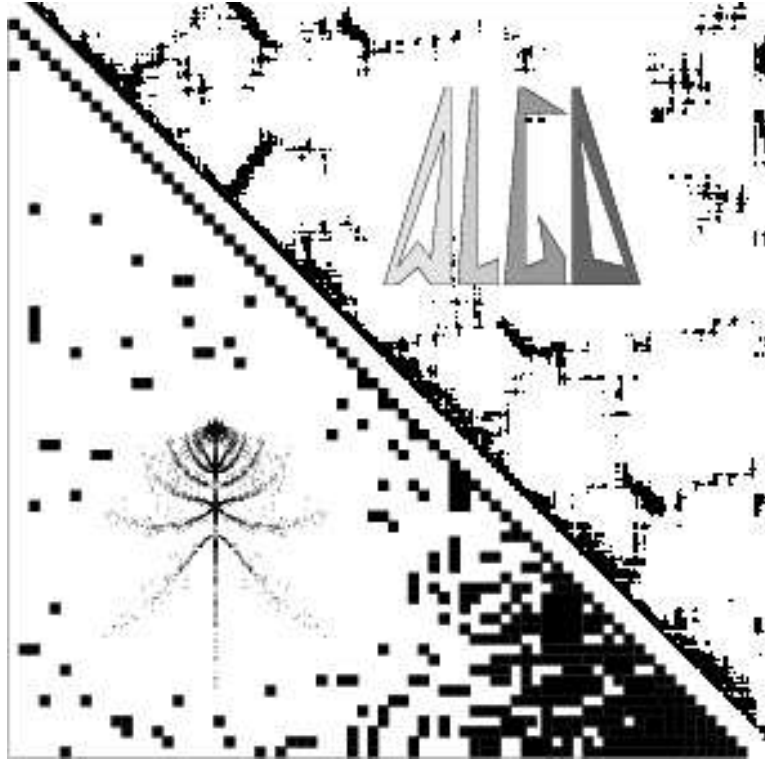


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ACTIVITY REPORT
of the
PARALLEL ALGORITHMS PROJECT
at
CERFACS

JANUARY 2003 - DECEMBER 2003

TR/PA/03/135

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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 the Parallel Algorithms Project can be found from the number of accesses to the CERFACS Web pages where about half of all the hits for CERFACS projects are on the Algo web pages.

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 INRIA-Lyon. The release currently being distributed is Version 4.3.2. Some research work that will most likely have an impact on future releases is discussed 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.

Most of the work discussed in Section 3 is concerned with the direct factorization of general sparse matrices and involves very innovative research that is very much work-in-progress. It is quite likely that this will have important consequences for the future development of sparse codes including MUMPS. We also report on the start of the three-year ACI-GRID Project with ENSEEIHT and others on developing a Grid based expert site for sparse matrices called GRID-Tlse.

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 notion of two-level schemes has also been implemented within a two level multigrid scheme for solving general unsymmetric problems and an examination comparing various ways of using spectral information has been conducted. An inner-outer scheme involving FGMRES at the outer level has been successfully combined with fast multipole software to solve very large electromagnetics problems efficiently. Other preconditioning techniques have been adapted for non-Newtonian fluid problems and nonlinear systems and the use of realistic stopping criteria have been developed for unsymmetric finite element problems. The power of combining OpenMP and MPI has been used to great effect in the solution of realistic and large problems in ocean circulation. Following investigations into matrix partitioning schemes for distributed matrix-vector multiplication, a wrapper is now being developed to embed the reverse-communication GMRES and FGMRES routines so that an entry will be provided that accepts a sparse matrix as input and automatically exploits parallelism in the matrix and vector operations. Since the GMRES and FGMRES routines are widely used and have been downloaded over 1000 times, this should result in a very popular software package.

