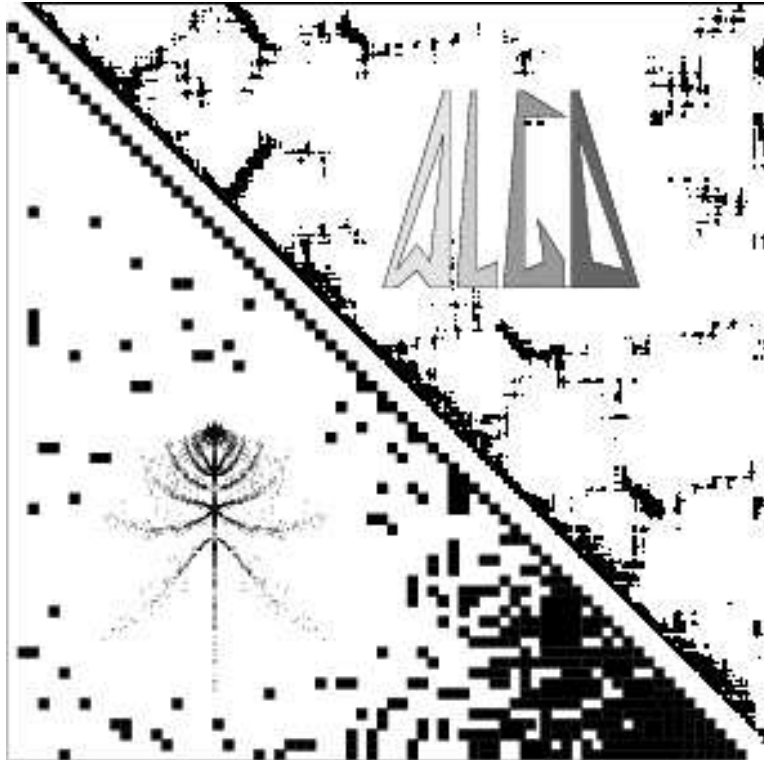


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ACTIVITY REPORT
of the
PARALLEL ALGORITHMS PROJECT
at
CERFACS

JANUARY 2002 - DECEMBER 2002

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Contents

1	Introduction (I. S. Duff)	5
2	List of Members of the Algo Team	9
3	Dense and Sparse Matrix Computations	10
3.1	Rank-revealing and Incremental Norm Estimation	10
3.2	Development of kernels for sparse numerical linear algebra	10
3.3	Development of the MUMPS package for solving sparse linear systems on distributed memory computers	11
3.4	Candidate-based dynamic scheduling for a distributed direct linear solver	12
3.5	Adapting a parallel sparse direct solver to SMP architectures	13
4	Iterative Methods and Preconditioning	14
4.1	A robust criterion for modified Gram-Schmidt with selective reorthogonalization	14
4.2	On the round-off error analysis of the iterated Classical Gram-Schmidt algorithm	14
4.3	A reorthogonalization procedure for the modified Gram-Schmidt algorithm based on a rank k update	15
4.4	A class of spectral two-level preconditioners	15
4.5	Exploiting spectral information in large electromagnetic calculations	16
4.6	Using symmetric Krylov solvers for solving electromagnetic problems using a fast multipole code	16
4.7	Domain decomposition methods in semiconductor device modelling	18
4.8	Some complementary investigations in inner-outer iterations	19
4.9	A set of GMRES routines for real and complex arithmetics on high performance computers	19
4.10	Experiments on Sparse Matrix Partitioning	20
4.11	Combining MPI and OpenMP: application to a Finite-Element program for acoustics	20
5	Qualitative Computing	22
5.1	Inner-Outer iterations	22
5.2	Inexact Computing and Homotopic Deviation	23
5.3	Arnoldi method and the happy breakdown	24
5.4	Virtual Reality	25
5.5	Geometric aspects of Computing	25
6	Nonlinear Systems and Optimization	27
6.1	Iterative techniques in variational data assimilation	27
6.2	Techniques for the Regularisation of Discrete Rank-Deficient Least Squares Problems	28
6.3	Out-of-core solvers for large dense linear least squares	28
7	Conferences and Seminars	30
7.1	Conferences and seminars attended by members of the Parallel Algorithms Project	30
7.2	Conferences and seminars organized by the Parallel Algorithms Project	33
7.3	Internal seminars organized within the Parallel Algorithms Project	34

8 Publications	35
8.1 Journal Publications	35
8.2 Theses	36
8.3 Technical Reports	36

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 in academic research, commerce, and industry. 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. In fact, it is very interesting to me how much the research directions of the Project are increasingly influenced by problems from the partners.

Members of the Team very much play their full part in the wider academic and research community. They are involved in Programme Committees for major conferences, are editors and referees for frontline journals, and are involved in research and evaluation committees. These activities both help CERFACS to contribute to the scientific life of France, Europe and the world while at the same time maintaining the visibility of CERFACS within these communities. Some measure of the visibility of CERFACS can be found from the statistics of accesses to the Algo Web pages at CERFACS where we are recording on average over 150 hits and over 100 downloads each day. Some of our most popular technical reports have been downloaded nearly 2000 times.

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 further developed the MUMPS package in conjunction with our colleagues at ENSEEIHT and elsewhere. The highlight of the year has been the release of Version 4.2 in December. This new version incorporates new ordering and scheduling strategies and includes a complex version. Some of the research work that was performed in support of this release is described in the following sections. The code continues to be downloaded on a daily basis by researchers throughout the world. The complex version has been accessed extensively and used in many applications, particularly in electromagnetics.

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. I am delighted to say that the new standard appeared this year as two special issues of the journal "High Performance Computing Applications". One of our main roles was the development of the Fortran 95 instantiation of the Sparse BLAS. This code is now accepted as an ACM TOMS algorithm and is available from the relevant pages of netlib.

Much attention has been paid in the last year to a deep analysis and understanding of the Gram-Schmidt orthogonalization process both at a theoretical and an implementational level. In particular, a new theoretical result has been obtained that proves that the computed orthogonal

factors are accurate in the sense that their norm is bounded by a quantity close to one. Julien Langou received an award for the best student paper for this work at the Copper Mountain meeting in April.

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 period, we have continued our work on developing such preconditioners, including two-level schemes that effectively and explicitly remove error components in a subspace spanned by eigenvectors corresponding to small eigenvalues of the already preconditioned system. The use of such a two-level spectral scheme has proved very powerful in the solution of very large problems in electromagnetics, including the industry standard COBRA test problem. The development of domain decomposition techniques in solving semiconductor device modelling problems was the subject of joint work with INRIA and was the topic of one of our PhD dissertations. Within this project, the direct solver MUMPS was used both as a solver for the local subproblems and on the Schur complement. The power of combining OpenMP and MPI has been used to great effect in the solution of realistic and large problems in underwater acoustics. Work has continued on analysing and experimenting with inner-outer iterations, in particular with consolidating the initial discoveries at CERFACS with more recent theoretical analysis by other groups. The GMRES and FGMRES codes that were discussed in a previous activity report have been further developed and continue to be available through the CERFACS web and have attracted over 1000 downloads, some from important establishments including partners of CERFACS. The technical papers describing these codes are the most popular ones for Web page access. Current investigations into matrix partitioning schemes for distributed matrix-vector multiplication will hopefully lead shortly to the embedding of the reverse-communication GMRES and FGMRES routines within a wrapper that accepts a sparse matrix as input and automatically exploits parallelism in the matrix and vector operations.

The main area of interest for the Qualitative Computing Group concerns a deep understanding of the influence of finite-precision computation on complex scientific numerical applications. The use of inner-outer iteration has continued in quite different applications. In Krylov methods where we have shown that reduced accuracy for the inner iteration can be accepted as the outer iteration converges; and in the power method where the accuracy needs to increase as the outer iteration proceeds. Solvers based on the former have been implemented in the ASTER code of EDF, while those based on the latter were incorporated into a neutronics code. Work has continued on the theory of homotopic perturbations now re-named homotopic deviations to emphasize that the “perturbation” may be very large (indeed may tend to infinity) although, of course, the rank of the perturbing matrix will be small. This theory has been used in a study of the acoustic wave equation and in an analysis of the Arnoldi method. A joint project with the TTN-group has resulted in the development of tools for studying large deviations. Algorithms and theory have been further developed for the use of hypercomplex numbers which can be a more natural way of representing actual physical processes.

A major focus of our work on nonlinear systems and optimization has been in joint work with the PALM Project and the Climate Modelling Group on data assimilation. We are particularly involved in a study of solution techniques for linear least-squares computations that lie at the heart of their algorithms. We are also involved in studies of rank-deficient least-squares computations from signal processing and in the solution of large scale dense least-squares problems from CNES using an out-of-core factorization of the normal equations matrix.

The Parallel Algorithms Project is heavily involved in the Advanced Training aspects of CERFACS' mission. We ran internal training courses for new recruits to all Projects 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 and feel that this is extremely useful to young scientists and engineers in both their training and their career choice. It can also help us to focus our research efforts and thus can benefit the work of the Team. A win-win situation. Stagiaires who successfully completed their training in the Team during the period included Mikael Doré (UJF, Grenoble), Romain Durdos (INSA, Rouen), Audrey Leal (INSA, Toulouse), and Stephane Pralet from ENSEEIHT who is now continuing with us to pursue a PhD degree. Members of the Team have assisted in many lecture courses at other centres, including ENSICA, INPT, Météo, Toulouse 1 and INSA. Two PhD theses were completed during the year with both defences being held on the same day in April. These were Bruno Carpentieri with a thesis on “Sparse preconditioners for dense complex linear systems in electromagnetic applications” and Jean Christophe Rioual whose topic was “Solving linear systems for semiconductor device simulations on parallel distributed computers”.

Our list of visitors is a veritable who’s who of numerical analysts, including many distinguished scientists from Europe and the United States. We have included a list of the visitors at the end of this introduction. In addition to inviting some of our visitors to give seminars, some of which are of general interest to other teams, we also run a 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.

The Parallel Algorithm Team hosted the now annual “Sparse Day” in June when we were able to take advantage of our visitors to design a very attractive programme that attracted nearly 50 participants from not only outside Toulouse but also outside France. Some researchers from the partners of CERFACS also participated. The speakers for this meeting are listed in Section 6.2 of this report.

