited the University of Genève, Switzerland, during three months, April-May-July, 2003.
- F. Guyomarc'h visited the University of Umeå, Sweden, and worked at the HPC2N, during three months, June-July-August 2003.
- B. Philippe is invited professor at ENIT, Tunis, Tunisia, during one year, from September 2003 until August 2004.

9.5.2. Visitors

The team has invited the following persons :

- A. Njifenjou, 2 months, from July 1 until August 31.
- D. Mehzer, 2 months, from July 10 until September 3.
- A. Murua, one week, from July 14 until July 23.
- E. Kontoghiorghes, one month, from July 21 until August 28.
- E. Kamgnia, three months, from August 1 until October 31.

10. Bibliography

Major publications by the team in recent years

- [1] A. AUBRY, P. CHARTIER. *On improving the convergence of Radau IIA methods when applied to index-2 DAEs.* in « SIAM Journal on Numerical Analysis », number 4, volume 35, 1998, pages 1347-1367.
- [2] A. AUBRY, P. CHARTIER. *Pseudo-symplectic Runge-Kutta methods.* in « BIT », number 3, volume 38, 1998, pages 439-461.
- [3] K. BURRAGE, J. ERHEL. *On the performance of various adaptive preconditioned GMRES.* in « Numerical Linear Algebra with Applications », volume 5, 1998, pages 101-121.

- [4] R. CHAN, P. CHARTIER, A. MURUA. *Post-projected Runge-Kutta methods for index-2 differential-algebraic equations*. in « Applied Numerical Mathematics », number 1-3, volume 42, 2002, pages 77-94.
- [5] R. CHOQUET, J. ERHEL. *Newton-GMRES algorithm applied to compressible flows*. in « International Journal for Numerical Methods in Fluids », volume 23, 1996, pages 177-190.
- [6] M. CROUZEIX, B. PHILIPPE, M. SADKANE. *The Davidson Method*. in « SIAM, Journal on Scientific and Statistical Computing », volume 15:1, 1994, pages 62-76.
- [7] H. HOTEIT, J. ERHEL, R. MOSÉ, B. PHILIPPE, P. ACKERER. *Numerical Reliability for Mixed Methods Applied to Flow Problems in Porous Media*. in « Computational Geosciences », volume 6, 2002, pages 161-194.
- [8] D. MEZHER, B. PHILIPPE. *Parallel computation of pseudospectra of large sparse matrices*. in « Parallel Computing », number 2, volume 28, 2002, pages 199-221.
- [9] Y. SAAD, M. YEUNG, J. ERHEL, F. GUYOMARC'H. *A deflated version of the Conjugate Gradient Algorithm*. in « SIAM Journal on Scientific Computing », number 5, volume 21, 2000, pages 1909-1926.

Books and Monographs

- [10] *Parallel Matrix Algorithms and Applications (PMAA '02)*. P. ARBENZ, E. GALLOPOULOS, B. PHILIPPE, Y. SAAD, editors, number 9, volume 29, September, 2003.

Articles in referred journals and book chapters

- [11] H. ABDALLAH. *Parallel Implementation of Uniformization to Compute the Transient Solution of Stochastic Automata Networks*. in « Parallel and Distributed Computing Practices », to appear.
- [12] J. BONNANS, P. CHARTIER, H. ZIDANI. *Discrete approximation of the Hamilton-Jacobi equation for an optimal control problem of a differential-algebraic system*. in « Control and Cybernetics », number 1, volume 32, 2003, pages 33-55.
- [13] M. BRIEU, J. ERHEL. *On the convergence of a non-incremental homogenization method for non-linear elastic composite materials*. in « Numerical Algorithms », volume 32, 2003, pages 141-161.
- [14] É. CANOT, L. DAVOUST, M. E. HAMMOUMI, D. LACHKAR. *Numerical simulation of the buoyancy-driven bouncing of a 2-D bubble at an horizontal wall*. in « Theor. and Comput. Fluid Dynamics », volume 17, 2003, pages 51-72.
- [15] F. CASTELLA, P. CHARTIER, E. FAOU. *Analysis of a Poisson system with boundary conditions*. in « C.R.A.S. », volume I336, 2003.
- [16] R. CHAN, P. CHARTIER, A. MURUA. *Reversible methods of Runge-Kutta type for Index-2 Differential-Algebraic Equations*. in « Numerische Mathematik », to appear.
- [17] J.-R. DE DREUZY, J. ERHEL. *Efficient algorithms for the determination of the connected fracture network*

and the solution to the steady-state flow equation in fracture networks. in « Computers and Geosciences », volume 29, 2003, pages 107-111.

