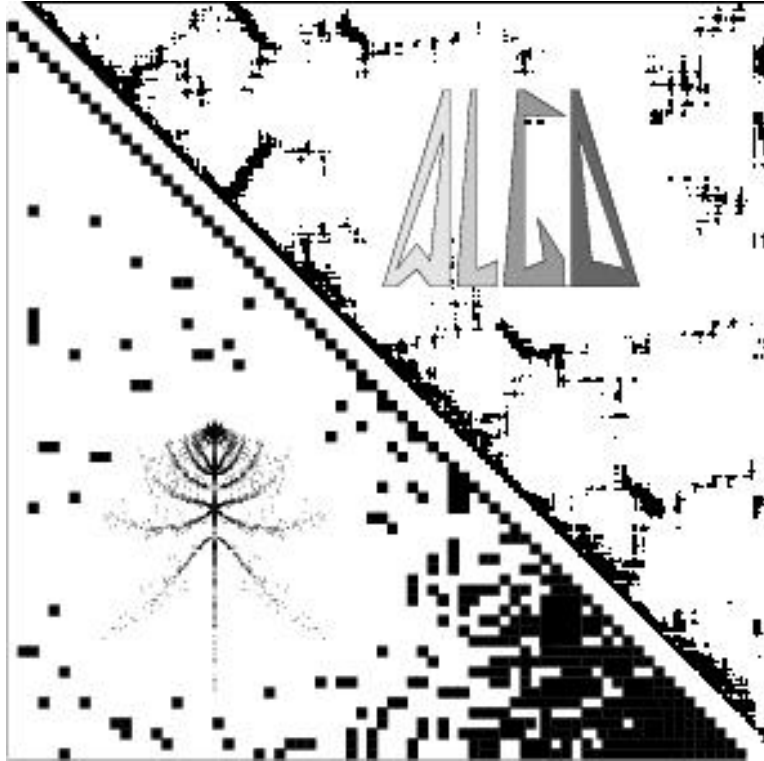


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ACTIVITY REPORT  
of the  
PARALLEL ALGORITHMS PROJECT  
at  
CERFACS

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# 1 Introduction

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## 1.1 Introduction

The research programme conducted by the Parallel Algorithms Project combines the excitement of basic research discoveries with their use in the solution of large-scale problems in science and engineering. We are concerned both with underlying mathematical and computational science research, the development of new techniques and algorithms, and their implementation on a range of high performance computing platforms.

The description of our activities is presented in several subsections, but this is only to give a structure to the report rather than to indicate any compartmentalization in the work of the Project. Indeed one of the strengths of the Parallel Algorithms Project is that members of the Team work very much in consultation with each other so that there is considerable overlap and cross-fertilization between the areas demarcated in the subsequent pages. This cross-fertilization extends to formal and informal collaboration with other teams at CERFACS, the shareholders of CERFACS, and research groups and end users elsewhere.

Our main approach in the direct solution of sparse equations continues to be the multifrontal technique originally pioneered at Harwell in the early 1980s. During this last period we have worked hard with our colleagues in ENSEEIHT and RAL to develop and tune the sparse direct code, MUMPS, in the PARASOL Project. The project finished in June and the final review meeting was held at CERFACS at the end of August. The reviewers were very pleased with the work done in the project and were particularly impressed by the MUMPS code which was used to solve a system of nearly 1 million degrees of freedom on an SGI Origin 2000 at the University of Bergen in Norway. Work is now continuing to incorporate this direct code within domain decomposition software both here at CERFACS and in the DDM code in Bergen.

At the level of international efforts for standards in numerical linear algebra, we have been very involved in the development of a new standard for the Basic Linear Algebra Subprograms (or BLAS) coordinated through the BLAST Technical Forum. In particular, we have been involved in the design of the new sparse BLAS and have developed a Fortran 95 instantiation of the resulting subprograms. Although iterative methods remove many of the bottlenecks of direct approaches, particularly regarding memory, it is now well established that they can only be used in the solution of really challenging problems if the system is preconditioned to create a new system more amenable to the iterative solver. During this last year we have continued our work on developing such preconditioners, including two-level schemes that avoid problems of degradation of convergence when the number of domains is increased to obtain more parallelism. We have coupled some of this work with the sparse direct approach discussed earlier and have used these algorithms and software in the solution of large problems in semi-conductor device modelling. We have also studied the parallel scalability of such methods and considered block versions of the iterative schemes that can be particularly powerful when many sets of equations are being solved. These block methods can also take great advantage of the BLAS kernels. We have continued our development of techniques to place large entries on the diagonal and our work has been used by ex-CERFACS collaborators in US Government laboratories to solve otherwise intractable large unsymmetric problems. Our work on developing sparse approximate inverses to precondition a dense matrix in an electromagnetics application from one of our shareholders continues and we have developed new algorithms that permit different sparsity patterns for approximating the matrix and its inverse and new criteria based on geometric

considerations rather than the magnitude of entries for determining the patterns. This work is designed to be used within a fast multipole approach for generating matrix-vector products and will be developed in collaboration with Aerospatiale and the electromagnetics Team at CERFACS.

The European project MYSHANET was completed during the year. This project developed a software tool for networks of PCs to help in the design of new industrial mechanical systems by performing parallel parametric multibody simulations.

The main area of interest for the Qualitative Computing Group concerns the reliability of numerical software in finite precision arithmetic. The major aspects of this that have been studied during this past years have been: homotopic perturbations, an analysis of the power method in the presence of multiple eigenvalues and determination of condition numbers for multiple defective eigenvalues, the development of tools and theory for inner-outer iterations, in particular for embedded solvers, and the use of quaternions for numerical computation. We have also continued a close collaboration with IRISA in Rennes involving, inter alia, the joint supervision of a PhD student working on hybrid methods for eigencomputation. We have completed work on the ZOOM Project for CNES on embedded solvers and are now heavily involved in the JASON Project with CNES concerning the determination of accurate orbits through GPS with respect to satellite positioning.

Although our senior scientist in the optimization area had to leave for family reasons during the year, she has continued to collaborate closely and will be visiting us frequently during the coming year. We also recruited a new postdoc towards the end of this year to ensure that this topic continues to have a high profile within the envelope of the Team's interests and expertise. Those of us who work in numerical linear algebra regard optimization as just an application area but indeed this activity can equally claim to be a major area in its own right that uses linear solvers almost as an elementary function. We accept that the truth lies between these extremes and have developed the optimization and nonlinear algebra activity significantly over the last year. Current areas of research include major work on trust-region algorithms involving a study of the influence and sensitivity of various controlling parameters and an investigation of the theory and practical implementation of primal-dual approaches, including the case of degenerate problems. Other research includes the development of sets of test problems for large scale optimization and the use of state-of-the-art techniques in meteorological data assimilation, in conjunction with our shareholders from Météo-France.

The Parallel Algorithms Team is heavily involved in the Advanced Training aspects of CERFACS' mission. We ran an internal training course for new recruits to all Teams at CERFACS to give them a basic understanding of high performance computing and numerical libraries. This course was also open to the shareholders of CERFACS. We are also involved in training through the "stagiaire" system. Members of the Team have assisted in many lecture courses at other centres, including ENSICA, INPT, INSA, Météo, Toulouse 1 and UPS. We run a regular series of "internal seminars" that are primarily for Team members to learn about each other's work and are also a good forum for young researchers to hone their presentational skills. We have also run a series of seminars from external people who are visiting the Team that attract a wider audience and for much of the year were responsible for the organization of the CERFACS seminar series. Team members have participated in many international conferences at both an invited and contributed level, and we have welcomed many visitors to CERFACS for both short and long periods. These visits have included young scientists from Taiwan and Japan eager to benefit from our experience in parallel computation. During this past year, Annick Sartenaer successfully defended her habilitation thesis at UPS and Patrick Amestoy, an ex-CERFACS student and postdoc, currently a Maître de Conférence at ENSEEIHT-IRIT, was also successful in obtaining his HDR qualification and is already the supervisor of a student at CERFACS. Thus the Parallel Algorithms Team already has grandchildren! Annick's thesis was principally on various aspects of large scale optimization and Patrick's was primarily on the solution of large sparse linear systems by direct methods on both shared memory and distributed memory computers.

The most major, and single most time-consuming, event in the Algo calendar in 1999 was the co-organization with ENSEEIHT-IRIT of the Euro-Par'99 conference at the beginning of September. One cannot overestimate the amount of work involved and all members of the local committee

dedicated many hours to the task of organizing this international meeting. Happily their efforts were rewarded by a record attendance of over 400 people and many plaudits both from the steering committee and from participants from all over the world. Truly an event that helped keep Toulouse at the heart of the technological map of Europe. The conference proceedings [ALG6] is a lasting testimony to the event and was co-edited by all members of the local committee.

I am very pleased to report that, over the past year, we have continued to increase our involvement in joint research projects with shareholders and with other teams at CERFACS. We have a major project on orbitography with CNES. We have two projects with Aerospatiale on block QMR and preconditioning techniques in electromagnetics, including a recently sponsored PhD on aspects of this work. We are involved in the training programme for the Mastere, organized by ENM. We have also two active collaborations with INRIA on domain decomposition and eigenvalues. We have had extensive discussions with CNES, EDF and CEA on both numerical linear algebra and their training needs and are in the process of planning training courses and workshops for these partners. In particular, in response to the interest of Aerospatiale, CNES, and EDF, we are currently preparing a workshop on inner-outer iterations and embedded software. We assist the other Teams at CERFACS on a daily basis but sometimes collaborate on a more substantial level as in the Dassault contract with CFD, and the use of ScaLAPACK and multipole methods with EMC.