I am very pleased to report that, over the reporting period, we have continued our involvement in joint research projects with shareholders and with other teams at CERFACS. We are involved in research committees such as the CCT of CNES. We have two projects with EADS on preconditioning techniques in electromagnetics and a sponsored PhD on the study of iterative solution techniques for multiple right-hand sides. We are involved in the training programme for the Mastere, organized by ENM. Our main collaboration with INRIA reached a major milestone with the successful defence of a PhD on domain decomposition techniques in semiconductor device modelling. We have completed a contract with EDF to utilize our finding on inner-outer iteration within their Aster code. We help the other Projects at CERFACS at all levels from the “over-a-coffee” consultancy to more major collaborations. These include advice on the ParELSA code of CFD and many aspects of algorithms and error analysis with TSI. We now have a strong and growing collaboration with the Climate Modelling Team on aspects of data assimilation and will be co-hosting a visit of a researcher from Belgium with the PALM Project of that Group. We are involved in close collaborations over linear solvers in electromagnetic codes with the EMC team.

As a postscript, one major highlight of the year was the recruitment of not one but two senior scientists so that, for the first time in some years, we have our full complement of seniors. My thanks to Luc Giraud, Serge Gratton, and Martin van Gijzen for doing all the hard work to ensure the smooth running of the Team.

Visitors to Parallel Algorithm Project in 2002

In alphabetical order, our visitors in the year 2002 included: YANNIS ALIFERIS (Université de Nice-Sophia Antipolis, France), MARIO ARIOLI (RAL, UK), MICHELE BENZI (Emory University, USA), OLIVIER BESSON (Université de Neuchâtel, Switzerland), PETTER BJØRSTAD (University of Bergen) ERIK BOMAN (Sandia National Labs, USA), BRUNO CARPENTIERI (Università di Bari,

Italy), DORON CHEN (Tel-Aviv University, Israel), FILOMENA D'ALMEIDA (Universidade do Porto, Portugal), TIM DAVIS (University of Florida, USA), FRÉDÉRIC DESPREZ (INRIA/LIP-ENS, France), CRISTIAN GATU (Université de Neuchâtel, Switzerland), JOHN GILBERT (Xerox Parc, USA), GENE GOLUB (Stanford University, USA), IVAN GRAHAM (University of Bath, UK), NICKY GRAVES GREGORY (University of Brighton, UK), LAURA GRIGORI (Lawrence Berkeley National Laboratory, USA), ABDOU GUERMOUCHE (LIP-ENS, France), PHILIPPE GUILLAUME (INSA, France), HUSSEIN HOTEIT (INRIA/IRISA, France), ALAIN HUARD (INSA, France), ERRICOS KONTOGHIORGHES (Université de Neuchâtel, Switzerland), JEAN-YVES L'EXCELLENT (INRIA/LIP-ENS, France), SÉBASTIEN LACROIX (IFP, France), ALEXANDRE LE BLANC (University of Artois, France), JOHN LEWIS (The Boeing Company, USA), OSNI MARQUES (Lawrence Berkeley National Laboratory, USA), JOSÉ MAS MARI (Universitat Politècnica de Valencia ETSE Agrunoms, Spain), AMERICO MARROCCO (INRIA-Rocquencourt, France), GÉRARD MEURANT (CEA, France), NANCY NICHOLS (University of Reading, UK), ESMOND NG (Lawrence Berkeley National Laboratory, USA), SUELY OLIVEIRA (The University of Iowa, USA), FRANÇOIS PELLEGRINI (LaBRI, France), BERNARD PHILIPPE (INRIA/IRISA, France), SERGE PIPERNO (CERMICS/INRIA, France), ROLDAN POZO (NIST, USA), PIERRE RAMET (LaBRI, France), JEAN ROMAN (LaBRI, France), MARIELBA ROJAS (Wake Forest University, USA), YOUSEF SAAD (University of Minnesota, USA), ROBERT SCHEICHL (University of Bath, UK), STEFAN SCHNEIDER (Technische Universitaet Dresden, Germany), JENNIFER SCOTT (RAL, UK), MASHA SOSONKINA (University of Minnesota Duluth, USA), WEI-PAI TANG (The Boeing Company, Seattle, USA), PHILIPPE TOINT (University of Namur) SIVAN TOLEDO (Tel-Aviv University, Israel), JEAN TSHIMANGA (University of Namur, Belgium), HENRY TUFO (University of Colorado at Boulder, USA), and MARINA VIDRASCU (INRIA-Rocquencourt, France).

Visitors from our partners have included: GUILLAUME ALLÉON (EADS-CCR, France), PATRICK AMESTOY (ENSEEIH-IRIT, France), DANIEL RUIZ (ENSEEIH, France), and GUILLAUME SYLVAND (EADS-CCR and CERMICS/INRIA, France).

Iain S. Duff.

2 List of Members of the Algo Team

IAIN DUFF - Project Leader
FRANÇOISE CHAITIN-CHATÉLIN - Qualitative Computing Group Scientific Advisor
MIKAEL DORÉ - Trainee
ROMAIN DURDOS - Trainee
LUC GIRAUD - Senior Researcher
SERGE GRATTON - Senior Researcher
JULIEN LANGOU - Ph.D. Student
DANIEL LOGHIN - Post. Doc.
EMERIC MARTIN - Ph.D. Student
TADAS MEŠKAUSKAS - Post. Doc., currently Vilnius University, Lithuania
STPHANE PRALET - Ph.D. Student
JEAN CHRISTOPHE RIOUAL - Ph.D. Student, currently NEC, UK
SONGKLOD RIYAVONG - Ph.D. Student
ELISABETH TRAVIESAS - Post. Doc., currently Transiciel, France
MARTIN VAN GIJZEN - Senior Researcher
CHRISTOF VÖMEL - Ph.D. Student
BRIGITTE YZEL - Administration

with the collaboration of

PATRICK AMESTOY (ENSEEIH-IRIT, France)
ERIC ANTERRIEU (CERFACS, Signal and Image Processing Team, France)
CAROLINE BOUSQUET (UPS, France)
BRUNO CARPENTIERI - (Università di Bari, Italy, currently CERFACS, France)
CHRISTOPHE DANIEL (UPS, France)
VALERIE FRAYSSÉ (KVASAR LLC, USA)
AUDREY LEAL (INSA, France)
AMERICO MARROCCO (INRIA-Rocquencourt, France)
GREGOIRE RICHARD (ENSEEIH-IRIT, France)
MIRO ROZLOŽNÍK (Academy of Sciences of the Czech Republic, Czech Republic)
ANTHONY T. WEAVER (Global Change Team, CERFACS, France)
AHMED N. ZAOUI

and with the contribution of ex-members who published papers this year on the work they developed during their time at CERFACS

DOMINIQUE ORBAN (Northwestern University, USA)
JUSSI RAHOLA (NOKIA, Finland)
MARIELBA ROJAS (Wake Forest University, USA)
SATU TISSARI (Finnish Center for Scientific Computing, Finland)

3 Dense and Sparse Matrix Computations

3.1 Rank-revealing and Incremental Norm Estimation

I. S. Duff: CERFACS, *France* and RUTHERFORD APPLETON LABORATORY, *England*;
C. Vömel: CERFACS, *France*

We have developed an incremental approach to 2-norm estimation for triangular matrices which is important for the detection of ill-conditioning, one of the basic problems arising in the numerical solution of linear systems. Applications of our scheme include the calculation of forward error bounds based on the condition number, robust pivot selection criteria and rank-revealing factorizations, in particular, when *inverse* factors arise in the factorization. In [2], we introduced such a scheme applicable for both dense and sparse matrices which can arise for example from a QR, a Cholesky or a LU factorization. If the explicit inverse of a triangular factor is available, as in the case of an implicit version of the LU factorization, we can relate our results to incremental condition estimation (ICE) presented in [1]. Incremental norm estimation (INE) extends directly from the dense to the sparse case without needing the modifications that are necessary for the sparse version of ICE. INE can be applied to complement ICE, since the product of the two estimates gives an estimate for the matrix condition number. Furthermore, when applied to matrix inverses, INE can be used as the basis of a rank-revealing factorization. The quality of our results on standard test cases is constantly high and demonstrates the general reliability of our scheme [3].

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- [1] C. H. Bischof. Incremental condition estimation. *SIAM J. Matrix Analysis and Applications*, 11:312–322, 1990.
 - [2] I. S. Duff and C. Vömel. Incremental Norm Estimation for Dense and Sparse Matrices. Technical Report TR/PA/00/83, CERFACS, Toulouse, France, 2000. Preliminary version of the article published in BIT, Numerical Mathematics, Volume 42, Issue 2 (June 2002), pp. 300–322. [Compressed PS](#).
 - [3] I. S. Duff and C. Vömel. Incremental Norm Estimation for Dense and Sparse Matrices. *BIT*, 42(2):300–322, 2002.

3.2 Development of kernels for sparse numerical linear algebra

I. S. Duff: CERFACS, *France* and RUTHERFORD APPLETON LABORATORY, *England*;
C. Vömel: CERFACS, *France*

It is with great pleasure that we can report on the release during this current year of the new Basic Linear Algebra Subprogram (BLAS) Standard developed and defined by the BLAS Technical Forum [2]. This involved many extensions to the earlier standards, including new functionalities, mixed precision BLAS, and sparse BLAS. A technical description of these can be found in the ACM TOMS paper [1]. Our main contribution to this effort was in the design, implementation, and testing of the sparse BLAS.

The design of the sparse BLAS is discussed in the paper [3]. This consists of a set of kernels providing basic operations for sparse matrices and vectors, including the multiplication of a dense vector or a set of dense vectors by a sparse matrix. A principal goal of the Sparse BLAS standard is to aid in

the development of iterative solvers for large sparse linear systems by specifying interfaces for a high-level description of vector and matrix operations for the algorithm developer while leaving enough freedom for vendors to provide the most efficient implementation of the underlying algorithms for their specific architectures.

The Sparse BLAS standard defines interfaces and bindings for the three target languages: C, Fortran 77 and Fortran 95. Our Fortran 95 implementation is intended as a reference model for the Sparse BLAS. The design is based on the idea of matrix handles so that the user need not be concerned with the details of the underlying storage schemes. It is envisaged that these kernels will be widely used in the solution of sparse equations by iterative methods. The software implementation has been published as TOMS algorithm [4].