Publications in Conferences and Workshops

- [18] H. ABDALLAH. *Méthodes numériques de calcul des performances des systèmes et réseaux informatiques.*, in « CIMNA1, premier Colloque International des Méthodes Numériques Appliquées », Beyrouth, Lebanon, November, 2003.
- [19] H. ABDALLAH. *Performance analysis of an ATM network via multidimensional Markov process.* in « PDPTA'2003, 2003 International Conference on Parallel and Distributed Processing Techniques and Applications », volume III, Las Vegas, USA, June, 2003.
- [20] É. CANOT, J. ERHEL. *Simulation de problèmes couplés d'hydro-géologie : utilisation d'une grille de calcul et d'un modèle de composants logiciels.* in « Renpar'15 », La Colle sur Loup, October, 2003.
- [21] P. CHARTIER. *Long-time averaging using symplectic solvers and applications to molecular dynamics.* in « Scicade'03 », Trondheim, Norway, July, 2003.
- [22] J.-R. DE DREUZY, P. DAVY, J. ERHEL. *Well test interpretation in heterogeneous media.* in « Synthèse du contrat européen SALTRANS », Majorque, Spain, October, 2003.
- [23] J. ERHEL, E. CANOT. *The inverse Electrocardiography Problem viewed as a General Linear Model.* in « ICIAM », Sydney, Australia, July, 2003.
- [24] J. ERHEL, J.-R. DE DREUZY. *A compact scheme for numerical simulation of flow circulation in highly heterogeneous porous media.* in « ICIAM », Sydney, Australia, July, 2003.
- [25] J. ERHEL, J.-R. DE DREUZY. *Modelling Flow and Transport in Subsurface Complex Fracture Networks.* in « SIAM GS », Austin, USA, March, 2003.
- [26] J. ERHEL, M. KERN. *Méthodes numériques pour le transport réactif.* in « MOMAS », Marseille, France, November, 2003.
- [27] E. FAOU. *Raman Laser Modeling: Mathematical and Numerical Analysis.* in « Scicade'03 », Trondheim, Norway, 2003.
- [28] F. GUYOMARC'H. *Résultats sur des variantes de la méthode d'Arnoldi.* in « Journées GAMNI-PSMN, Problèmes de valeurs propres et paramètres critiques », Lyon, France, December, 2003.
- [29] D. MEZHER, B. PHILIPPE. *Parallel incomplete multifrontal QR decomposition.* in « PMAA », November, 2002.
- [30] R. SIDJE, K. BURRAGE, B. PHILIPPE. *An Augmented Lanczos Algorithm for the efficient computation of a dot-product of a function of a large sparse symmetric matrix..* in « Computational Science - ICCS 2003 », series LNCS, number 2659, Springer Verlag, P. M. A. SLOOT, D. ABRAMSON, A. V. BOGDANOV, J. J.

DONGARRA, A. Y. ZOMAYA, Y. E. GORBACHEV, editors, pages 693–704, 2003.

- [31] D. VADILLO, É. CANOT, B. LOPEZ, A. SOUCEMARIANADIN. *Collisions of single and multiple drops onto solid walls*. in « ICLASS'2003 », Sorrento, Italy, July, 2003.

Internal Reports

- [32] M. W. BERRY, D. MEZHER, B. PHILIPPE, A. SAMEH. *Parallel computation of the singular value decomposition*. Research Report, number RR-4694, INRIA, January, 2003, <http://www.inria.fr/rrrt/rr-4694.html>, to appear in Handbook on Parallel Computing and Statistics, publisher : Marcel Dekker.
- [33] E. CANCÈS, F. CASTELLA, P. CHARTIER, E. FAOU, C. L. BRIS, F. LEGOLL, G. TURINICI. *High-order averaging schemes with error bounds for thermodynamical properties calculations by MD simulations*. Research Report, number 4875, INRIA, July, 2003, <http://www.inria.fr/rrrt/rr-4875.html>.
- [34] F. CASTELLA, P. CHARTIER, E. FAOU, D. BAYART, F. LEPLINGARD, C. MARTINELLI. *Raman Laser Modeling: Mathematical and Numerical Analysis*. Research Report, number 4776, INRIA, March, 2003, <http://www.inria.fr/rrrt/rr-4776.html>.
- [35] E. FAOU. *Multiscale Expansions for Linear Clamped Elliptic Shells*. Research Report, number 4956, INRIA, October, 2003, <http://www.inria.fr/rrrt/rr-4956.html>.

Bibliography in notes

- [36] A. BJÖRCK. *Numerical methods for least-squares problems*. SIAM, 1996.
- [37] A. BRUASET. *A survey of preconditioned iterative methods*. series Pitman Research Notes in Mathematics Series, Longman Scientific and Technical, 1995.
- [38] J. E. DENNIS, R. B. SCHNABEL. *Numerical Methods for Unconstrained Optimization and Nonlinear Equations*. Prentice-Hall series in Computational Mathematics, 1983.
- [39] I. DUFF, A. ERISMAN, J. REID. *Direct Methods for Sparse Matrices*. Oxford Science Publications, 1986.
- [40] S. K. GODUNOV, O. P. KIRILJUK, V. I. KOSTIN. *Spectral portrait of matrices and criteria of spectrum dichotomy*. in « Computer arithmetic and enclosure methods », J. HERZBERGER, L. ATHANASSOVA, editors, 1991.
- [41] P. C. HANSEN. *Rank-deficient and discrete ill-posed problems*. SIAM, 1997.
- [42] G. MEURANT. *Computer solution of large linear systems*. North Holland, Amsterdam, 1999.
- [43] J. ORTEGA, W. RHEINBOLDT. *Iterative Solution of Nonlinear Equations in Several Variables*. series Computer science and applied mathematics, Academic Press, 1970.
- [44] Y. SAAD. *Iterative methods for sparse linear systems*. PWS publishing, 1995.

-
- [45] G. L. G. SLEIJPEN, H. A. VAN DER VORST. *A Jacobi-Davidson iteration method for linear eigenvalue problems*. in « SIAM J. Matrix Anal. Appl. », volume 17, 1996.
- [46] L. N. TREFETHEN. *Pseudospectra of matrices*. in « Numerical Analysis », Longman Scientific and Technical, D. F. GRIFFITHS, G. A. WATSON, editors, 1991.