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## 2 Dense and Sparse Matrix Computations

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### 2.1 MUMPS - a distributed memory multifrontal solver (P. R. Amestoy, I. S. Duff, J.-Y. L'Excellent and J. Koster)

The European project PARASOL had as its main goal the design and development of a library of scalable sparse matrix solvers for distributed memory computers. CERFACS, in collaboration with ENSEEIHT-IRIT and the CLRC Rutherford Appleton Laboratory, was responsible for the direct solvers. In this context, we developed a MULTifrontal MASSively Parallel Solver (MUMPS) [1, ALG20].

MUMPS has been designed to solve symmetric positive definite, general symmetric, and unsymmetric linear systems whose coefficient matrices are possibly rank deficient. The MUMPS package uses a multifrontal approach to factorise the matrix [2, 3]. Similar to serial HSL solvers, the parallel MUMPS package solves in three main steps: an analysis step, a factorization step and a solution step.

MUMPS achieves high performance by exploiting two kinds of parallelism: tree parallelism that comes from the sparsity of the problem and node parallelism from dense matrix kernels. MUMPS uses dynamic data structures and dynamic scheduling of computational tasks to accommodate extra fill-in in the factors due to numerical considerations (not taken into account during the analysis step). This dynamic approach also allows the parallel code to cope with load variations on the processors. MUMPS overlaps computation with communication by using asynchronous communication.

In 1999, there were several important upgrades to the MUMPS package. Figure 2.i lists the major releases of the package for partners in the PARASOL project. The continuous development and incorporation of new features requested by the partners has resulted in a software package (currently MUMPS version 4.1.1) that is unique amongst sparse direct solvers.

The MUMPS software is written in Fortran 90. It requires MPI for message passing and makes use of BLAS, LAPACK, BLACS, and ScaLAPACK subroutines. MUMPS was developed and tested on an IBM SP2, an SGI Power Challenge, and an SGI Origin 2000. The software has recently been ported to a Cray T3E.

So far, the MUMPS software has mainly been used for solving problems from the industrial partners in the PARASOL project. Typical PARASOL test cases are from application areas such as computational fluid dynamics, structural mechanics, modelling compound devices, modelling ships and mobile offshore platforms, industrial processing of complex non-Newtonian liquids, and modelling car bodies and engine components. Table 2.ii shows the performance of the MUMPS factorization and solution phases on a symmetric positive definite matrix (provided by MSC) that comes from the modelling of an inline skater. The matrix is of order 503,712 and has 18.7 million nonzeros in its lower triangular part. The factorization requires  $1.4 \times 10^{11}$  floating-point operations and the factors contain 175 million entries. The largest problem we have solved to date is a model of an AUDI crankshaft. The corresponding linear system is symmetric positive definite and of order 943,695 with more than 39 million entries in its lower triangular part. With the best ordering of the unknowns that we tried, MUMPS created 1.4 billion entries in the factors and required  $5.9 \times 10^{12}$  floating-point operations for the factorization.

[1] P. R. Amestoy, I. S. Duff, and J.-Y. L'Excellent, (1998), Multifrontal parallel distributed symmetric and unsymmetric solvers, Tech. Rep. TR/PA/98/22, CERFACS, Toulouse, France. To appear in special issue of *Comput. Methods in Appl. Mech. Eng.* on Domain Decomposition and Parallel Computing.

Version	Important new features	Release month
1.0	MPI version using only tree parallelism.	5/97
2.0	Uses both node and tree parallelism. Uses ScaLAPACK at root node of elimination tree. Better data management enables solution of larger problems. Uses PARASOL interface (host-node paradigm).	2/98
2.1	Version for symmetric positive definite matrices	5/98
2.2	Available with Fortran 90 interface: Ability to handle general symmetric matrices. Hybrid host version (including serial code). Basic version of rank estimate and null-space.	9/98
2.2	Available with PARASOL interface: Includes orderings based on METIS and other graph partitioning strategies.	10/98
3.1	Version with entry for unassembled matrices. Improved strategies for rank estimation and null-space.	1/99
3.2	Capability of handling distributed matrix input.	2/99
4.0	Final code for PARASOL partners. Better tuned/interface for other PARASOL codes. Ability to return a Schur complement matrix.	4/99
4.1.1	Current version.	12/99

Table 2.i: The versions of MUMPS in 1998/1999.

number of processors	elapsed time	
	factorization	solution
1	723	18.5
2	385	10.7
4	222	8.8
8	151	5.0
12	97	4.4
16	68	4.2
32	62	4.4

Table 2.ii: Factorisation and solution time (in seconds) for MUMPS on the INLINE500K test case (503,712 unknowns) on an SGI Origin 2000 (195Mhz) machine.

- [2] I. S. Duff and J. K. Reid, (1983), The multifrontal solution of indefinite sparse symmetric linear systems, *ACM Trans. Math. Softw.*, **9**, 302–325.
- [3] I. S. Duff and J. K. Reid, (1984), The multifrontal solution of unsymmetric sets of linear systems, *SIAM J. Scientific and Statistical Computing*, **5**, 633–641.

## 2.2 Development of kernels for dense and sparse numerical linear algebra (I. S. Duff, M. J. Daydé and C. Vömel)

Matrix-matrix multiplication (of dense matrices) can be performed at often close to peak rates on a wide range of computers although a highly tuned code is sometimes required. This is because the regular structures involved allow various forms of partitioning and blocking that can be used to exploit caches, vector registers, or parallelism to ensure that the normal bottleneck of high performance computing, namely access to memory, is avoided. Daydé and Duff have designed the Level 3 BLAS kernel for matrix-matrix multiply (GEMM), using only Fortran, so that it performs well on RISC based computers. They have also designed the other Level 3 BLAS routines so that they can use either this GEMM kernel or one supplied by the computer vendor. Their paper on this work has recently appeared in ACM Trans Math Software [ALG3]. Their intention is to develop these codes further when new architectures appear. The current codes are freely available from the anonymous ftp site <ftp.enseeiht.fr> in directory `pub/numerique/BLAS/RISC`.

We have also been involved in discussions on the design of basic Linear Algebra Subprograms for Level 2 and Level 3 kernels for sparse matrices. A paper on User Level codes has appeared in ACM Trans Math Software [5] and ideas from this paper have influenced the design of the kernels within the BLAS being developed by the BLAS Technical forum <http://www.netlib.org/cgi-bin/checkout/blast/blast.pl>. A key part of this design is the idea of matrix handles so that the user need not be concerned with the details of the storage schemes for the sparse matrix. It is envisaged that these kernels will be widely used in the solution of sparse equations by iterative methods. After some preliminary work by Laurent Sutra, a summer student at CERFACS, we have designed and developed a Fortran 95 instantiation of the sparse BLAS for the BLAS Technical forum project [4].

- [4] I. S. Duff and C. Vömel, (2000), Level 2 and Level 3 Basic Linear Algebra Subprograms for sparse matrices: a Fortran 95 instantiation, Tech. Rep. (To appear), CERFACS, Toulouse, France.
- [5] I. S. Duff, M. Marrone, G. Radicati, and C. Vittoli, (1997), Level 3 Basic Linear Algebra Subprograms for sparse matrices: a user level interface, *ACM Trans. Math. Softw.*, **23**, 379–401.

## 2.3 Permuting large entries to the diagonal (I. S. Duff and J. Koster)

We have continued the development of several algorithms based on bipartite weighted matching algorithms for permuting a matrix so that the entries on the diagonal of the permuted matrix are large relative to the off-diagonal entries. We have also implemented a scaling with one of the options which gives a unit diagonal with no off-diagonal entries larger than one. This work is based on earlier work reported in [7] and is described in detail in [8]. A highly efficient Fortran code MC64 has been written to implement this algorithm.

We have experimented with using these algorithms to preorder matrices prior to using various factorization and solution schemes and have sometimes found a dramatic effect. For example, when used with the MA41 multifrontal code, far fewer operations and considerably less storage are needed for the factorization of unsymmetric systems because the multifrontal factorization does not perturb the initial selection of pivots by so much. Other researchers, for example [9], have used our code so

that they can predetermine a pivot sequence and avoid subsequent dynamic scheduling in a parallel implementation of their supernodal factorization.

We have also found that the robustness and performance of preconditioned iterative solvers can be greatly improved by using MC64 as a preprocessing step. For example, the scaling option in the code has a profound influence on the convergence of the Block Cimmino iterative scheme. Some problems do not converge without the reordering and scaling but require only a few iterations if such preprocessing is performed. Extensive experiments with our orderings as a preprocessing step in the solution of indefinite and nonsymmetric linear systems has confirmed our findings that the convergence of Krylov subspace methods preconditioned with standard incomplete factorizations can be greatly improved [6]. They observed similar gains for other preconditioning techniques such as factored sparse approximate inverses when preprocessed using our scheme.