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- [1] L. S. Blackford, J. Demmel, J. Dongarra, I. S. Duff, S. Hammarling, G. Henry, M. Heroux, L. Kaufman, A. Lumsdaine, A. Petit, R. Pozo, K. Remington, and R. C. Whaley. An updated set of Basic Linear Algebra Subprograms (BLAS). *ACM Transactions on Mathematical Software (TOMS)*, 28(2):135–151, June 2002.
 - [2] BLAS Technical Forum. Special Issue: On Basic Linear Algebra Subprograms Technical BLAST Forum Standard -I and II. *The International Journal of High Performance Computing Applications*, 16(1–2), 2002.
 - [3] I. S. Duff, M. A. Heroux, and R. Pozo. An overview of the Sparse Basic Linear Algebra Subprograms: the new standard from the BLAS Technical Forum. *ACM Trans. Math. Softw.*, 28(2):239–267, 2002.
 - [4] I. S. Duff and C. Vömel. Algorithm 818: A Reference Model Implementation of the Sparse BLAS in Fortran 95. *ACM Trans. Math. Softw.*, 28(2):268–283, 2002.

3.3 Development of the MUMPS package for solving sparse linear systems on distributed memory computers

P. R. Amestoy: ENSEEIHT-IRIT, *France*, **C. Bousquet:** UPS, *France*, **C. Daniel:** UPS, *France*, **I. S. Duff:** CERFACS, *France* and RUTHERFORD APPLETON LABORATORY, *England*;
G. Richard: ENSEEIHT-IRIT, *France*

We were fortunate to have three stagiaires working on the MUMPS Project principally supervised by Patrick Amestoy of ENSEEIHT-IRIT. They were working from the base of Version 4.1 of the MUMPS package [1] and they performed some preliminary work that has proved of assistance for the development of Version 4.2 of MUMPS that was released at the end of 2002.

The work performed at ENSEEIHT-IRIT by Gregoire Richard [3] concerned coupling and testing other ordering packages within MUMPS. This was important since we had already observed that different orderings can have a significant effect on the performance of the code in terms of work, memory and parallelism. Version 4.1 had only one integrated ordering (AMD) and an interface to other orderings through acceptance of a input permutation. In Version 4.2, several orderings are more tightly coupled to the package.

The work of Caroline Bousquet and Christophe Daniel [2] concerned the development of a much requested complex version (that now exists in Version 4.2) and the design and development of a rigorous test deck for the code, an essential tool for the verification and development of any package, particularly one so large and complicated as the MUMPS package.

This work together with that described in Sections 3.4 and 3.5 has been very important for the future development of the MUMPS package and, in particular, for the Version 4.2 release.

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- [1] P. R. Amestoy, I. S. Duff, J.-Y. L'Excellent, and J. Koster. A fully asynchronous multifrontal solver using distributed dynamic scheduling. *SIAM J. Matrix Analysis and Applications*, 23(1):15–41, 2001.
 - [2] C. Bousquet and C. Daniel. Complex version and validation of MUMPS, Multifrontal Massively Parallel Solver. Working Notes WN/PA/02/34, CERFACS, Toulouse, France, 2002. Memoire de Maîtrise Ingénierie Mathématique, UPS III. [Compressed PS](#), [PDF](#).
 - [3] G. Richard. Coupling MUMPS and ordering software. Working Notes WN/PA/02/24, CERFACS, Toulouse, France, 2002. [Compressed PS](#), [PDF](#).

3.4 Candidate-based dynamic scheduling for a distributed direct linear solver

P. R. Amestoy: ENSEEIHT-IRIT, *France*; **I. S. Duff**: CERFACS, *France* and RUTHERFORD APPLETON LABORATORY, *England*; **C. Vömel**: CERFACS, *France*

The asynchronous distributed memory multifrontal solver MUMPS [1, 2] can be described by a computational graph in the form of a tree (the so-called *assembly tree*) where the computation at a node of the tree is equivalent to several steps of Gaussian elimination on a dense submatrix (the *frontal matrix*) and the remaining Schur complement from this partial factorization (the so-called *contribution block*) is sent to the parent of the node of the tree and is summed (or *assembled*) with contribution blocks from other children and data from the original matrix to form another frontal matrix at the parent. MUMPS exploits both the parallelism inherent in the tree (by processing independent branches in parallel) as well as parallelism within tree nodes with a large enough contribution block. A master process is assigned to the node to factorize the pivot block and this in turn distributes the work of generating the contribution block to a set of slave processes that are assigned dynamically during the numerical factorization.

While the *master* processor of each node in the tree (i.e. the one that is responsible for the factorization of the block of fully summed variables) is chosen during the analysis phase, the *slaves* for the parallel update of large contribution blocks are only chosen during the factorization phase. This dynamic task scheduling takes place in order to balance the work load of the processors at run time. Problems can arise if too much freedom is offered to the dynamic scheduling. If every processor is a candidate for a slave then, on each processor, enough workspace has to be reserved during the analysis phase for the corresponding computational tasks. However, during the factorization, typically not all processors are actually needed as slaves (and, on a large number of processors, only a very few are needed), so the prediction of the required workspace will be overestimated. Thus the size of the problems that can be solved is reduced unnecessarily because of this difference between the prediction and allocation of memory in the analysis phase and the memory actually used during the factorization.

With the concept of *candidate processors* it is possible to address this issue. The concept originates in an algorithm presented in [4] and extends efficiently to MUMPS. For each node that requires slaves to be chosen dynamically during the factorization because of the size of its contribution block, we introduce a limited set of processors from which the slaves can be selected. While the master previously chose slaves from among all less loaded processors, the freedom of the dynamic scheduling can be reduced so that the slaves are only chosen from the candidates. This effectively allows us to exclude all non-candidates from the estimation of workspace during the analysis phase and leads to a more realistic prediction of workspace needed. Furthermore, the candidate concept allows us to better structure the computation since we can explicitly restrict the choice of the slaves to a certain group of processors and enforce a ‘subtree-to-subcube’ mapping principle.

Our new approach significantly improves the scalability of the solver in terms of execution time and storage. By comparison with the previous version of MUMPS, we demonstrate the efficiency and the scalability of the new algorithm on up to 512 processors. Our test cases include matrices from regular 3D grids and irregular ones from real-life applications [3].

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- [1] P. R. Amestoy, I. S. Duff, J.-Y. L'Excellent, and J. Koster. A fully asynchronous multifrontal solver using distributed dynamic scheduling. *SIAM J. Matrix Analysis and Applications*, 23(1):15–41, 2001.
 - [2] P. R. Amestoy, I. S. Duff, J.-Y. L'Excellent, and X. S. Li. Analysis, tuning and comparison of two general sparse solvers for distributed memory computers. Technical Report TR/PA/00/72, CERFACS, Toulouse, France, 2000. Preliminary version of the article published in *ACM Trans. Math. Softw.*, vol. 27, pp 388-421. [Compressed PS](#).
 - [3] P. R. Amestoy, I. S. Duff, and C. Vömel. Task scheduling in an asynchronous distributed memory multifrontal solver. Technical Report TR/PA/02/105, CERFACS, Toulouse, France, 2002. [Compressed PS](#), [PDF](#).
 - [4] A. Pothén and C. Sun. A Mapping Algorithm for Parallel Sparse Cholesky Factorization. *SIAM J. Scientific Computing*, 14(5):1253–1257, 1993.

3.5 Adapting a parallel sparse direct solver to SMP architectures

P. R. Amestoy: ENSEEIHT-IRIT, *France*; **I. S. Duff:** CERFACS, *France* and RUTHERFORD APPLETON LABORATORY, *England*; **S. Pralet:** CERFACS, *France*; **C. Vömel:** CERFACS, *France*

In the context of the direct solution of general sparse linear systems, we consider the problem of task scheduling on SMP architectures with non-uniform cost of communication. Our main target type of computer architecture can be defined as a so called two-level architecture. Each level is composed of a set of identical processors sharing a common memory (that is, is an SMP node). The work in [2] about MUMPS implicitly assumed that our target computer was a distributed memory computer with uniform memory access and uniform cost of communication. We show the limitations of this approach on machines with a two-level architecture and indicate how we can remedy these limitations in [1]. Our modifications of the algorithms affect both the symbolic factorization and the numerical factorization phase. Our experiments on the IBM SP from CINES (Montpellier) with 16 processors per SMP node and up to 128 processors show that we can significantly reduce both the amount of inter-node communication and the factorization time. The algorithms have been integrated into Version 4.2 of MUMPS.

We note that these algorithms, although only experimented on such target computers, will naturally adapt to a more general framework of computers with heterogeneous processors and multilevel architectures. Most of the additional effort that has still to be done is in the development of middleware tools that will permit a good estimation (with probable dynamic readjustments) of the parameter characterizing the multilevel architectures. This will clearly require further significant work that will benefit from the algorithms and results presented in [1].

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- [1] P. R. Amestoy, I. S. Duff, S. Pralet, and C. Vömel. Adapting a parallel sparse direct solver to SMP architectures. Technical Report TR/PA/03/5, CERFACS, Toulouse, France, 2003. Submitted to *Parallel Computing Journal*, Special issue on Parallel and Distributed Scientific and Engineering Computing. [Compressed PS](#).
 - [2] P. R. Amestoy, I. S. Duff, and C. Vömel. Task scheduling in an asynchronous distributed memory multifrontal solver. Technical Report TR/PA/02/105, CERFACS, Toulouse, France, 2002. Submitted to *SIAM Journal of Matrix Analysis and Applications*. [Compressed PS](#), [PDF](#).

4 Iterative Methods and Preconditioning

4.1 A robust criterion for modified Gram-Schmidt with selective reorthogonalization

L. Giraud: CERFACS, *France*; **J. Langou:** CERFACS, *and* EADS-CCR, *France*

In this work we investigate a new criterion for selective reorthogonalization in the modified Gram-Schmidt algorithm that is referred to as the L -criterion.. This criterion depends on a single parameter L . When L is chosen smaller than 1 (e.g. $L = 0.99$), for numerically nonsingular matrices, this criterion is able to realize the compromise between saving useless reorthogonalization and giving a set of computed vectors that are orthogonal up to machine precision level. We study its behaviour in the presence of rounding errors. We give some counter-examples which prove that the standard criteria might fail. Through numerical experiments, we illustrate that our new criterion seems also suitable for the classical Gram-Schmidt algorithm. More details on this work can be found in [1, 2].