- [6] M. Benzi, J. C. Haws, and M. Tũma, (1997), Preconditioning Highly Indefinite and Nonsymmetric Matrices, Tech. Rep. LA-UR-99-4857, Los Alamos National Laboratory, Los Alamos, NM, USA.
- [7] I. S. Duff and J. Koster, (1999a), The design and use of algorithms for permuting large entries to the diagonal of sparse matrices, *SIAM J. Matrix Analysis and Applications*, **20**, 889–901.
- [8] I. S. Duff and J. Koster, (1999b), On algorithms for permuting large entries to the diagonal of a sparse matrix, Tech. Rep. TR/PA/99/13, CERFACS, Toulouse, France. Submitted to *SIAM J Matrix Analysis and Appl.*
- [9] X. S. Li and J. W. Demmel, (1998), Making Sparse Gaussian Elimination Scalable by Static Pivoting, In *Proceedings of Supercomputing*, Orlando, Florida.

## 2.4 Parallelization of the *ELU* algorithm (R. Suda)

In transient circuit analysis, linear systems with sparse coefficient matrices must be solved. Direct solvers are usually used to solve them, because most iterative solvers fail to converge. To speedup the linear solution in circuit transient analysis, we have proposed the *ELU* (Ensparsed *LU*) decomposition algorithm [10]. Assuming Newton-Raphson iterations are used, it is designed as an approximate linear solver. It solves a linear system  $\tilde{A}\tilde{x} = b$ , where  $\tilde{A}$  is a modified coefficient matrix so that the *LU* factorization of  $\tilde{A}$  has a smaller number of nonzero entries than the *LU* factorization of the original matrix  $A$ . The factorization can be computed by updating the previous factorization with a small number of floating-point operations. The magnitude of the error matrix  $\tilde{A} - A$  is controlled by a threshold parameter.

On our visit to CERFACS, we studied the efficient parallelization of the *ELU* decomposition algorithm. As the first step, we have parallelized an *ELU* code with a parallelization scheme similar to MUMPS [ALG20]. Its parallel efficiency was almost the same as that of the underlying parallel *LU* factorization. Our next research theme will involve further exploitation of the parallelism of *ELU*.

- [10] R. Suda and Y. Oyanagi, (1998), The Ensparsed LU Decomposition Method for Large Scale Circuit Transient Analysis, In *Proceedings ASP-DAC '98*, Yokohama, Japan, 507–512.

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## 3 Iterative Methods and Preconditioning

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### 3.1 Sparse preconditioning of dense problems from electromagnetism applications (B. Carpentieri, I.S. Duff and L. Giraud)

The analysis of wave propagation phenomena is required in the simulation of many industrial processes ranging from radar cross section to antenna design, absorbing materials, electromagnetic compatibility, and so on. A reliable approach to address these problems solves the Maxwell equations in the frequency domain leading to dense complex linear systems which are very challenging to solve. Nowadays the typical problem size in the electromagnetic industry is continually increasing, and direct dense methods based on Gaussian elimination become impractical even on large parallel platforms because of their high computational cost. A promising alternative is the iterative solution via Krylov subspace solvers, provided we have fast matrix-vector multiplications and robust preconditioners. Two projects were completed focusing on the design of robust preconditioning techniques, a key component of Krylov methods in that context.

In the first project [ALG23] we investigate and compare the performance of different types of preconditioners, both of implicit and explicit form, in connection with some popular Krylov solvers. Sparse approximate inverse techniques prove to be the best candidates to precondition this class of problems efficiently. In particular, the Frobenius-norm minimization approach can greatly accelerate the convergence of iterative solvers, if compared with the implicit approach based on incomplete factorizations. This method requires the selection of a sparse nonzero pattern for the preconditioner that captures the large entries of the inverse. Different heuristics based on the magnitude of the entries of the coefficient matrix  $A$  of the linear system are considered for that purpose. A major concern is the issue of cost, usually a bottleneck for this family of methods. To reduce the computational effort, the preconditioning matrix is obtained by using a sparse approximation of  $A$ , constructed by using the same pattern to that of the preconditioner. On more difficult problems, retaining more large entries from  $A$  can improve substantially the quality of the preconditioner without increasing the computational cost much.

In the second project [ALG22], we propose some sparse pattern selection strategies both for the preconditioner and for the selection of the entries of  $A$  in order to develop a robust Frobenius norm minimization method for electromagnetic scattering problems. The novelty of our approach comes from using a different nonzero pattern selection for the original matrix to that for the preconditioner and from exploiting geometrical or topological information from the underlying meshes in addition to using methods based on the magnitude of the entries. The numerical and computational efficiency of the proposed preconditioners are illustrated on a set of model problems arising both from academic and from industrial applications. Our numerical experiments, compared to those observed with some classical preconditioners of both explicit and implicit form, suggest that the new strategies are viable approaches for the solution of large-scale electromagnetic problems using preconditioned Krylov methods. In particular, our strategies exploit only physical information related to the near field, so that they are applicable when fast multipole techniques are used for the matrix-vector product on parallel distributed memory computers. A paper related to this work has been submitted for the *special issue* of the conference *Preconditioning Techniques for Large Sparse Matrix Problems in Industrial Applications* (Hubert H. Humphrey Institute, University of Minnesota, Minneapolis, 10–12 June 1999).

### 3.2 A two-level preconditioner for the Schur complement and application to semi-conductor device modeling (L. Giraud and J.-C. Rioual)

In the framework of a joint research project between INRIA (A. Marrocco, P. Le Tallec) and CERFACS (L. Giraud, J. C. Rioual) we are developing a parallel domain decomposition code for the solution of the drift diffusion equation involved in semiconductor device modelling.

The model describes the stationary state of a transistor (when  $t \rightarrow \infty$ ) when a tension is applied on its bounds. This model is a system of six nonlinear partial differential equations totally coupled. This system is decoupled and discretized in time by an implicit nonlinear scheme. At each time step we have to solve three systems of two nonlinear partial differential equations. The first system is associated with the electrostatic potential, the second one with the negative charges (electrons) and the last one with the positive charges (holes).

Each of these systems is discretized in space by a mixed finite-element method defined on 2D unstructured meshes and then solved by a Newton-Raphson method. At each step of the Newton-Raphson method a linear system of equations has to be solved.

In order to solve these linear systems, we investigate domain decomposition techniques without overlap.

The only local component enabling convergence is a block diagonal preconditioner where each block corresponds to the assembled local Schur complement matrices associated with one subdomain [12], [ALG24]. (i.e. the exact Schur complement matrix restricted to each subdomain interface). While this preconditioner is numerically relevant, we needed efficient sparse software to make it computationally competitive.

Using classical sparse direct solver, the computation of the local Schur complement matrices is usually too time consuming. We used some functionalities of the multifrontal parallel solver MUMPS [11] to compute it efficiently.

The local component of the preconditioner works well, but the condition number of the preconditioned system still depends on the number of subdomains. To avoid this drawback, we are looking for a two-level strategy, with a coarse grid preconditioner with one degree of freedom for each subdomain. This is ongoing work.

[11] P. R. Amestoy, I. S. Duff, and J.-Y. L'Excellent, (1998), Multifrontal Parallel Distributed Symmetric and Unsymmetric Solvers, Tech. Rep. TR/PA/98/22, CERFACS, Toulouse, France. To appear in special issue of Comput. Methods in Appl. Mech. Eng. on domain decomposition and parallel computing.

[12] L. Carvalho, (1997), *Preconditioned Schur complement methods in distributed memory environments*, PhD thesis, INPT/CERFACS, Toulouse, France. TH/PA/97/41, CERFACS.

### 3.3 Block Krylov solvers (L. Giraud and J. Langou)

In collaboration with the CCR Aerospatiale Matra we are investigating Krylov methods able to handle simultaneously several right-hand sides. Our preliminary study focuses on the block variant of the GMRES algorithm and more precisely on the deflation technique that should be implemented to manage situations where the solutions associated with some right-hand sides converge faster than for the others.

### 3.4 European project MYSHANET, parallel Multi-body simulation for SHock absorber design on PC NETwork (L. Giraud and U. Martin-Martin)

The PST projects aim at transferring technology to small and medium enterprises that are newcomers in the field of high performance computing and networking. The Parallel Algorithms Project has coordinated one PST project entitled MYSHANET (Project no 97 051 EP 26 441) that is connected to the Italian Transfer Technology Node NOTSOMAD. The partners of the MYSHANET consortium are the developers CEIT (Spain), CERFACS, and end-users Donerre (France, small company with less than 10 people) and Marzocchi (Italy) that are shock absorber manufacturers. In the framework of this 18 month project that ended in June 1999, a code originally developed for Unix platforms [ALG1] has been ported to networks of PCs running the NT operating system. The resulting software tool, installed on industrial end-users networks of PCs, helps in the design of new industrial mechanical systems by performing parallel parametric multi-body simulations.

### 3.5 Local preconditioners for two-level non-overlapping domain decomposition methods (L. M. Carvalho, L. Giraud and G. Meurant)

We consider additive two-level preconditioners, with a local and a global component, for the Schur complement system arising in non-overlapping domain decomposition methods. We propose two new parallelizable local preconditioners. The first one is a computationally cheap but numerically relevant alternative to the classical block Jacobi preconditioner. The second one exploits all the information from the local Schur complement matrices and demonstrates an attractive numerical behaviour on heterogeneous and anisotropic problems. We also propose two implementations based on approximate Schur complement matrices that are cheaper alternatives to construct the given preconditioners but preserve their good numerical behaviour. We compare their numerical performance with well-known robust preconditioners such as BPS [13] and the balanced Neumann-Neumann method [14].

[13] J. Bramble, J. Pasciak, and A. Schatz, (1986), The Construction of Preconditioners for Elliptic Problems by Substructuring I., *Math. Comp.*, **47**, 103–134.

[14] J. Mandel, (1993), Balancing Domain Decomposition, *Communications in Numerical Methods in Engineering*, **9**, 233–241.

### 3.6 Parallel scalability of two-level non-overlapping domain decomposition methods (L. Giraud and F. Guevara)

In order to study the parallel scalability of the preconditioners described in Section 3.5, those numerical techniques have been implemented on distributed memory platforms. The parallel implementation intensively used the new functionality of the MUMPS code [ALG20] that explicitly computes the local Schur complement. This enables us to easily construct our preconditioners and to perform the matrix-vector product with the Schur complement matrix using a simple Level 2 BLAS routine.

### 3.7 Preconditioning in domain decomposition (D. Lee)

Dr. Daniel Lee, from the National Center for High-Performance Computing in Taiwan, visited CERFACS for a research study in parallel processing with applications using a domain decomposition

method. During his three-month visit, from January 16 to April 15, he attended the regular internal seminars and gave a talk on “Solving PDEs by FV and DD Methods” on March 11.

He had very helpful discussions with Iain Duff and Luc Giraud. Also thanks to the interactive environment and the Sun cluster, he designed and implemented in some detail several preconditioners. In his nonlinear approach to fluids computation, based on a domain decomposition method, he regards the interface problem as a preconditioner for a nonlinear block Jacobi DD approach, with an optional fine level interface problem solved to obtain a further preconditioner. Also a (global) coarse level preconditioner is considered. These are discussed in the report [16].

A relaxation type strategy, in simple or hybrid form, can be used to accelerate the convergence on the interface variables, providing an interface preconditioner for the global problem. Furthermore, one can even over-relax the setup of the interface problems resulting in an accelerated interface preconditioner. These are discussed in the report [15].

Such preconditioned nonlinear DD methods exhibit impressive improvement over the basic non-preconditioned parallel Newton-Jacobi method. In summary, the interface problem is relatively small in size, easier to solve by an approximate matrix-free Newton-iterative method, and the solution should provide more accurate interior boundary condition at the interface variables in an efficient way. That is, the acceleration on only the interface variables yields a preconditioner for subsequent (nonlinear) DD iterations.

[15] D. Lee and M. Yu, (2000), Parallel flow computation with domain based SOR type interface preconditioner. Accepted for HPC-Asia-2000 Conference.

[16] D. Lee, (1999), On the interface and two-level preconditioners in Newton-Schwarz method. Presented at Domain Decomposition Conference Chiba, Japan, August 1999.

## 4 Qualitative Computing

*Group members: Françoise Chaitin-Chatelin, Amina Bouras, Sargis Dallakyan, Sébastien Goldstein, Valérie Frayssé, Abderrazak Ilahi, Elisabeth Traviesas and Ahmed Zaoui.*

The central question studied in the Qualitative Computing Group concerns the reliability of numerical software and methods in finite-precision arithmetic. This problem has been addressed through different aspects including a theory of computability in finite precision, convergence of iterative methods in finite precision, perturbation theory (conditioning and backward error analysis) in linear algebra, eigenvalue computations. Our research is motivated and enriched by applications on physical and technological problems arising from both academic and industrial worlds.

Our on-going collaboration with CNES concerns now not only accurate orbitography but addresses also the question of the convergence of embedded solvers. This topic seems to attract a wide industrial interest since we have also been approached by EDF and Aerospatiale. This will result in a joint workshop with these three shareholders in September 2000.

We now discuss some points that have been particularly investigated during the year 1999.

### 4.1 Homotopic perturbations

We consider a deviation matrix  $E$  and a homotopic (resp. normwise) normalisation factor  $\alpha_H$  (resp.  $\alpha_N$ ). The notions of backward error and pseudospectrum have been studied in [ALG28, ALG38] for the case of a perturbation  $\Delta A = tE$ ,  $t \in \mathbb{C}$ , and the norm  $|t|/\alpha_H$ . For a given  $\varepsilon > 0$ , the comparison between the homotopic  $\varepsilon$ -pseudospectrum  $\sigma_\varepsilon^{\mathcal{H}(E)}(A)$  and the normwise  $\varepsilon$ -pseudospectrum  $\sigma_\varepsilon^{\mathcal{N}}(A)$  depends on the values  $\alpha_N$  and  $\alpha_H$ . When the structure  $E$  of the perturbation  $\Delta A$  is known, and for an appropriate choice of  $\alpha_H$  and  $\alpha_N$ ,  $\sigma_\varepsilon^{\mathcal{H}(E)}(A)$  can give us much better information about the localisation of the eigenvalues of  $A$  than  $\sigma_\varepsilon^{\mathcal{N}}(A)$ . Can we have an easy way to find the border of  $\sigma_\varepsilon^{\mathcal{H}(E)}(A)$ ? Is the border of  $\sigma_\varepsilon^{\mathcal{H}(E)}(A)$ , called  $\Gamma_\varepsilon(A, E)$ , the same set as all the eigenvalues of  $A(t) = A + tE$ ,  $|t| = \varepsilon$ ? In the general case, the border of  $\sigma_\varepsilon^{\mathcal{H}(E)}(A)$  is included in  $\Gamma_\varepsilon(A, E)$ . Only for a matrix  $E$  of rank 1 are these two sets equal.

For  $\varepsilon = 1$ , the set  $\Gamma_\varepsilon(A, E)$  is the *spectral curve*  $\Gamma$  associated with  $(A, E)$ . What are the properties of this *spectral curve*  $\Gamma$ ?

- If the solution  $x(t)$  of the linear system  $(A(t) - zI)x(t) = b$  is known, and if  $z$  is outside the curve  $\Gamma$  associated with  $(A, E)$ , the solution  $x(t)$  can be computed by means of a convergent Neumann series from the solution  $x$  of  $(A - zI)x = b$ .
- Only if  $E$  is of rank 1, the spectrum of  $A(t)$ ,  $|t| = 1$  is located on  $\Gamma$  and the spectrum of  $A(t)$ ,  $|t| > 1$  is located outside  $\Gamma$ . For example, for  $H_k$  and  $V_k = \{v_1, \dots, v_k\}$  from an Arnoldi process, all the eigenvalues of  $H_k$  are located on the spectral curve  $\Gamma$  associated with  $A$  and with the deviation matrix  $-h_{k+1,k}v_{k+1}v_k^*$  of rank 1.
- Only if  $E$  is of rank 1, because the spectrum of  $A$  lies inside the curve  $\Gamma$  associated with  $(A, E)$  as well as on  $\Gamma'$  associated with  $(A + E, E)$ , the use of spectral curves allows us to better locate the eigenvalues of  $A$ .

The main part of this work was presented at the "Second Workshop on Large-Scale Scientific Computations", Sozopol, Bulgaria, June 2-6, 1999. The reference [ALG28] has been accepted for publication.

## 4.2 An analysis of the convergence of the Power method for multiple eigenvalues

Although the Power method for the computation of the dominant eigenvalue is the most basic eigensolver, its convergence has been mostly studied in the case where the matrix is diagonalisable and when the dominant eigenvalue is simple or semi-simple. We provide a complete convergence analysis in the most general case where the dominant eigenvalue can be defective, assuming however that there is only one distinct eigenvalue of largest modulus. In [ALG21], we assume that the arithmetic is exact and we relate the convergence properties, in terms of backward error, with the Jordan structure of the matrix and the choice of the initial vector. Future work will include the analysis of the convergence in finite-precision arithmetic.

## 4.3 Condition numbers for multiple defective eigenvalues

We study the the Hölder-continuous mapping from a matrix to one of its eigenvalues when it is multiple and defective [ALG27]. Two asymptotic Hölder-condition numbers are considered: one (resp. the other) is associated with a generalization of the Fréchet (resp. Gateaux) derivative. We illustrate on an exhaustive set of  $3 \times 3$  examples why these asymptotic condition numbers may not be appropriate to analyze eigencomputations performed in finite precision. We present the complementary view point of differential geometry which is based on the stratification diagram in  $\mathbb{C}^{3 \times 3}$ . The distance to the stratum indicates when this complementary viewpoint is required.

## 4.4 Eigenvalue computations—Collaboration with INRIA

We have developed the hybrid eigensolver ISA : Itérations Simultanées - Arnoldi, by coupling the Arnoldi code ArnoldiB (IRISA) and the Simultaneous Iterations code SRRIT (Bai and Stewart) [17, 18]. The code is intended to compute the  $r$  eigenvalues (counted with multiplicities) which are the closest to a given complex number  $\sigma$ . To enhance the robustness of the code, we have introduced level 3 BLAS routines. The numerical quality of the code is assessed on test examples based on results in [19]. This work is done in the framework of the CERFACS-INRIA collaboration.

Part of the work was presented at the Doctoriales 99, a meeting between Ph.D. students and industry representatives. The presentation of A. Zaoui was awarded the “best exposition” prize.

[17] Z. Bai and G. W. Stewart, (1997), Algorithm 776: SRRIT: A Fortran Subroutine to Calculate the Dominant Invariant Subspace of a Nonsymmetric Matrix, *ACM Trans. Math. Software*, **23**, 494–513.

[18] F. Chatelin, (1988), *Valeurs propres de matrices*, Masson, Paris.

[19] E. Traviesas, (2000), *Convergence des méthodes de Krylov : arithmétique exacte vs arithmétique à précision finie*, Ph.D. dissertation, Université Toulouse I. to appear.