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4.2 On the round-off error analysis of the iterated Classical Gram-Schmidt algorithm

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M. Rozložník: INSTITUTE OF COMPUTER SCIENCE, ACADEMY OF SCIENCES OF THE CZECH REPUBLIC, *Czech Republic*

In this work we analyse the numerical behaviour of the classical Gram-Schmidt algorithm with one iterative refinement/reorthogonalization step. Assuming numerical nonsingularity of the matrix we prove that two steps of the Classical Gram-Schmidt process are enough for preserving the orthogonality of the computed vectors close to machine-precision level. We give a rounding error analysis and relate our results to the approach used in the Kahan-Parlett [4] “twice is enough” algorithm as well as to results given by Abdelmalek, Daniel et al [1], Hoffmann [3] and others. More details on this work can be found in [2]

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4.3 A reorthogonalization procedure for the modified Gram–Schmidt algorithm based on a rank k update

L. Giraud: CERFACS, *France*; **S. Gratton:** CERFACS, *France*; **J. Langou:** CERFACS, and EADS-CCR, *France*

The modified Gram–Schmidt algorithm is a well-known and widely used procedure to orthogonalize the column vectors of a matrix. When applied to ill-conditioned matrices in floating-point arithmetic, the orthogonality among the computed vectors may be lost. In this work, we propose an *a posteriori* reorthogonalization technique based on a rank k update of the computed vectors. The set of vectors built is orthogonal up to machine precision assuming a large enough k is chosen. Moreover, we show that the rank of the update can be tuned to monitor the orthogonality quality. We illustrate the efficiency of this approach in the framework of the GMRES-Seed technique for the solution of an unsymmetric linear system with multiple right-hand sides. In particular, we report experiments on numerical simulations in electromagnetic applications where such problems arise.

A complete description of this work is available in [1, 2]

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 - [2] J. Langou. *Résolution d'un système linéaire à plusieurs second membres par des methodes itératives. Application à la méthode multipôle rapide en électromagnétisme*. PhD thesis, Institut National des Sciences Appliquées de Toulouse, 2003. Defense scheduled for the end of March 2003.

4.4 A class of spectral two-level preconditioners

B. Carpentieri: CERFACS, *France*; **I. S. Duff:** CERFACS, *France* and RUTHERFORD APPLETON LABORATORY, *England*; **L. Giraud:** CERFACS, *France*

It is well known that the convergence of Krylov methods for solving linear systems often depends to a large extent on the eigenvalue distribution. In many cases, it is observed that “removing” the smallest eigenvalues can greatly improve the convergence. Several techniques have been proposed in the past few years that attempt to tackle this problem. The proposed approaches can be split into two main families depending on whether the scheme enlarges the generated Krylov space or adaptively updates the preconditioner. In this work, we follow the second approach and propose a class of preconditioners both for unsymmetric and for symmetric linear systems that can also be adapted for symmetric positive definite problems. We effectively solve the preconditioned system exactly in the low dimensional space associated with the smallest eigenvalues and use this to update the preconditioned residual. This update results in shifting eigenvalues from close to the origin to near to one for the new preconditioner. This is ideal when there are only a few eigenvalues near the origin while all the others are close to one because the updated preconditioned system becomes close to the identity. We illustrate the performance of our method through extensive numerical experiments on a set of general linear systems.

More details are available in [2] as well as examples on two different applications in [1, 3]. Finally, we refer to Section 4.5 for the use of this technique for large electromagnetic simulations.

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4.5 Exploiting spectral information in large electromagnetic calculations

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L. Giraud: CERFACS, *France*; **J. Langou:** CERFACS, *and* EADS-CCR, *France*;
E. Martin: CERFACS, *France*

In the last couple of years we have been working on preconditioning techniques suitable for preconditioning large dense complex linear systems arising from the discretization of the Maxwell's equations via boundary-element techniques [1, 3]. In this work we have introduced a class of two-level preconditioners [2] that implement low-rank updates aimed at removing the possible bad effect of the smallest eigenvalues.

In this study we investigate several techniques that attempt to take advantages of spectral information of the preconditioner based on the Frobenius norm-minimization implemented in a parallel Fast Multipole code [5]. In particular we show that our recent spectral two-level preconditioner is still effective for the solution of large industrial electromagnetics problems.

More details on this work are available in [4].

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4.6 Using symmetric Krylov solvers for solving electromagnetic problems using a fast multipole code

R. Durdos: CERFACS, *France*; **L. Giraud:** CERFACS, *France*; **J. Langou:** CERFACS, *and* EADS-CCR, *France*

In this work we investigate the use of symmetric QMR [4] for the solution of symmetric dense linear systems arising from electromagnetic applications. Symmetric QMR (SQMR) is a hybrid version of QMR that benefits from the symmetry of the matrix so dividing by two the cost compared to QMR. The advantage over solvers like GMRES is that SQMR uses a short term recurrence and therefore requires only a few vectors to be stored while the number of dot products is also considerably reduced. The main drawback is an observed delay in the convergence due in general to a loss of orthogonality among the computed vectors. In our experiments, the matrix-vector products are performed using a fast multipole code [6] with three different formulations. Even though, in exact arithmetic, the dense matrix is symmetric, the use of floating-point arithmetic combined with the approximations made in the three implementations of the fast multipole method deteriorate this property. We therefore end up by using a non-symmetric matrix-vector product in a symmetric solver. In Figure 4.1, we plot the backward error as a function of the iterations for three formulations of the multipole expansion (denoted by fmm1, fmm2 and fmm3) and two different arithmetics (i.e. single or double

precision). These experiments indicate that SQMR converges well down to a level that is related to the symmetry of the computed matrix (only accessible through mat-vec product); this latter also greatly influences the rate of convergence. The better the symmetry is, the better the convergence. In Figure 4.1, we also plot the convergence of GMRES as a reference. When the matrix is nearly symmetric, the behaviour of SQMR is close to that of GMRES. SQMR, which is very appropriate for those problems when the matrix is fully assembled [1], may also be applied with the multipole method but requires careful implementation to maintain the symmetry of the multipole expansion. Finally, preliminary experiments on small problems have been conducted to embed SQMR in flexible FQMR [7] iterations. The behaviour of the resulting inner-outer procedure is rather disappointing and does not exhibit the nice convergence observed with its counterpart based on GMRES [2]. More details on this work can be found in [3, 5].

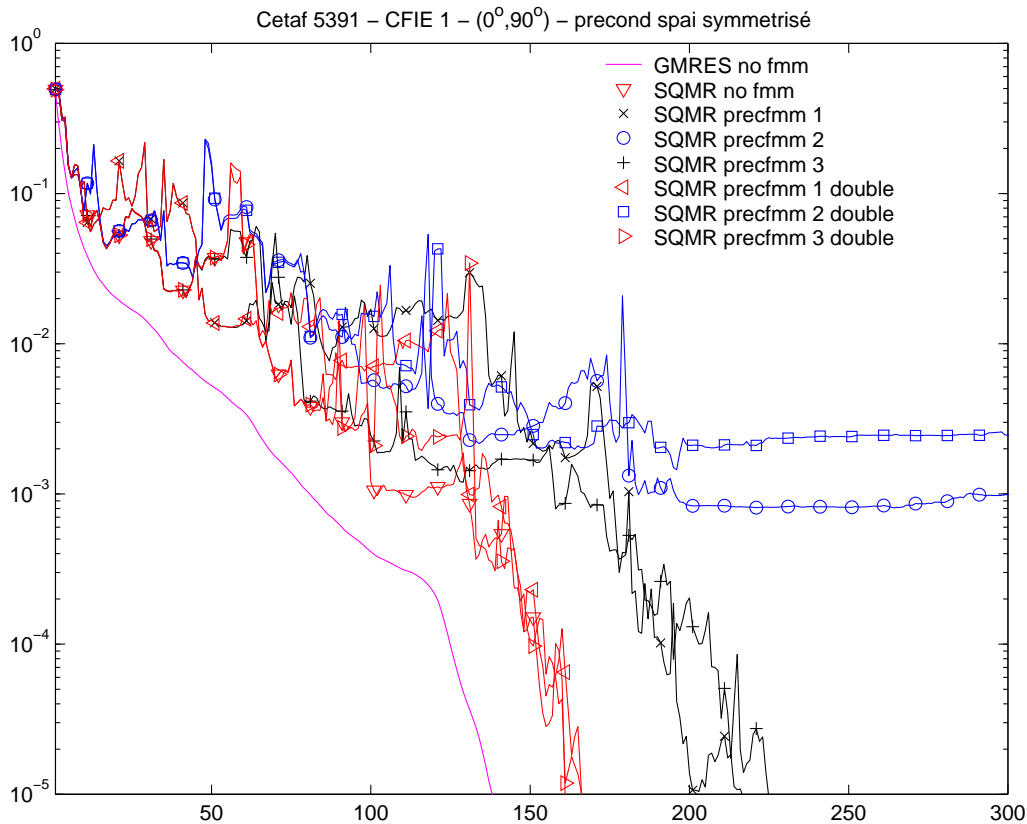


Figure 4.1: Convergence behaviour of GMRES and SQMR with various fast multipole calculations.

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4.7 Domain decomposition methods in semiconductor device modelling

L. Giraud: CERFACS, France; **J.-C. Rioual:** CERFACS, France; **A. Marrocco:** INRIA, France

The numerical simulation of semiconductor devices is extremely demanding in term of computational time because it involves complex embedded numerical schemes. At the kernel of these schemes is the solution of very ill-conditioned large linear systems. In this work, we investigate the effects of the various ingredients of our hybrid iterative schemes that play a central role in the robustness of those solvers when they are embedded in other numerical schemes. On a set of bidimensional unstructured mixed finite-element problems representative of large semiconductor simulations, we perform a fair and detailed comparison between parallel iterative and parallel direct linear solvers. We show that iterative solvers can be robust enough to solve the very challenging linear systems that appear in those simulations. This study greatly benefits from and makes intensive use of MUMPS [1, 2] (see Section 3.5).