## 4.5 Convergence of embedded solvers

Iterative processes are widely used in Linear Algebra for treating large sets of data. It becomes more and more common now that one iterative solver has to be embedded in an outer one: this is the case, for instance, for solving eigenproblems with inverse iteration or with a Krylov method with invert. The question then arises: *what is the best strategy for stopping the inner iterations to ensure the convergence of the outer iterations while minimizing the global computational cost ?*

This question has been partially addressed by numerical experts only very recently [20, 25, 24, 22, 21, 23]. The proposed strategies have been so far extremely problem-dependent.

Our purpose is to improve our understanding of the numerical behaviour of embedded solvers through a large set of experiments. We are targeting first the embedded iterations arising in shift-and-invert

techniques for large eigenproblems, and inner-outer processes in domain decomposition techniques. Part of this work is being developed in the framework of the Zoom contract with CNES.

- [20] S. C. Eisenstat and H. F. Walker, (1996), Choosing the forcing terms in an inexact Newton method, *SIAM J. Sci. Comput.*, **17**, 16–32.
- [21] E. Giladi, G. H. Golub, and J. B. Keller, (1998), Inner and outer iterations for the Chebyshev algorithm, *SIAM J. Numer. Anal.*, **35**, 300–319.
- [22] G. H. Golub and M. L. Overton, (1988), The convergence of inexact Chebyshev and Richardson iterative methods for solving linear systems, *Numer. Math.*, **53**, 571–593.
- [23] G. Golub and Q. Ye, (1999), Inexact Inverse Iterations for the Generalized Eigenvalue Problems, scsm-99-02, Stanford University.
- [24] G. H. Golub, Z. Zhang, and H. Zha, (1998), Large sparse symmetric eigenvalue problems with homogeneous linear constraints: the Lanczos process with inner-outer iterations.
- [25] P. Smit and M.-H.-C. Paardekooper, (1999), The effects of inexact solvers in algorithms for symmetric eigenvalue problems, *Lin. Alg. Appl.*, **287**, 337–357.

## 4.6 Jason contract with CNES

We are continuing our collaboration with CNES on accurate orbitography, for which we are in charge of performing an analysis of speed, efficiency and numerical robustness of the available software. The carrier phase ambiguity resolution is the main problem for reaching centimeter level accuracy in Global Positioning System. Mathematically the ambiguity resolution can be presented as a mixed least-squares problem. To find the numerical solution to this problem an efficient method, called Least-squares AMBiguity Decorrelation Adjustment (LAMBDA) method, has been developed by Professor P.J.G. Teunissen from Delft University of Technology. Based on a MATLAB implementation of the LAMBDA method, extensive numerical tests have been done in [ALG25]. The result of these tests show that the LAMBDA method itself is a robust and reliable method for the GPS carrier phase ambiguity resolution. There was a minor bug in the distributed software which has been fixed, and the optimization has been carried out, which can lead to a significant improvement in the performance.

Following the work initiated in [27], the condition numbers for the  $L^TDL$  factorization have been computed on a preliminary set of real data: this showed that this key part of the computation seems rather insensitive to perturbations. We also investigated the influence that errors on the estimated ambiguities may have on the final least-squares solution [26]. More should be done in this direction, in particular with real data.

In [ALG26], an overview of carrier phase differential GPS and the latest developments in the field of GPS carrier phase ambiguity resolution are presented.

We hope that the test cases, provided recently by CNES, will help us address important questions related to the control of the quality of the resolved ambiguities.

- [26] S. Goldstein, (1999), Traitement d’ambiguïtés entières - Etude de sensibilité. Rapport de Stage de deuxième année CUST-Clermont-Ferrand & CERFACS.
- [27] S. Gratton, (1995), Utilisation du produit de Kronecker pour le calcul du conditionnement en norme de Frobenius, Tech. Rep. Annexe du rapport FR/PA/95/28, CERFACS.

## 4.7 Multiplication of hypercomplex numbers

How complex can a number be such that it is still possible to compute with it ? That is, that we cannot only add, but multiply and divide (except by 0) ? It was discovered in the 19<sup>th</sup> century that

(in addition to the reals) this was possible on vectors of  $\mathbb{R}^n$ , of dimension  $n = 2$  (complex numbers),  $n = 4$  (quaternions) and  $n = 8$  (octonions). And it was proved in 1958 that this was possible only for these 4 values  $n = 1, 2, 4$  and  $8$ . This remarkable result has remained almost unnoticed by the practitioners of computation. However, it seems likely that octonions are to Biology what quaternions are to Physics [ALG30]. The computing power of Geometry was presented, on invitation, at the 1999 Dundee conference [ALG10]. We are currently investigating new directions for computation along these lines. Some of the new perspectives toward a self-evolving Information Theory have been presented in [ALG29]. Reference [28] has been accepted for publication.

[28] F. Chaitin-Chatelin and S. Gratton, (1998), On the condition number associated with the polar factorization of a rectangular matrix, Technical Report TR/PA/98/25, CERFACS, Toulouse, France. To appear in *Num. Lin. Alg. Appl.*

## 4.8 Visualization of bifurcations

It is difficult to overestimate the role of visualization in classifying and describing a large variety of bifurcation points in dynamical systems. At the bifurcation points, the asymptotic behaviour of dynamical systems changes qualitatively, a phenomenon that is well known in modern physics. An interesting example of this can be found in the theory of critical phenomena, where bifurcation points represent continuous phase transition points, separating different phases. Because a large number of parameters control the phase transition points (e.g. temperature, pressure, external magnetic field, etc.), a good visualization of multiparametric bifurcation is necessary for better understanding of the phase structure of a system under consideration.

In Ref. [ALG33] several difficulties related to visualization of Figure 8.3 have been presented.

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## 5 Nonlinear Systems and Optimization

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### 5.1 Constrained and Unconstrained Testing Environment (CUTE) v. 3.0. (A.R. Conn, N.I.M. Gould, D. Orban and Ph.L. Toint)

The Constrained and Unconstrained Testing Environment (CUTE) [29] is a versatile environment for testing small to large-scale nonlinear programming problems arising from both real practical applications and from academic circles. It provides Fortran tools for computing function values, gradients, Hessians, matrix-vector products and handles both dense and sparse problems. It has been designed with multi-platform environments in mind and the test problems are written using the SIF (Standard Input Format) description language, formerly used by LANCELOT [30]. CUTE also provides tools to help the users build their own interface to their optimization package, as well as ready-to-use interfaces to famous existing packages like MINOS and OSL.

The purpose of this research is to make the CUTE environment available on more platforms, including the quickly growing Linux. Its installation phase should also be made more efficient, making better use of available disk space and memory, as well as allowing multiple installations with different settings. We shall provide more tools, with enhanced capabilities, that implement recent developments in dense and sparse linear algebra.

[29] I. Bongartz, A. R. Conn, N. I. M. Gould, and P. L. Toint, (1995), CUTE: Constrained and Unconstrained Testing Environment, *Transactions of the ACM on Mathematical Software*, **21**, 123–160.

[30] A. R. Conn, N. I. M. Gould, and P. L. Toint, (1992), *LANCELOT: a Fortran package for large-scale nonlinear optimization (Release A)*, Springer Series in Computational Mathematics, Springer Verlag, Heidelberg, Berlin, New York.

### 5.2 Local convergence of the newton/log-barrier method for degenerate problems (S.J. Wright and D. Orban)

We examine the sequence of local minimizers of the log-barrier function for a nonlinear program near a solution at which second-order sufficient conditions and the Mangasarian-Fromovitz constraint qualifications are satisfied, but the active constraint gradients are not necessarily linearly independent [ALG39]. In trying to retrieve results similar to those contained in the seminal book [31], we obtained the following. When a strict complementarity condition is satisfied, we show uniqueness of the local minimizer of the barrier function in the vicinity of the nonlinear program solution, and obtain a semi-explicit characterization of this point. When strict complementarity does not hold, we obtain several other interesting characterizations, in particular an estimate of the distance between the minimizers of the barrier function and the nonlinear program in terms of the barrier parameter, and a result about the direction of approach of the sequence of minimizers of the barrier function to the nonlinear programming solution.

[31] A. V. Fiacco and G. P. McCormick, (1968), *Nonlinear Programming: Sequential Unconstrained Minimization Techniques*, J. Wiley and Sons, Chichester, England. Reprinted as *Classics in Applied Mathematics*, SIAM, Philadelphia, USA, 1990.

### 5.3 A primal-dual interior-point trust-region algorithm for non-convex, nonlinear programming (A.R. Conn, N.I.M. Gould, D. Orban and Ph.L. Toint)

In this project, we globalized a primal-dual interior point algorithm by means of trust-regions in order to minimize a non-convex function subject to nonlinear inequality and linear equality constraints [ALG31]. By globalizing, we mean ensuring convergence (of the sequence of iterates or a subsequence thereof) to a critical point from *any* starting point. Primal-dual interior point methods for nonlinear programming have indeed received increasing interest these last years, given their success in linear programming (see [33]). This research is partly based on the work of Conn, Gould and Toint [32] where a linesearch strategy is used. The present method uses a primal-dual model of the logarithmic barrier function, which is iteratively approximately minimized in a trust region. The method is globally convergent to weak second-order stationary points. The algorithm has been implemented in the Harwell Subroutine Library as HSLVE12 and has been successfully tested on both convex and non-convex, low to high-dimensional quadratic programming problems from the CUTE [29] collection, in the case where the inequality constraints are simple bounds.