A complete description of this work is available in [3, 4]

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4.8 Some complementary investigations in inner-outer iterations

V. Frayssé: KVASAR LLC, USA; L. Giraud: CERFACS, France; S. Gratton: CERFACS, France

Embedded iterative linear solvers are more and more often used in Linear Algebra. An important issue is how to tune the level of accuracy of the inner solver to guarantee the convergence of the outer solver at the best global cost. As a first step towards the challenging goal of controlling embedded linear solvers, inexact Krylov methods are used as a model of inner-outer iterations with an external Krylov scheme. This work aims at completing the pioneering work described in the reports [1, 2] in order to address the symmetric and positive definite situation with Conjugate Gradients as well as further investigate other Krylov methods than GMRES. Various new relaxation strategies have also been considered that are based on polynomials of the residual norm, while only experiments with the residual norm were reported in the earlier work. Finally the bibliography of the previous paper has been updated to include recent theoretical studies [3, 4] that attempt to explain the observed phenomenon. We notice that these studies were motivated by the earlier version of our work.

The experiments have been integrated into the revised version of [1] submitted to the *SIAM Journal of Matrix Analysis and Applications*.

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4.9 A set of GMRES routines for real and complex arithmetics on high performance computers

V. Frayssé: KVASAR LLC, USA; L. Giraud: CERFACS, France; S. Gratton: CERFACS, France;
J. Langou: CERFACS, and EADS-CCR, France

Because the CERFACS public domain GMRES package has become fairly widely used (more than 700 downloads since December 1997 from all over the world) we decide to make a major release in order to take into account the recent update of the BLAS standard [1] and to introduce a few new features. One of these enables the user to avoid an extra matrix-vector product at each restart. This is of interest when the matrix-vector product is expensive such as in our applications in electromagnetism using a Fast Multipole expansion (see Section 4.5) and in non-overlapping domain decomposition (see Section 4.7).

The associated User's guide [3] has been updated and supersedes [2]. In this report, we describe the implementations of the GMRES algorithm for both real and complex, and single and double precision arithmetics that are suitable for serial, shared memory and distributed memory computers. For the sake of portability, simplicity, flexibility and efficiency the GMRES solvers have been implemented in Fortran 77 using the reverse communication mechanism for the matrix-vector product, the preconditioning and the dot product computations. For distributed memory computation, several orthogonalization procedures have been implemented to reduce the cost of the dot product calculation, that is a well-known efficiency bottleneck for the Krylov methods. Finally, various stopping criteria based on normwise backward error are available.

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4.10 Experiments on Sparse Matrix Partitioning

S. Riyavong: CERFACS, France

We have undertaken experiments to determine the comparative quality of four graph partitioners: PaToH [1, 2], hMeTiS [5], Mondriaan [6], and Monet [4] with application to sparse matrix partitioning. A large selection of application-driven matrices from the Rutherford-Boeing Collection [3] are partitioned and then permuted so that the resulting form exhibits block structures. This form is useful for implementing sparse matrix-vector multiplication in a parallel computing environment where each block will be assigned to a single computing node. The details will be given in a working note.

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4.11 Combining MPI and OpenMP: application to a Finite-Element program for acoustics

L. Giraud: CERFACS, France; **M. van Gijzen:** CERFACS, France

Finite-Element programs are usually parallelized either at a low level by exploiting fine-grain loop parallelism or at a much higher level by exploiting the coarse grain parallelism of a mesh splitting in a domain decomposition type approach. On clusters of Symmetric Multi-Processors (SMP's) these two approaches can be combined by, on the one hand mapping separate subdomains onto separate nodes, and on the other hand exploiting the loop parallelism within a node.

Following the work described in [1], we have made a combined fine grain/coarse grain parallel implementation of the vectorized, Finite-Element program SIMPLE for ocean-acoustic simulations. We have used OpenMP to parallelize the vectorized loops and MPI to implement communication between nodes.

When solving the linear system, the coarse grain parallelism based on domain decomposition techniques degrades the numerical properties of the preconditioner when the number of subdomains is increased because of the lack of a global mechanism in the preconditioner. As a result, iterative methods like the Conjugate Gradient method take more iterations as the number of subdomains increases. The combination of OpenMP and MPI is of particular interest for reducing the adverse effect of the domain decomposition on the preconditioner. By using OpenMP within each subdomain handled by the nodes, and MPI between the nodes, the number of subdomains can be reduced from the number of processors to the number of nodes. Consequently, the undesired numerical deterioration is alleviated while keeping the number of processors involved in the calculation unchanged. This highlights a situation where mixing Open-MP and MPI enables us to find a satisfactory trade-off between the efficiency of the numerical scheme and the efficiency of the parallel implementation. More details can be found in [2].

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5 Qualitative Computing

Group members: Françoise Chaitin-Chatelin, Mikael Doré, Audrey Leal, Tadas Meškauskas, Elisabeth Traviesas, Martin van Gijzen, and Ahmed N. Zaoui.

The work of the Qualitative Computing Group is a collaborative effort to assess the validity of computer simulations. The central question is to give meaning to computer results which are seemingly wrong such as in chaotic computations. This goal can be reached by uncovering the laws of computation which govern finite-precision computations in the neighbourhood of singularities. Some of these laws are now well understood. For example, one can cite i) the role of the normwise backward error to assess the reliability of numerical software in finite precision, ii) the role of nonnormality which makes approximated singularities appear much closer than they are in exact arithmetic.

A number of new laws have emerged more recently, which have been the focus of the Group's attention in recent years. The new laws concern in particular:

- a) *inexact computing* and the associated homotopic pseudospectrum and backward error as a fruitful framework to understand approximate numerical methods, in exact arithmetic,
- b) the unreasonable robustness of Krylov-type methods to perturbations in the data,
- c) the (underestimated) role of Geometry in Scientific Computing.

Our research and understanding is vitally nourished by work on practical numerical software applications in Physics and Technology, which come from CERFACS partners. We review below the work accomplished in 2002 in five related areas.

5.1 Inner-Outer iterations

T. Meškauskas: CERFACS, *France*; **F. Chaitin-Chatelin:** CERFACS, *France*; **M. van Gijzen:** CERFACS, *France*

It is well known that *asymptotic* methods, such as Newton-like methods for systems and the power method for eigenvalues, need to be performed with more and more accuracy as one gets closer to the solution.

On the contrary, *direct* methods such as Krylov-type methods exhibit a remarkable robustness to perturbations in the data. The only requirement is that, when the incomplete Krylov method is used *iteratively*, as in the *restarted* versions, the first steps in each new iteration loop are computed to full working accuracy, which can be later relaxed as the convergence proceeds inside the loop [1]. In the first phase of a project, supported by the CERFACS industrial partner EDF, such a relaxation strategy has successfully been implemented in the eigenmode solver code ASTER [2].

The second phase of the project aimed at reducing the number of inner iterations of a code for neutronics. This code implements the Shift-and-Invert Power method with Chebychev acceleration. The Power method is a Newton rather than a Krylov method. For this reason a relaxation technique as described above did not work. This fact was numerically verified. However, a great reduction in the number of inner iterations was obtained by applying the classical refinement technique for Newton methods, that is, the inner systems are solved increasingly accurately as the outer loop converges [3].

After the successful completion of the project with EDF, an overview was given to the CERFACS industrial partners [4] about recent progress on this subject.

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5.2 Inexact Computing and Homotopic Deviation

F. Chaitin-Chatelin: CERFACS, *France*; **A. Leal:** INSA, *France*; **E. Traviesas:** CERFACS, *France*; **M. van Gijzen:** CERFACS, *France*

In many areas of classical mathematics, singularities can be forgotten because they are locally non-generic and disappear under small perturbation. But the viewpoint of the classical theory of singularities may not be appropriate in Inexact Computing, which models situations when the accuracy on the data is intrinsically limited, as in the phenomenological world of Natural Sciences. It is our experience that singularities cannot be ignored in finite-precision computation and that their influence can be enormous [3]. Even if the arithmetic is exact, there is most often a discretisation error, when solving partial differential equations, for example. Analytic perturbation theory is the favourite tool for studying the phenomena of Inexact Computing locally.

However, there may be *non-local* effects. To study such a possibility we developed the theory of Homotopic Deviation [5] which analyses the eigenvalues of the matrix family

$$\mathbf{A}(\tau) = \mathbf{A} + \tau\mathbf{E}, \mathbf{A}, \mathbf{E} \in \mathbb{C}^{n \times n}, \quad (5.1)$$

where the homotopy parameter $\tau = re^{i\theta} \in \mathbb{C}$. Classical Homotopic Perturbation corresponds to $r = |\tau| \in [0, 1]$. In contrast, we obtain unexpected results for the case $r \rightarrow \infty$, when the deviation matrix \mathbf{E} is rank deficient. The results correspond to *non-local* effects induced on $\mathbf{A}(\tau)$ by the singularities of \mathbf{A} : they may disappear locally (for $|\tau|$ small enough) but not completely at a global level. The effects become visible for $|\tau|$ large enough.

Homotopic Deviation with a complex parameter is a versatile computational tool which allows the point of view to evolve continuously from a local ($|\tau|$ small) to a global ($|\tau|$ large enough) position, and conversely, to analyse the properties of the matrix resolvent field $z \rightarrow \mathbf{R}(\tau, z) = (\mathbf{A}(\tau) - z\mathbf{I})^{-1}$ for $\mathbf{A}(\tau)$, with $\tau \in \mathbb{C}$, as well as its vector spectral field $\tau \rightarrow \lambda(\tau)$. Generically, for any $z \in \mathbb{C}$, the resolvent matrix $\mathbf{R}(\tau, z)$ is defined for any $\tau \in \mathbb{C}$ but for at most n values τ_i , for which z is an eigenvalue of $\mathbf{A}(\tau_i) = \mathbf{A} + \tau_i\mathbf{E}$. We characterise a class of deviation matrices \mathbf{E} of rank $\hat{r} < n$ for which there may exist at most $n - \hat{r}$ points in \mathbb{C} , introduced in [5] as *critical points*, such that $\mathbf{R}(\tau, z)$ exists for any $\tau \in \mathbb{C}$ and $\mathbf{R}(\tau, z)$ has a finite representation as a polynomial of degree \hat{r} in τ . The singularities of the resolvent vanish at these critical points. Interestingly, $n - 1$ critical points always exist for rank 1 deviation matrices. In this case, $\mathbf{R}(\tau, z) - \mathbf{R}(0, z)$ is linear in τ [5, 6].