[32] A. R. Conn, N. I. M. Gould, and P. L. Toint, (1999), A Primal-Dual Algorithm for Minimizing a Nonconvex Function Subject to Bound and Linear Equality Constraints, In *Nonlinear Optimization and Applications 2*, G. D. Pillo and F. Giannessi, eds., Dordrecht, The Netherlands, Kluwer Academic Publishers. To appear.

[33] S. J. Wright, (1997), *Primal-Dual Interior-Point Methods*, SIAM, Philadelphia, USA.

### 5.4 Superlinear convergence of primal-dual interior point algorithms for nonlinear programming (N.I.M. Gould, D. Orban, A. Sartenaer and Ph.L. Toint)

We have analyzed local convergence properties of the primal-dual trust-region interior point method [ALG31], described in Section 5.3. This method is designed to minimize a nonlinear, nonconvex, objective function subject to linear equality constraints and general inequalities by means of a log-barrier approach. The presented analysis follows that of [ALG39, 34, 35, 36], the first of which is described in Section 5.2. Asymptotically, for each value of the barrier parameter, a single primal-dual linear system is solved and interpreted as a predictor-corrector-like extrapolation of the central path. Stepping along the direction thereby given yields a point that already matches the barrier subproblem stopping tolerances and Q-superlinear convergence, which can be as close to quadratic as one wishes, is achieved. Moreover, this fast asymptotic convergence occurs componentwise. Since the Inner Minimization phase — used in [ALG31] to solve a barrier subproblem — is not required asymptotically, we observe that the drawn conclusions hold independently of the Inner Minimization procedure. The theoretical results that have been drawn are encouraging and exhibit a convergence rate for barrier methods that is essentially as fast as that previously obtained for exterior penalty methods [36].

We also examine the achievable rates of convergence when the aforementioned extrapolation step is followed by one or several further Newton steps. In this case, the primal-dual merit function is dramatically reduced in the following manner: we show that the barrier parameter may decrease at a  $(2^q - 1)$  rate if  $q$  further Newton steps are taken. We expect to retrieve a Q- $(2^q - 1)$  rate of convergence in the sequence of iterates as well.

[34] A. R. Conn, N. I. M. Gould, and P. L. Toint, (1994), A note on using alternative second-order models for the subproblems arising in barrier function methods for minimization, *Numerische Mathematik*, **68**, 17–33.

- [35] J.-P. Dussault, (1995), Numerical stability and efficiency of penalty algorithms, *SIAM Journal on Numerical Analysis*, **32**, 296–317.
- [36] N. I. M. Gould, (1989), On the convergence of a sequential penalty function method for constrained minimization, *SIAM Journal on Numerical Analysis*, **26**, 107–126.

## 5.5 On the practical dependency of a trust-region algorithm on its parameters (N.I.M. Gould, D. Orban, A. Sartenaer and Ph.L. Toint)

Trust region techniques are known to be robust and competitive methods for large-scale nonlinear optimization. Their efficiency depends in particular on a good choice for the updating rules of the trust-region radius in the course of the solution. Our purpose is to investigate the determination of optimal parameters regarding both the update of the trust region and the acceptance of the trial step. With this in mind, we have implemented a code that allows such a determination of optimal parameters by covering a very large sample of potential values, each of which is being tested on a large set of problems from the CUTE [29] collection. The whole set of runs took several months and was completed at the end of the year. Using statistical tools, we have now to draw general conclusions from the extensive set of results to determine optimal values for the parameters. We will thereafter publish these conclusions.

- [37] A. R. Conn, N. I. M. Gould, and P. L. Toint, (2000), *Trust Region Methods*, SIAM, Philadelphia, USA. To appear.
- [38] A. Sartenaer, (1997), Automatic determination of an initial trust region in nonlinear programming, *SIAM Journal on Scientific Computing*, **18**, 1788–1803.

## 5.6 Improved minimization techniques in meteorological data assimilation (J. Nocedal, A. Sartenaer, R. Waltz and S.J. Wright)

The aim of this project is to propose new optimization techniques for three-dimensional and four-dimensional assimilation of data in meteorology. Our goal is to reduce the computer time needed in the assimilation process and to increase the reliability of the results. The proposed research consists of experimental work closely coordinated with a theoretical study of both the physical problems and the algorithms. The new optimization techniques will include for instance enriched limited memory quasi-Newton methods for the minimization of nonlinear cost functions and automatic preconditioners to accelerate the conjugate gradient method. We have completed a first stage that has consisted of several meetings with people of Météo France, in order for the team involved in the project to understand meteorological data assimilation better and to get an idea of the current needs in the field from the optimization point-of-view.

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## 6 Conferences and Seminars

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### 6.1 Conferences and seminars attended by members of the Parallel Algorithms Project

#### January

IRISA, Projet ALADIN, Rennes, France, January 21 and April 26. A. ZAOUI, *Valeurs propres intérieures complexes*, talk.

#### February

Seminar, NAg Ltd, Oxford, February 1. I. DUFF, *Multifrontal solvers within the PARASOL environment*, seminar.

#### March

Inter-university third cycle in mathematical programming organized by the Belgian National Fund for Scientific Research, Han-sur-Lesse, Belgium, March 4–5. A. SARTENAER, *On the accuracy of the solution and the behavior of the gradient in nonlinear optimization*, talk.

Inter-university third cycle in mathematical programming organized by the Belgian National Fund for Scientific Research, Han-sur-Lesse, Belgium, March 4–5. D. ORBAN, *A primal-dual trust-region algorithm for constrained nonlinear programming: global and local analysis*, talk.

HPCI Seminar: Parallel Sparse Matrix Solvers, EPCC, Edinburgh, March 15. I. DUFF, *Direct solution of sparse linear equations on parallel computers*, invited talk.

IFP, Rueil Malmaison, France, March 18. L. GIRAUD, *Domain decomposition and parallel computing*, invited speaker.

Computational Cattle Breeding '99, Helsinki, Finland, March 18-20. I. DUFF, *Parallel algorithms for solving large sparse equation systems*, invited talk.

SIAM Parallel Processing '99, San Antonio, Texas, March 20-24. I. DUFF, *The PARASOL Project and the multifrontal parallel solver for sparse systems*, invited minisymposium talk.

SIAM Parallel Processing '99, San Antonio, Texas, March 20-24. I. DUFF, *Higher level BLAS for sparse matrices*, invited minisymposium talk.

International Conference on Optimization, Trier, Germany, March 22–24. A. SARTENAER, *em On the accuracy of the solution and the behavior of the gradient in nonlinear optimization*, talk.

#### April

Seminar, University of Kentucky, Lexington, April 21. I. DUFF, *The PARASOL Project and the multifrontal parallel solver for sparse systems*, seminar.

Seminar, University of Tennessee, Knoxville, April 23. I. DUFF, *The PARASOL Project and the multifrontal parallel solver for sparse systems*, seminar.

## May

Seminar, INRIA, Rocquencourt, May 6. I. DUFF, *International Conference on Preconditioning Techniques for Large Sparse Matrix Problems in Industrial Applications*, seminar.

Sixth SIAM Conference on Optimization, Atlanta, Ga., USA, May 10–12. D. ORBAN, *A primal-dual trust-region algorithm for constrained nonlinear programming: global and local analysis*, talk.

1999 SIAM Annual Meeting, Atlanta, Ga., USA, May 12–15. D. ORBAN, attendee.

Congrès d'Analyse Numérique, Ax-les-thermes, France, May 17–21. A. BOURAS, *Solveurs itératifs emboîtés pour le calcul de valeurs propres de grandes matrices*, poster.

Congrès d'Analyse Numérique, Ax-les-thermes, France, May 17–21. E. TRAVIESAS, *Convergence des méthodes de Krylov*, poster.

INRIA, Sophia Antipolis, France, May 19. L. GIRAUD, *Domain decomposition and parallel computing*, invited speaker.

Université des Sciences, Rabat, Morocco, May 26. V. FRAYSSÉ, *L'analyse inverse des erreurs : Récentes avancées*, invited talk.

## June

International Conference on Preconditioning Techniques for Large Sparse Matrix Problems in Industrial Applications, Minneapolis, Minnesota, June 9–12. I. DUFF, *Sparse preconditioning of dense problems from electromagnetic applications*, talk.

Householder Symposium, Whistler, Canada, June 13–19. I. DUFF, *Sparse preconditioning of dense problems from electromagnetic applications*, talk.

18th Biennial Conference on Numerical Analysis, University of Dundee, June 29–July 2. F. CHAITIN-CHATELIN, *The computing power of Geometry*, invited speaker.

## July

ICIAM'99, Edimburgh, July 5–9. V. FRAYSSÉ, *Pseudospectra at CERFACS*, talk. Minisymposium 163, Parallel software for sparse matrices and applications, Edinburgh, Scotland, July 5-9.

I. DUFF, *Sparse matrix software in the PARASOL Project*, talk.

## August

Eighth International Colloquium on Numerical Analysis and Computer Science with Applications, Plovdiv, Bulgaria, August 13-17. I. DUFF, *Direct solution of sparse linear equations on parallel computers*, keynote talk.

EuroPar'99, Toulouse, France, August 31–September 3. I. DUFF, *Sparse direct methods and software for systems of equations*, tutorial talk.

## September

Ecole 99 de Calcul Numérique et Symbolique / Algèbre Linéaire, Rabat, Morocco, September 13–17. V. FRAYSSÉ, *Numerical solution of large eigenvalue problems*, invited talk.  
L. GIRAUD, *Méthodes itératives pour la résolution parallèle de systèmes linéaires*, invited talk.

Summer School on Advances in parallel processing with applications, Natal, Brazil, September 27–October 5. I. DUFF, *Parallel Direct Methods for Solving Systems of equations*, invited talks.

## October

EDF, October 21. F. CHAITIN-CHATELIN, *Le Calcul Qualitatif*, invited talk.

First Workshop on Nonlinear Optimization: “Interior Point and Filter Methods”, Coimbra, Portugal, October 27–30. D. ORBAN, *A primal-dual trust-region algorithm for constrained nonlinear programming: global and local analysis*, talk.

Seminar, CNR Pavia, Italy, October 29. I. DUFF, *The PARASOL Project and MUMPS, a multifrontal parallel solver for sparse systems*, seminar.

## November

ISPRS Workshop on Direct Versus Indirect Methods of Sensor Orientation, Barcelona, Spain, November 25–26. S. DALLAKYAN, attendee.

Doctoriales 99, Boussens, France, November 28–December 3. A. ZAOUI, *Calcul de valeurs propres*, poster.

## December

CCT Calcul Scientifique et Modélisation, CNES, December 7. V. FRAYSSÉ and L. GIRAUD, *Introduction aux techniques performantes en Algèbre Linéaire*, invited talk.

## 6.2 Conferences and seminars organized by the Parallel Algorithms Project

### January

PHILIPPE BOUGEAULT (Meteo-France, Toulouse), *Opportunities for progress in mesoscale weather prediction*, January 12.

### February

PIERRE DEGOND (UPS, Toulouse), *Mathematical modelling and scientific computing: some examples of applications to plasmas*, February 5.

### March

SHERRY LI (NERSC, Lawrence Berkeley National Laboratory), *Scalable sparse LU decomposition with static pivoting*, March 1.

GEORGES BALMINO (CNES, Toulouse), *The gravity field of the earth and other solar system bodies*, March 9.

STEPHEN WRIGHT (Argonne National Lab), *The Wide impact of interior-point methods*, March 16.

## April

JEAN-CLAUDE NEDELEC (CMAP - Ecole Polytechnique, Paris), *Modelisation and numerical methods in electromagnetism*, April 1.

## July

D.C. SORENSEN (Rice University, Houston), *Krylov subspace projection methods for model reduction*, July 22.

J. DONGARRA (University of Tennessee & Oak Ridge National Laboratory), *NetSolve: A Network server for solving computational science problems*, July 23.

## 6.3 Internal seminars organized within the Parallel Algorithms Project

### Februrary

BRUNO CARPENTIERI, *Continuation techniques in numerical bifurcation*.

SERGUEI SOKOL, *Multi Coarse correction with Suboptimal Operators (MCSO) method as linear solver in NSMB code*.

JEAN-CHRISTOPHE RIOUAL, *A deterministic approach for rounding-error analysis. Implementation via automatic differentiation*.

DOMINIQUE ORBAN, *A primal-dual trust-region algorithm for minimizing a non-convex function subject to bounds and equality constraints. Part I: Introduction*.

### March

LUC GIRAUD, *Parallel subdomain-based preconditioner for non-overlapping domain decomposition methods*.

DANIEL LEE, *Solving PDE by finite volume and domain decomposition method - my experience*.

### June

BRUNO CARPENTIERI, *Sparse preconditioning of dense problems from electromagnetic applications (joint work with I. Duff and L. Giraud)*.

### September

GHISLAIN LARTIGUE, *Etude d'un solveur parallèle en vue de son implantation dans le code industriel AETHER*.

### October

REIJI SUDA, *A sparsified LU factorization for circuit transient analysis*.

## 7 Publications

### 7.1 Journal Publications

- [ALG1] S. Baldini, L. Giraud, J. M. Jimenez, L. M. Matey, and J. G. Izaguirre, (1999), High Performance Computing in multi-body system design, *Int J. Supercomputer Applications*, **13**, 99–106.
- [ALG2] T. A. Davis and I. S. Duff, (1999), A combined unifrontal/multifrontal method for unsymmetric sparse matrices, *ACM Trans. Math. Softw.*, **25**, 1–20.
- [ALG3] M. J. Daydé and I. S. Duff, (1999), The RISC BLAS: A blocked implementation of Level 3 BLAS for RISC Processors, *ACM Trans. Math. Softw.*, **25**, 316–340.
- [ALG4] I. S. Duff and J. Koster, (1999), The design and use of algorithms for permuting large entries to the diagonal of sparse matrices, *SIAM J. Matrix Analysis and Applications*, **20**, 889–901.
- [ALG5] L. Giraud and R. S. Tuminaro, (1999), Schur complement preconditioners for anisotropic problems, *IMA J. Numerical Analysis*, **19**, 1–17. Also published as Sandia Nat. Lab Technical Report 98-8488J.

### 7.2 Conference Proceedings and Book Chapters

- [ALG6] P. AMESTOY, P. BERGER, M. DAYDÉ, I. DUFF, V. FRAYSSÉ, L. GIRAUD, AND D. RUIZ, eds., *EuroPar'99 Parallel Processing*, Lecture Notes in Computer Science, No. 1685, Berlin, Heidelberg, New York, Springer-Verlag.
- [ALG7] P. R. Amestoy, I. S. Duff, J.-Y. L'Excellent, and P. Plecháč, (1999), PARASOL. An integrated programming environment for parallel sparse matrix solvers, In *High-Performance Computing*, R. J. Allan, M. F. Guest, A. D. Simpson, D. S. Henty, and D. A. Nicole, eds., New York, Kluwer Academic/Plenum Publishers, 79–90.
- [ALG8] L. Carvalho and L. Giraud, (1999a), Block diagonal preconditioners for the Schur complement method, In *Innovative computational methods for structural mechanics*, M. Papadrakakis and B. Topping, eds., Edinburgh, UK, Saxe-Coburg publications, 61–82.
- [ALG9] L. Carvalho and L. Giraud, (1999b), Parallel subdomain-based preconditioner for the Schur complement, In *EUROPAR'99 Parallel Processing*, P. Amestoy, P. Berger, M. Daydé, V. Frayssé, L. Giraud, and D. Ruiz, eds., vol. 1685, Lecture Notes in Computer Science, Springer-Verlag, 1032–1039. Preliminary version published as CERFACS Tech. Rep. TR/PA/99/04.
- [ALG10] F. Chaitin-Chatelin, (1999), The computing power of Geometry, In *Numerical Analysis 1999*, D. F. Griffiths and G. A. Watson, eds., CRC Press LLC.
- [ALG11] F. Chalot, G. Chevalier, Q. Dinh, and L. Giraud, (1999), Some investigations of domain decomposition techniques in parallel CFD, In *EUROPAR'99 Parallel Processing*, P. Amestoy, P. Berger, M. Daydé, V. Frayssé, L. Giraud, and D. Ruiz, eds., vol. 1685, Lecture Notes in Computer Science, Springer-Verlag, 595 – 602. Preliminary version published as CERFACS Tech. Rep. TR/CFD/99/06.
- [ALG12] I. S. Duff and J. A. Scott, (1998), A comparison of frontal software with other Harwell Subroutine Library sparse direct solvers, In *High performance algorithms for structured Matrix problems*, P. Arbenz, M. Paprzycki, A. Sameh, and V. Sarin, eds., NOVA Science Publishers, Inc., Commack, NY, 1–25. Actually appeared in May 1999.
- [ALG13] I. S. Duff and J. A. Scott, (1999), MA62 – A frontal code for sparse positive-definite symmetric systems from finite element applications, In *Innovative computational methods for structural mechanics*, M. Papadrakakis and B. Topping, eds., Edinburgh, Saxe-Coburg Publications, 1–25.

- [ALG14] I. S. Duff, (1999a), A brief bibliography of recent research and software for the parallel solution of large sparse linear equations, In *Proceedings of the Computational Cattle Breeding '99 Workshop, Tuusula, Finland, March 18-20, 1999*, Bulletin No 20, Uppsala, Sweden, International Bull Evaluation Service, 43–46.
- [ALG15] I. S. Duff, (1999b), Matrix Methods, In *Supercomputing, collision processes and applications*, K. L. Bell, K. A. Berrington, D. S. F. Crothers, A. Hibbert, and K. T. Taylor, eds., New York, Kluwer Academic, 119–136.
- [ALG16] L. Giraud, R. Guivarch, and J. Stein, (1999), A parallel distributed fast 3D Poisson solver for MésoNH, In *EUROPAR'99 Parallel Processing*, P. Amestoy, P. Berger, M. Daydé, V. Frayssé, L. Giraud, and D. Ruiz, eds., vol. 1685, Lecture Notes in Computer Science, Springer-Verlag, 1431 – 1434.
- [ALG17] P. Jabouille, R. Guivarch, P. Kloos, D. Gazen, N. Gicquel, L. Giraud, N. Asencio, V. Ducrocq, J. Escobar, J.-L. Redelsperger, J. Stein, and J.-P. Pinty, (1999), Parallelization of the french meteorological mesoscale model MésoNH, In *EUROPAR'99 Parallel Processing*, P. Amestoy, P. Berger, M. Daydé, V. Frayssé, L. Giraud, and D. Ruiz, eds., vol. 1685, Lecture Notes in Computer Science, Springer-Verlag, 1417 – 1422.
- [ALG18] F. Mazzia and R. A. McCoy, (1999), Numerical experiments with a shifted SSOR preconditioner, In *Iterative methods in scientific computation II*, D. R. K. et. al., ed., IMACS, 00–00.