Homotopic methods are often used in Mathematical Analysis, either in a computational context, under the name of continuation methods, or in a theoretical one to investigate questions related to convergence and analyticity. In such methods, the homotopy parameter is constrained by $|\tau| \in [0, 1]$. See references [1, 2, 3, 4, 5, 6, 8, 10]. The typical situation corresponds to a local analysis. It is characterised by i) $\tau \rightarrow 0$, to analyse $\mathbf{A}(\tau)$ by perturbation techniques, or by ii) $0 \leq \tau \leq 1$ to relate \mathbf{A} to \mathbf{B} by means of $\mathbf{A}(\tau) = \mathbf{A} + \tau(\mathbf{B} - \mathbf{A})$. However, the important case $|\tau| \rightarrow \infty$, which is required

by a global analysis, had never been looked at in the literature to date.

An important domain of application for Homotopic Deviation is the area of Quadratic Eigenvalue Problems [2] which are of fundamental importance in questions related to stability. A specific class of Quadratic Eigenvalue Problems that we have studied with the Homotopic Deviation theory stems from Acoustics [7]. In particular, we have studied the acoustic wave equation (in 1D and 2D) where the boundary conditions are partly pressure release (homogeneous Dirichlet) and partly impedance, with a complex impedance parameter ζ . The translation of context from Acoustics to Homotopic Deviation implies that $\tau = \frac{1}{\zeta}$ is the classical homotopy parameter. Therefore $|\tau| \rightarrow \infty$ is equivalent to $\zeta \rightarrow 0$, which supports the physical interpretation that the impedance condition is transformed into a pressure release condition. Moreover, the notion of critical points, which is a key notion in Homotopic Deviation theory, can be interpreted as points that can never correspond to a resonance frequency, irrespective of the value of the impedance. The results are reported in [7] and have been submitted to Linear Algebra and its Applications. A related report is [9].

Another important area of application for Homotopic Deviation is the convergence of Krylov type methods. This is reported in the next item.

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5.3 Arnoldi method and the happy breakdown

F. Chaitin-Chatelin: CERFACS, *France*; **E. Travesias:** CERFACS, *France*;
A.N. Zaoui: CERFACS, *France*

A convincing theory of the convergence of an iterative Arnoldi method is still a tantalizing goal for numerical analysts in Linear Algebra. We approach this question by considering the incomplete Arnoldi method on a matrix of order n as a *finite*, or *direct* (as opposed to iterative or asymptotic) method. In this approach, it is of prime importance to understand the relation between the starting vector v_1 and the happy breakdown at step $k_0 \ll n$. This requires, in particular, eliminating the conventional assumption that the matrix is non-derogatory. Because, if the matrix is non-derogatory,

no early happy breakdown can occur unless the starting vector lies exactly in an invariant subspace in exact arithmetic.

As was already shown in [2, 6], the incomplete Arnoldi method at step k can be cast in the Homotopic Deviation framework with a deviation matrix $\mathbf{E}_k = \mathbf{v}_k \mathbf{v}_{k+1}^H$, which is defective: $\mathbf{v}_{k+1}^H \mathbf{v}_k = 0$. This defectiveness of \mathbf{E} provides an algorithmically important class of applications, where the assumption that the eigenvalue 0 of \mathbf{E} is *semi-simple* is *not* satisfied. As a result, the analysis of the convergence at step k requires one to look at step $k - 1$ as well as at step $k + 1$ [5].

Further references are [1, 3, 4].

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5.4 Virtual Reality

M. Doré: INP, GRENoble, France; **F. Chaitin-Chatelin:** CERFACS, France;
M. van Gijzen: CERFACS, France; **A. N. Zaoui:** CERFACS, France, with support of the TTN-group

Visualisation of homotopic spectral portraits with MATLAB has already brought unexpected new insights in 2001 [2]. It has, for example, led to the notion of critical points. In order to use more advanced visualisation tools than MATLAB, an interface has been made with the Virtual Reality equipment of CERFACS. This work has mainly been performed in the context of a traineeship [3] in collaboration with the TTN-group. Partly as a result of this work, the emphasis on the development of the Homotopic Deviation theory has shifted to the study of large deviations, in particular to the case $|\tau| \rightarrow \infty$. This leads to the notion of kernel points [1].

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5.5 Geometric aspects of Computing

F. Chaitin-Chatelin: CERFACS, France; **A. N. Zaoui:** CERFACS, France

In conventional scientific computing, the four arithmetic operations (+, −, ×, /) are usually defined on scalars or real numbers, that is 1D vectors. Linear Algebra is performed on matrices and vectors

of potentially very large dimension, but the numbers themselves are either real scalars (1 dimension) or complex scalars (2 dimensions). Hypercomplex scalars are usually not used in Numerical Linear Algebra. However, it is known since the days of Hamilton and Graves that one can multiply and divide real vectors of dimension 2^k , $k = 0, 1, 2, \dots$, which define algebras of hypercomplex numbers. This requires introducing an additional geometric operation, the conjugation. These 5 operations define the arithmetic-geometric core of Nature's Computation. For example, the laws of Classical Mechanics and of Maxwell's electromagnetism can be written most efficiently by using products of quaternions, which are 4D vectors. The real component can be interpreted as Time and the 3 imaginary components as Space [4].

The first four real hypercomplex algebras A_k are well known: $A_0 = \mathbb{R}$, $A_1 = \mathbb{C}$, $A_2 = \mathbb{H}$ (quaternions) and $A_3 = \mathbb{G}$ (octonions). By comparison the corresponding four binary algebras B_k on $\mathbb{Z}_2 = \{0, 1\}$ are hardly known [6]. They have been the focus of our attention [4, 5]. We discovered that with an appropriate ordering, B_1 has the structure of \mathbb{Z}_4 . The numbering $0 = (00)$, $1 = (10)$, $2 = (11)$, and $3 = (01)$ defines the complex multiplication on sequences of 2 bits with multiplication mod 4. Weaker results are obtained for parts of B_2 (mod 8) and B_3 (mod 16) [5]. B_1 is given an important interpretation related to Quantum Computing on qu-bits (i.e. quantum bits): the logical gate $\sqrt{\text{not}}$ is a rotation of angle $\pi/2$ [4]. These results have been presented at [1, 2, 3].

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 - [3] F. Chaitin-Chatelin. Hasard et créativité: le calcul de la vie, September 27, 2002. *Grand Séminaire*, Observatoire Midi Pyrénées, Toulouse, September 27, 2002, talk.
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6 Nonlinear Systems and Optimization

6.1 Iterative techniques in variational data assimilation

L. Giraud: CERFACS, *France*; **S. Gratton:** CERFACS, *France*; **J. Langou:** CERFACS, *and* EADS-CCR, *France*; **A. T. Weaver:** CERFACS, *France*

In this work, we intend to develop algorithms for large-scale data assimilation problems arising in oceanography. In the framework of an ocean incremental variational assimilation algorithm [7], we define the quadratic functional J by

$$J(w) = \frac{1}{2}w^T (UU^T)^{-1} w + \frac{1}{2}(Hw - d)^T (SS^T)^{-1}(Hw - d),$$

where UU^T and SS^T are positive definite (covariance) matrices, S is a square matrix, often diagonal, and U is a $k \times n$ rectangular matrix, $k \geq n$. The functional J has a unique global minimizer w^* that can be obtained either directly by solving the symmetric linear system $\nabla J = 0$ or indirectly by solving the full rank linear least squares problem

$$\min_x \left\| \begin{pmatrix} I_n \\ S^{-1}HU \end{pmatrix} x - \begin{pmatrix} 0 \\ S^{-1}d \end{pmatrix} \right\|_2, \quad (6.1)$$

because the solution x^* to (6.1) is related to w^* by the relation $w^* = Ux^*$. In our applications, the matrices H , S and U can neither be formed explicitly nor stored (the size of w is typically several million) but their application to a vector can be computed. For instance, in the assimilation algorithm, the operation $y = Ux$ is performed via the time-step integration of a generalized diffusion equation [6]. In that framework, the only viable method to solve (6.1) is an iterative scheme that only requires the result of matrix-vector products.

We investigate the use of the following four methods: 1) Limited-memory quasi-Newton (implementation of [3]); 2) Conjugate Gradient (CG) algorithm (implementations of [1], [2]); 3) Conjugate Gradient for Least-Squares (CGLS); 4) LSQR algorithm using Lanczos bidiagonalization [4]. Here, we apply the methods 1) and 2) on Problem 6.1 considered as an unconstrained quadratic optimization problem, whereas the methods 3) and 4) are chosen for their numerical reliability on linear least-squares problems. It is important to note that, for Problem 6.1, all the above iterative methods yield the same iterates in exact arithmetic, so that the discrepancies often observed in practice illustrate the robustness, or lack thereof, of the different methods in the presence of round-off.

In ocean data assimilation, the computational cost of some of the matrix-vector evaluations is extremely high. In that respect, re-orthogonalization strategies in CG or LSQR become effective and affordable. Such techniques have already been used in other applications occurring in Structural Mechanics [5], and Numerical Weather Forecasting [1]. In this work, we consider variants of these techniques that ensure a fast convergence on our problems.

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6.2 Techniques for the Regularisation of Discrete Rank-Deficient Least Squares Problems

E. Anterrieu: CERFACS, *France*; **S. Gratton:** CERFACS, *France*

The solution of least-squares problems, with a very ill-conditioned coefficient matrix, is likely to be contaminated by many error sources, such as rounding errors or noise in the data.

However, for some applications, the solution can be stabilized by introducing appropriate a priori information, which takes for instance the form of a penalty added to the least-squares criterion in the Tikonov regularisation.

We compare two regularization strategies, S_1 and S_2 , on an inverse problem arising in the reconstruction of the brightness temperature by a band-limited space-borne instrument in the framework of the SMOS project. Our formulation leads to an underdetermined linear least-squares problem, where the coefficient matrix and the right-hand side are both complex, but whose solution should be real because of the physical properties of the problem. In Strategy S_1 the *real* solution of minimum norm is computed using a decomplexification of the problem and an SVD on a real matrix. Strategy S_2 makes use of the band property to give a full rank linear least-squares problem in real arithmetic that is solved using orthogonal transformations. Both strategies S_1 and S_2 are compared using simulated data that are perturbed using a zero mean Gaussian noise whose covariance is obtained from a physical model of the instrument. It follows from the simulations that S_2 is superior to S_1 in the sense that the perturbations on the solution resulting from perturbations of the data are smaller for S_2 than for S_1 . This fact is confirmed by a first order analysis.