### 7.3 Theses

- [ALG19] A. Sartenaer, (1999), *Développement d'algorithmes en optimisation non-linéaire : de l'étude théorique à l'expérimentation numérique*, Thèse d'Habilitation à Diriger les Recherches, Université Paul Sabatier.

### 7.4 Technical Reports

- [ALG20] P. Amestoy, I. Duff, J.-Y. L'Excellent, and J. Koster, (1999), A fully asynchronous multifrontal solver using distributed dynamic scheduling, Technical Report TR/PA/99/28, CERFACS, Toulouse, France.
- [ALG21] A. Bouras, F. Chaitin-Chatelin, V. Frayssé, and A. Ilahi, (1999), Nouvelles analyses de la méthode de la puissance. Partie 1 : Etude asymptotique générale, Technical Report TR/PA/99/35, CERFACS, Toulouse, France.
- [ALG22] B. Carpentieri, I. Duff, and L. Giraud, (1999a), Sparse pattern selection strategies for robust Frobenius norm minimization preconditioners in electromagnetism., Technical Report TR/PA/00/05, CERFACS, Toulouse, France. To appear in Numerical Linear Algebra with Applications.
- [ALG23] B. Carpentieri, I. Duff, and L. Giraud, (1999b), Sparse preconditioning of dense problems from electromagnetic applications., Technical Report TR/PA/00/04, CERFACS, Toulouse, France.
- [ALG24] L. Carvalho, L. Giraud, and G. Meurant, (1999), Local preconditioners for two-level non-overlapping domain decomposition methods, Tech. Rep. TR/PA/99/38, CERFACS, Toulouse, France, France.
- [ALG25] F. Chaitin-Chatelin, S. Dallakyan, and V. Frayssé, (1998), On the GPS carrier phase ambiguity resolution. The LAMBDA method: an analysis of speed, efficiency and numerical robustness, Contract Report IR/PA/99/23, CERFACS, Toulouse, France.
- [ALG26] F. Chaitin-Chatelin, S. Dallakyan, and V. Frayssé, (1999), An overview of carrier phase differential GPS, Contract Report IR/PA/99/50, CERFACS, Toulouse, France.
- [ALG27] F. Chaitin-Chatelin, A. Harrabi, and A. Ilahi, (1999), About Hölder condition numbers and the stratification diagram for defective eigenvalues, Technical Report TR/PA/99/19, CERFACS, Toulouse, France. To appear in IMACS Journal on Mathematics of Computation.
- [ALG28] F. Chaitin-Chatelin, V. Toumazou, and E. Traviesas, (1999), Accuracy assessment for eigencomputations: variety of backward errors and pseudospectra, Tech. Rep. TR/PA/99/03, CERFACS, Toulouse, France. To appear in the proceedings of the “International Workshop on Accurate Solution of Eigenvalues Problems” - Special issue of *Lin. Alg. Appl.*

- [ALG29] F. Chaitin-Chatelin, (1999a), Le Sens de la Vie, Technical Report TR/PA/99/20, CERFACS, Toulouse, France.
- [ALG30] F. Chaitin-Chatelin, (1999b), The computing power of Geometry, Technical Report TR/PA/99/24, CERFACS, Toulouse, France. To appear in Proceedings of 18th Biennial Conference on Numerical Analysis, Dundee, June 1999.
- [ALG31] A. Conn, N. Gould, D. Orban, and P. Toint, (1999), A primal-dual trust-region algorithm for non-convex nonlinear programming, Technical Report TR/PA/99/27, CERFACS, Toulouse, France. To appear in Mathematical Programming B.
- [ALG32] S. Dallakyan, N. Ananikian, and R. Ghulghazaryan, (1999), Thermodynamic chaos and infinitely many critical exponents in the Baxter-Wu model, Technical Report TR/PA/00/06, CERFACS, Toulouse, France. Submitted for publication to Physica D, cond-mat/9909289.
- [ALG33] S. Dallakyan, (1999), A note on the visualization of multiparametric bifurcations, Technical Report TR/PA/00/07, CERFACS, Toulouse, France. To appear in Computers and Graphics.
- [ALG34] I. S. Duff and H. A. van der Vorst, (1999), Developments and trends in the parallel solution in linear systems, Technical Report TR/PA/99/10, CERFACS, Toulouse, France.
- [ALG35] I. S. Duff, (1999a), A brief bibliography of recent research and software for the parallel solution of large sparse linear equations, Technical Report TR/PA/99/12, CERFACS, Toulouse, France. AMS(MOS) subject classifications: 65F05, 65F50.
- [ALG36] I. S. Duff, (1999b), The impact of high performance Computing in the solution of linear systems: trends and problems, Technical Report TR/PA/99/41, CERFACS, Toulouse, France.
- [ALG37] S. Gratton, V. Frayssé, and V. Toumazou, (1999), Structured backward error and condition number for linear systems of the type  $A^*Ax = b$ , Technical Report TR/PA/99/05, CERFACS, Toulouse, France. To appear in BIT.
- [ALG38] V. Toumazou and E. Traviesas, (1999), A note on homotopic backward error and pseudospectra for the generalized eigenproblem, Tech. Rep. TR/PA/99/14, CERFACS, Toulouse, France.
- [ALG39] S. J. Wright and D. Orban, (1999), Properties of the log-barrier function on degenerate nonlinear programs, Technical Report TR/PA/99/36, CERFACS, Toulouse, France. Submitted for publication to Mathematics of Operations Research.

## 8 Appendix: Pictures

### 8.1 A geometrical approach for preconditioning dense problems from electromagnetism

Relevant physical information extracted from the underlying mesh can be exploited to construct an effective sparse approximate inverse preconditioner for dense linear systems of equations which arise in computational electromagnetics. In the density colouring graph of Figure 8.1 we plot for a cylindrical geometry the distance in terms of wavelength among pairs of edges in the mesh with respect to the magnitude of their associated entries in the inverse of the coefficient matrix of the system. The different colouring of the points refer to the density of the pattern computed for the preconditioner. For each value of distance/wavelength in the y-axis, the colouring tells us the percentage of density of the pattern computed if we retain all the edges up to there, according to the right colourbar. Most of the entries in the inverse matrix come from weak far-away interactions in the mesh, and the largest ones are strongly localized. An effective and very sparse pattern for the preconditioner can be obtained by selecting for each edge all those edges within a sufficiently large sphere defining a geometric neighbourhood. This selection strategy is referred to as the *geometrical strategy* [ALG22].



Figure 8.1: Geometrical localization in the mesh for the large entries of  $A^{-1}$  for a cylinder with a hollow inside.

## 8.2 Homotopic perturbations

According to Section 4.1, if  $E$  is of rank 1, the spectrum of  $A$  lies on the spectral curve

$$\Gamma' = \{z \in \text{Re}(A + E), \rho(E(A + E - zI)^{-1}) = 1\}$$

associated with  $(A + E, E)$ . For a  $z \in \Gamma'$ , the quantity  $\rho(E(A + E - zI)^{-1})$  is equal to 1 in exact arithmetic but can differ from 1 in finite-precision computations. We illustrate this fact by choosing

- a matrix  $A$  like a Jordan block of size 4 associated with the eigenvalue 0,
- a deviation matrix  $E = e_4 e_1^T$ .

The three-dimensional plot of Fig. 8.2 shows the quantity

$$\phi(z) = |\rho(E(A + E - zI)^{-1}) - 1|, \quad z \in \mathbb{C}$$

computed in finite precision. If  $z = 0$  is the eigenvalue of  $A$  of multiplicity 4, it lies on  $\Gamma'$  in exact arithmetic, but the quantity  $\phi(z)$  is not exactly zero in this case. The curve  $\Gamma'$  computed in finite precision arithmetic may differ from the exact curve  $\Gamma'$  and may thus not contain the spectrum of  $A$ .



Figure 8.2:  $|\rho(E(A + E - zI)^{-1}) - 1|$  computed ( $A$  a Jordan block of size 4 and  $E = e_4 e_1^T$ )

### 8.3 Visualization of bifurcations

The plot of magnetization  $m$  versus external magnetic field  $h$  and temperature  $T$  for the Baxter-Wu model is presented in Figure 8.3. To draw this graph, first one needs to map the three-dimensional space of  $m, h$  and  $T$  onto a two-dimensional computer display. This can be done with proper transformations: translation, rotation and projection. Due to the physical constraints, magnetization is bounded in the interval  $[-1, 1]$ , so the parameters of the above mentioned transformations are relatively easy to obtain. The main difficulties which one faces is the fact that a large number of iterations are necessary for stabilizing the attractor of the map near bifurcation points (critical slowing down). On the other hand, using a large number of iterations in the whole range of parameters makes the drawing process impossible to complete in a reasonable time. Note that software that stores all the 3D points is not suitable for our purpose, due to extremely large number of points ( $\sim 10^8$ ). Instead one could use a virtual screen in a memory to store only a 2D picture, but we also ruled this out since a real-time processing of the data is necessary.

Nevertheless, by changing the number of iteration and colors manually we were able to obtain the 3D graphics of magnetization as a function of temperature and external magnetic field. Figure 8.3 shows the main phase structure of our model and what kind of behavior to expect in a real experiment.

We hope that with a proper pre-processing of the data, many of the above mentioned visualization problems can be avoided.



Figure 8.3: Plot of  $m$  - (magnetization) versus  $h$  - (external magnetic field) and  $T$  - (temperature). See Section 4.8