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6.3 Out-of-core solvers for large dense linear least squares

L. Giraud: CERFACS, *France*; **S. Gratton:** CERFACS, *France*

The long term objective of our work is to design a least-squares solver with out-of-core capabilities to tackle very large problems on distributed memory computers with two features that will make the code original compared to existing public domain software [1, 2]:

1. computation of some parts of the covariance matrix $(A^T A)^{-1}$,
2. possibility of carrying out incremental solutions, i.e. of updating the solution after appending a set of rows to A and b .

For the sake of the numerical robustness of the code, we plan to use orthogonal transformations. However, we decided to start with a normal equation implementation of the code because we believe that this first step will enable us to become more familiar with some aspects of out-of-core solvers such as the efficient use of I/O systems on various platforms.

So far we have designed a parallel code that computes the upper-triangular part of the normal equation matrix $A^T A$ and the right-hand side $A^T b$. The matrix A and the vector b are stored out-of-core, but the triangular matrix is in-core. This code combines MPI and OpenMP and runs currently on various internal CERFACS platforms that include the bi-processor Pentium III cluster, the Itanium I and the COMPAQ Alpha-Server. Similarly to the manufacturer tuned DGEMM kernel, the overall code achieves a sustained Megaflops rate close to the peak performance on each processor[3]. Similar experiments will soon be undertaken on a four node cluster of quadri-processor Itanium II as well as on a Power 4 based IBM SP machine.

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7 Conferences and Seminars

7.1 Conferences and seminars attended by members of the Parallel Algorithms Project

January

Visiting Lecturer in the Centre for Mathematics and its Applications (CMA), School of Mathematical Sciences, ANU, Canberra, Australia, January 12-24. I. S. DUFF.

Summer School in Computational Mathematics, Australian National University, Canberra, January 14-19. I. S. DUFF, *Series of lectures on direct methods for sparse matrices*, invited speaker.

February

Institute of Computer Science, Prague, Czech Republic, February 5. J. LANGOU, *TMGS - A "twice is enough" reorthogonalization algorithm*, joint work with L. Giraud, seminar.

Latsis Symposium, Iterative Solvers for Large Linear Systems celebrating 50 years of the conjugate gradient method and Professor Gene H. Golub's 70th birthday, ETH Zurich, Switzerland, February 18-21. L. GIRAUD, *Inner-Outer schemes for large dense complex linear systems in electromagnetic applications*, joint work with B. Carpentieri, I. S. Duff and G. Sylvand, contributed talk.

Latsis Symposium, Iterative Solvers for Large Linear Systems celebrating 50 years of the conjugate gradient method and Professor Gene H. Golub's 70th birthday, ETH Zurich, Switzerland, February 18-21. I. S. DUFF, attendee.

March

Dublin City University, March 1. I. S. DUFF, *Preconditioning for numerical solution of BE problems in electromagnetics*, joint work with B. Carpentieri and L. Giraud, seminar.

7th Copper Mountain Conference on Iterative Methods, Copper Mountain, Colorado, USA, March 24-29. L. GIRAUD, *A class of spectral two-level preconditioners*, joint work with B. Carpentieri, I. S. Duff and J.-C. Rioual, contributed talk.

7th Copper Mountain Conference on Iterative Methods, Copper Mountain, Colorado, USA, March 24-29. J. LANGOU, *When modified Gram-Schmidt generates a well-conditioned set of vectors*, joint work with L. Giraud, contributed talk.

7th Copper Mountain Conference on Iterative Methods, Copper Mountain, Colorado, USA, March 24-29. I. S. DUFF, attendee and program committee.

April

NERSC, Lawrence Berkeley National Laboratory, California, USA, April 3. I. S. DUFF, *Preconditioning for numerical solution of BE problems in electromagnetics*, joint work with B. Carpentieri and L. Giraud, seminar.

University of Liverpool, England, April 11. I. S. DUFF, *Preconditioning for numerical solution of BE problems in electromagnetics*, joint work with B. Carpentieri and L. Giraud, seminar.

British Applied Mathematics Symposium, University of Warwick, England, April 12. I. S. DUFF, *Preconditioning for numerical solution of BE problems in electromagnetics*, joint work with B. Carpentieri and L. Giraud, invited minisymposium speaker.

May

Congrs National d'Analyse Numrique (CANUM2002), Anglet, France, May 27-31 MARTIN VAN GIJZEN, *Solving large linear systems on parallel computers: the CERFACS experience*, contributed talk.

June

Householder Symposium XV, Peebles, Scotland, June 17-21. I. S. DUFF, *The use of a sparse indefinite solver in optimization packages*, invited plenary talk.

Householder Symposium XV, Peebles, Scotland, June 17-21. F. CHAITIN-CHATELIN, *Computing beyond limits*, contributed talk.

Householder Symposium XV, Peebles, Scotland, June 17-21. L. GIRAUD, *Multi-level preconditioning techniques for the solution of large dense linear systems in electromagnetism*, joint work with B. Carpentieri and I. S. Duff, contributed talk.

NAG/Oxford University Computing Lab Workshop on Preconditioning, Oxford, England, June 25. I. S. DUFF, *Sparse pattern selection strategies for robust Frobenius norm minimization preconditioners in electromagnetism*, joint work with B. Carpentieri and L. Giraud, invited talk.

Workshop on Fast Multipole Methods in electromagnetism applications, CNES, June 27. L. GIRAUD, *Preconditioners for FMM and FMM as a preconditioner*, joint work with B. Carpentieri, I. S. Duff and G. Sylvand, invited talk.

July

IMA 2002 Summer Program in Scientific Computing, University of Kentucky, USA, July 14-20. I. S. DUFF, *Sparse Matrix Methods*, invited lecturer.

University of Tennessee at Knoxville, USA, July 24. I. S. DUFF, *A Short Overview of the GRID-TLSE Project*, jointly prepared with M. Daydé, seminar.

Argonne National Laboratory, Illinois, USA, July 31. I. S. DUFF, *The Use of a Sparse Indefinite Solver in Optimization Packages*, seminar.

August

Computational Linear Algebra with Applications, Milovy, Czech Republic, August 4-10. I. S. DUFF, *How direct methods make iterative methods work*, invited talk.

Computational Linear Algebra with Applications, Milovy, Czech Republic, August 4-10. J. LANGOU, *A reorthogonalization procedure for MGS applied to a low rank deficient matrix*, joint work with L. Giraud and S. Gratton, contributed talk.

International conference on integral methods in science and engineering (IMSE2002), St Etienne, France, August 7-10. MARTIN VAN GIJZEN, *Large scale acoustic simulations on clusters of multiprocessors*, contributed talk.

September

Grand Séminaire, Observatoire Midi Pyrenées, Toulouse, France, September 27. F. CHAITIN-CHATELIN, *Hasard et Créativité: le Calcul de la Vie*, talk.

October

2003 Conference of the Dutch-Flemish Numerical Analysis Communities, Woudschoten, Netherlands, October 1-3. MARTIN VAN GIJZEN, attendee.

Department of Mathematics colloquiums, Wake Forest University, Wake Forest, USA, October 23. MARTIN VAN GIJZEN, *Large-scale scientific computing at CERFACS*, invited talk.

November

Oxford University, November 2002. I. S. DUFF, *MSc Course on Sparse Direct Methods*, presented jointly with J. Scott, invited lecturer.

2nd International Workshop on Parallel Matrix Algorithms and Applications (PMAA'02), Neuchâtel, Switzerland, November 9-10. I. S. DUFF, *Direct Methods for sparse matrices*, invited tutorial.

2nd International Workshop on Parallel Matrix Algorithms and Applications (PMAA'02), Neuchâtel, Switzerland, November 9-10. I. S. DUFF, *The symbiosis of direct and iterative methods for solving large sparse systems*, invited talk.

2nd International Workshop on Parallel Matrix Algorithms and Applications (PMAA'02), Neuchâtel, Switzerland, November 9-10. J. LANGOU, attendee.

Computational Science and Engineering Seminar, Delft University of Technology, Delft, Netherlands, November 22. MARTIN VAN GIJZEN, *Large-scale scientific computing at CERFACS*, invited talk.

December

Oxford University, December 2002. I. S. DUFF, *MSc Course on Sparse Direct Methods*, presented jointly with J. Scott, invited lecturer.

Alan Curtis Day in Oxford, December 5. I. S. DUFF, Chairman and organizer.

International Workshop on Computational Codes: the Technological Aspects of Mathematics advances in computing and software development for Differential Equations, University of Bari, December 18-20. B. CARPENTIERI, attendee.

7.2 Conferences and seminars organized by the Parallel Algorithms Project

February

Randomness and Creativity in Numbers. February 13. F. CHAITIN-CHATELIN (CERFACS). Wide Interest CERFACS Seminar.

What's new since the SIAM lectures in 1996. February 13-14. N. GRAVES GREGORY (University of Brighton).

Computational Ocean Acoustics: Do Finite Element Models have a future?. February 27. M. VAN GIJZEN (CERFACS). Wide Interest CERFACS Seminar.

April

Sparse preconditioners for dense complex linear systems in electromagnetic applications. April 23. B. CARPENTIERI (CERFACS), Ph.D Thesis defense.

Jury: G. Alléon (EADS), M. Daydé (ENSEEIH), I. S. Duff (CERFACS and RAL), L. Giraud (CERFACS), G. Meurant (CEA), Y. Saad (University of Minnesota), S. Piperno (INRIA-CERMICS).

Solving linear systems for semiconductor device simulations on parallel distributed computers. April 23. J.-C. RIOUAL (CERFACS), Ph.D Thesis defense.

Jury: A. Marrocco (INRIA), I. G. Graham (University of Bath), M. Vidrascu (INRIA), P. Amestoy (ENSEEIH-IRIT), I. S. Duff (CERFACS and RAL), L. Giraud (CERFACS), G. Meurant (CEA).

Iterative computation of PDE eigenvalues. April 24. I. G. GRAHAM (University of Bath).

May

Structure prediction for sparse LU factorization with partial pivoting. May 23. L. GRIGORI (Loria).

June

Sparse Days Meeting, June 24-25.

Support Theory and Preconditioning, ERIK BOMAN (Sandia National Laboratories). *Support preconditioners in TAUCS*, SIVAN TOLEDO (Tel-Aviv University). *Subset preconditioning*, DORON CHEN (Tel-Aviv University). *Crout Versions of ILUT*, YOUSEF SAAD (University of Minnesota). *Preconditioners for indefinite problems*, MICHELE BENZI (Emory University). *AISM: A factorized sparse approximate inverse preconditioner*, JOSE MAS MARÍ (Universitat Politècnica de València). *Reducing communication latency in applying incomplete factor preconditioner*, ESMOND NG (Lawrence Berkeley National Laboratory). *Using numerical values in sparse matrix reorderings for ILU and ARMS preconditioners*, MASHA SOSONKINA (University of

Minnesota Duluth). *Linear systems and mixed finite elements in hydrogeology*, HUSSEIN HOTEIT (INRIA/IRISA). *On iterative solution of linear systems in reservoir simulation*, SEBASTIEN LACROIX (IFP). *Decoupling and parallel preconditioning for sedimentary basin simulations*, ROBERT SCHEICHL (University of Bath). *Condition numbers in projection methods for integral equations*, FILOMENA D'ALMEIDA (Universidade do Porto).

July

Predicting QR Fill-In. July 9. S. OLIVEIRA (University of Iowa).

November

Inexact Krylov subspace methods for linear systems: analysis and practice. November 13. J. VAN DEN ESHOF (Utrecht University).

December

Terascale Spectral Element Algorithms and Implementations. December 12. H. TUFO (University of Colorado at Boulder, National Center for Atmospheric Research).

Solving acoustic problems. December 19. A. LE BLANC (University of Artois).

7.3 Internal seminars organized within the Parallel Algorithms Project

March

Introduction to Automatic Differentiation. March 13. E. FONTDECABA.

September

Homotopic deviation. Recent results using advanced visualisation techniques. September 12. M. VAN GIJZEN.

Study and improvement of a sparse multifrontal solver on SMP architecture. September 12. S. PRALET.

8 Publications

8.1 Journal Publications

- [PUB1] L. S. Blackford, J. Demmel, J. Dongarra, I. S. Duff, S. Hammarling, G. Henry, M. Heroux, L. Kaufman, A. Lumsdaine, A. Petitet, R. Pozo, K. Remington, and R. C. Whaley. An updated set of Basic Linear Algebra Subprograms (BLAS). *ACM Trans. Math. Softw.*, 28(2):135–151, June 2002.
- [PUB2] I. S. Duff, M. A. Heroux, and R. Pozo. An overview of the Sparse Basic Linear Algebra Subprograms: the new standard from the BLAS Technical Forum. *ACM Trans. Math. Softw.*, 28(2):239–267, 2002.
- [PUB3] I. S. Duff and C. Vömel. Algorithm 818: A Reference Model Implementation of the Sparse BLAS in Fortran 95. *ACM Trans. Math. Softw.*, 28(2):268–283, 2002. Implementation available from URL: <http://www.netlib.org/netlib/toms/818>.
- [PUB4] I. S. Duff and C. Vömel. Incremental Norm Estimation for Dense and Sparse Matrices. *BIT*, 42(2):300–322, 2002.
- [PUB5] L. Giraud. Combining shared and distributed memory programming models on clusters of symmetric multiprocessors: Some basic promising experiments. *International Journal of High Performance Computing Applications*, 16(4):425–430, 2002.
- [PUB6] L. Giraud and J. Langou. When modified Gram-Schmidt generates a well-conditioned set of vectors. *IMA Journal of Numerical Analysis*, 22(4):521–528, 2002.
- [PUB7] N. I. M. Gould, D. Orban, A. Sartenaer, and Ph. L. Toint. Componentwise fast convergence in the solution of full-rank systems of nonlinear equations. *Mathematical Programming Serie B*, 92(3):481–508, 2002.
- [PUB8] D. Kay, D. Loghin, and A. J. Wathen. A preconditioner for the Steady-State Navier-Stokes equations. *SIAM J. Scientific Computing*, 24(1):237–256, 2002.
- [PUB9] D. Loghin and A. J. Wathen. Schur complement preconditioners for the Navier-Stokes equations. *Int. J. Num. Meth. in Fluids*, 40(3–4):403–412, 2002.
- [PUB10] D. Orban and S. J. Wright. Properties of the Log-Barrier Function on Degenerate Nonlinear Programs. *Mathematics of Operations Research*, 27(3):585–613, 2002.
- [PUB11] J. Rahola and S. Tissari. Iterative solution of dense linear systems arising from the electrostatic integral equation in MEG. *Physics in Medicine and Biology*, 47(6):961–975, 2002.
- [PUB12] M. Rojas and D. C. Sorensen. A trust-region approach to the regularization of large-scale discrete ill-posed problems. *SIAM J. Scientific Computing*, 26(3):1843–1861, 2002.
- [PUB13] M. Rojas and T. Steihaug. An interior-point trust-region-based method for large-scale nonnegative regularization. *Inverse Problems*, 18(5):1291–1307, 2002.

8.2 Theses

- [THS1] B. Carpentieri. *Sparse preconditioners for dense complex linear systems in electromagnetic applications*. Ph.D. dissertation, INPT, April 2002. TH/PA/02/48.
- [THS2] J.-C. Rioual. *Solving linear systems for semiconductor device simulations on parallel distributed computers*. Ph.D. dissertation, INPT, April 2002. TH/PA/02/49.

8.3 Technical Reports

- [TRP1] P. R. Amestoy, I. S. Duff, and C. Vömel. Task scheduling in an asynchronous distributed memory multifrontal solver. Technical Report TR/PA/02/105, CERFACS, Toulouse, France, 2002. [Compressed PS](#), [PDF](#).
- [TRP2] C. Bousquet and C. Daniel. Complex version and validation of MUMPS, Multifrontal Massively Parallel Solver. Working Notes WN/PA/02/34, CERFACS, Toulouse, France, 2002. Memoire de Maîtrise Ingénierie Mathématique, UPS III. [Compressed PS](#), [PDF](#).
- [TRP3] B. Carpentieri, I.S. Duff, and L. Giraud. A class of spectral two-level preconditioners. Technical Report TR/PA/02/55, CERFACS, Toulouse, France, 2002. To appear in SIAM J. Scientific Computing. [Compressed PS](#), [PDF](#).
- [TRP4] F. Chaitin-Chatelin. About Singularities in Inexact Computing. Technical Report TR/PA/02/106, CERFACS, Toulouse, France, 2002. [Compressed PS](#), [PDF](#).
- [TRP5] F. Chaitin-Chatelin, T. Meškauskas, and A. N. Zaoui. Hypercomplex division in the presence of zero divisors on \mathbb{R} and \mathbb{Z}_2 . Technical Report TR/PA/02/29, CERFACS, Toulouse, France, 2002. [Compressed PS](#), [PDF](#).
- [TRP6] F. Chaitin-Chatelin and E. Traviasas. PRECISE and the reliability of Numerical Software. Technical Report TR/PA/02/57, CERFACS, Toulouse, France, 2002. To appear in Handbook of Computation, Bo Einarsson ed., SIAM Philadelphia. [Compressed PS](#), [PDF](#).
- [TRP7] F. Chaitin-Chatelin and E. Traviasas. Qualitative Computing. Technical Report TR/PA/02/58, CERFACS, Toulouse, France, 2002. To appear in Handbook of Computation, Bo Einarsson ed., SIAM Philadelphia. [Compressed PS](#), [PDF](#).
- [TRP8] F. Chaitin-Chatelin and A. N. Zaoui. Hypercomputation in $\{0,1\}$. Technical Report TR/PA/02/73, CERFACS, Toulouse, France, 2002. [Compressed PS](#), [PDF](#).
- [TRP9] R. Durdos. Krylov solvers for large symmetric dense complex linear systems in electromagnetism: some numerical experiments. Working Notes WN/PA/02/97, CERFACS, Toulouse, France, 2002. [Compressed PS](#), [PDF](#).
- [TRP10] L. Giraud and J. Langou. Another proof for modified Gram-Schmidt with reorthogonalization. Working Notes WN/PA/02/53, CERFACS, Toulouse, France, 2002. [Compressed PS](#), [PDF](#).
- [TRP11] L. Giraud and J. Langou. Robust selective Gram-Schmidt reorthogonalization. Technical Report TR/PA/02/52, CERFACS, Toulouse, France, 2002. [Compressed PS](#), [PDF](#).
- [TRP12] L. Giraud, J. Langou, and M. Rozložník. On the round-off error analysis of the Gram-Schmidt algorithm with reorthogonalization. Technical Report TR/PA/02/33, CERFACS, Toulouse, France, 2002. [Compressed PS](#), [PDF](#).

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- [TRP13] L. Giraud, A. Marrocco, and J.-C. Rioual. Iterative versus direct parallel substructuring methods in semiconductor device modeling. Technical Report TR/PA/02/114, CERFACS, Toulouse, France, 2002. [Compressed PS](#), [PDF](#).
- [TRP14] L. Giraud and M. B. van Gijzen. Large scale acoustic simulations on clusters of SMPs. Technical Report TR/PA/02/116, CERFACS, Toulouse, France, 2002. To appear in the proceedings of the IMSE2002 conference. [Compressed PS](#), [PDF](#).
- [TRP15] N. I. M. Gould, D. Orban, and Ph. L. Toint. General CUTEr documentation. Technical Report TR/PA/02/13, CERFACS, Toulouse, France, 2002. [Compressed PS](#), [PDF](#).
- [TRP16] N. I. M. Gould, D. Orban, and Ph. L. Toint. General SifDec documentation. Technical Report TR/PA/02/14, CERFACS, Toulouse, France, 2002. [Compressed PS](#), [PDF](#).
- [TRP17] G. Richard. Coupling MUMPS and ordering software. Working Notes WN/PA/02/24, CERFACS, Toulouse, France, 2002. [Compressed PS](#), [PDF](#).