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. A nested approach using flexible Krylov methods has been investigated in a system involving global ocean circulation. Work has continued on the theory and practical applications of homotopic deviations. The applications have included the analysis of parameterised quadratic eigenproblems in computational acoustics and the study of Krylov type methods. 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 and Global Change 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 and have established that one of the major algorithms used by the climate community is Gauss-Newton. This insight has led to the consideration of more powerful schemes. We have also examined regularization techniques for the solution of rank-deficient least-squares problems in synthetic aperture imaging applications from signal processing. The work on the solution of large scale dense least-squares problems using an out-of-core factorization of the normal equations matrix has resulted in a code that is competitive with ScaLAPACK but only requires half the storage. Although interior-point methods have become very popular for linear programs, there are still many cases when the SIMPLEX algorithm should be preferred and we have developed some techniques involving sparse matrix techniques for improving the efficiency of this algorithm.

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 Laurie Delmas (INSA, Rouen), Clément Lacourt (ENSEEIHT), and Marc Baboulin 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, Toulouse 1 and INSA. Two PhD theses were completed during the year. These were Christof Vöemel in March with a thesis on “Contributions to research in high performance scientific computing for sparse matrices” and Julien Langou whose topic was “Iterative methods for solving linear systems with multiple right-hand sides” and who defended his theses during the St Girons meeting in June. Both were successful in obtaining excellent postdoctoral appointments in the USA: Christof with Jim Demmel in Berkeley, and Julien with Jack Dongarra in Tennessee. We should also extend our congratulations to Bruno Carpentieri, one of last year’s graduands, who was awarded the Léopold Escande prize for the best INPT thesis.

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. Three of our visitors for this year stayed for a reasonably long period. These were: Julian Hall (sparse matrices and linear programming), Shane Mulligan (numerical solution of 3-dimensional PDEs), and Marielba Rojas (optimization). In addition to inviting 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. At the beginning of the year, Martin van Gijzen accepted the baton for running the CERFACS wide interest seminars and has run a very active and energetic programme in support of these more general seminars.

This year we expanded the annual “Sparse Day” to a three-day meeting on “Sparse matrices and grid computing” that we held in St Girons, Ariège. The conference was highly successful and evoked memories of the meeting that we held in St Girons in 1994 effectively to launch the International Year of Linear Algebra. The “St Girons Deux” meeting attracted 83 participants from 12 countries that included many world recognized researchers in sparse matrices and in grid computing, which theme was chosen because of our involvement in the GRID-Tlse Project supported by the ACI-Grid initiative. The list of attendees is given in Section 7.2.

I am very pleased to record that, over the reporting period, we have continued our involvement in joint research projects with shareholders and with other teams at CERFACS. We are represented in the CCT of CNES on orbitography and have developed a strong collaboration with them in the parallel distributed generation of normal equations and their subsequent Choleski factorization for applications in geodesy. 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. One of the stagiaires worked on an EADS project of implementing a dense out-of-core direct solver. We have had detailed discussions with EDF on parallel linear solvers. Our work on the optimization and linear algebraic aspects of data assimilation has been of great interest to and the subject of some discussions with Météo France. 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 elsA 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 and Global Change Team on aspects of data assimilation and have co-hosted 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. We have also interacted with the CSG group on issues concerning new computer chips and technologies.

As a postscript, I should record my thanks to my three seniors, Luc Giraud, Serge Gratton, and Martin van Gijzen, for doing all the hard work to ensure the smooth running of the Team.

Iain S. Duff.

Visitors to Parallel Algorithm Project in 2003

In alphabetical order, our visitors in the year 2003 included:

GUILLAUME ALLÉON (EADS-CCR, France), ABDELLATIF EL GHAZI (Université Mohammed V, Rabat, Morocco) PATRICK AMESTOY (ENSEEIH-IRIT, France), MARIO ARIOLI (CLRC-Rutherford Appleton Laboratory, UK) AKE BJÖRCK (Linköping University, Sweden) MATTHIAS BOLLHOEFER (TU Berlin, Germany) JACK DONGARRA (University of Tennessee, USA) JASPER VAN DEN ESHOF (University of Utrecht, Netherlands) ENRIC FONTDECABA (Industrias de Optica S.A., Spain) JULIAN HALL (University of Edinburgh, UK) PER CHRISTIAN HANSEN (Technical University of Denmark) ABDERRAZAK ILAHI (Facult des Sciences de Gabès, Tunisia) JACKO KOSTER (Parallab, BCCS, Bergen, Norway) FELIX KWOK (McGill University, Montreal, Quebec, Canada) SHERRY LI (Lawrence Berkeley National Laboratory, Berkeley, CA, USA) PIERRE MARECHAL (Université de Montpellier II) SHANE MULLIGAN (Dublin Institute of Technology, Dublin, Ireland) ESMOND NG (Lawrence Berkeley National Laboratory, Berkeley, CA, USA) ALEX POTHEN (Old Dominion University, Norfolk VA, USA) MARIELBA ROJAS (Wake Forest University, Winston-Salem, USA) JEAN ROMAN (INRIA Futurs, LaBRI, Talence, FRANCE) DANIEL RUIZ (ENSEEIH, France), and YOUSEF SAAD (University of Minnesota, USA) JENNIFER SCOTT (Rutherford Appleton Laboratory, UK) GERARD SLEIJPEN (PAYS-BAS) ANNICK SARTENAER (The University of Namur, Belgium) MICHAEL SAUNDERS (Stanford University, USA) MASHA SOSONKINA (Ames Laboratory/DOE Iowa State University, USA) GUILLAUME SYLVAND (EADS-CCR and CERMICS/INRIA, France). PHILIPPE TOINT (The University of Namur, Belgium) JEAN TSHIMANGA (The University of Namur, Belgium) MIROSLAV TŮMA (Academy of Sciences of the Czech Rep., Prague, Czech Republic)

2 List of Members of the Algo Team

IAIN DUFF - Project Leader
FRANÇOISE CHAITIN-CHATELIN - Qualitative Computing Group Scientific Advisor
LUC GIRAUD - Senior Researcher
SERGE GRATTON - Senior Researcher
MARTIN VAN GIJZEN - Senior Researcher
BRUNO CARPENTIERI - Post. Doc.
DANIEL LOGHIN - Post. Doc.
MARC BABOULIN - Ph.D. Student
JULIEN LANGOU - Ph.D. Student, currently University of Tennessee, US
EMERIC MARTIN - Ph.D. Student
STEPHANE PRALET - Ph.D. Student
SONGKLOD RIYAVONG - Ph.D. Student
CHRISTOF VÖMEL - Ph.D. Student, currently U.C. Berkeley, California, US
JULIAN HALL - Visitor, currently University of Edinburgh, UK
SHANE MULLIGAN - Visitor, currently Dublin Institute of Technology, Ireland
MARIELBA ROJAS - Visitor, currently Wake Forest University, US
LAURIE DELMAS - Trainee
CLEMENT LACOURT - Trainee
BRIGITTE YZEL - Administration

3 Dense and Sparse Matrix Computations

3.1 Symmetric weighted matching and application to indefinite multifrontal solvers

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

S. Pralet: CERFACS, *France*

We study techniques for scaling and choosing pivots when using multifrontal methods in the LDL^T factorization of symmetric indefinite matrices where L is a lower triangular matrix and D is a block diagonal matrix with 1×1 and 2×2 blocks.

For the LU factorization of a matrix A , MC64 [3] can be used to get a maximum weighted matching so that the corresponding permutation will place large entries on the diagonal. The matrix can then be scaled so that diagonal entries have modulus one and off-diagonals have modulus less than or equal to one. This has been found to greatly improve the numerical stability of the subsequent LU factorization.

If, however, MC64 is applied to a symmetric matrix the resulting permutation will not normally preserve symmetry. We examine ways in which MC64 can be used while still preserving symmetry. Then an ordering (for example, AMD [1]) can be computed on the permuted matrix to get a symmetric permutation in order to decrease the fill-in in the factors.

We use our “symmetric” MC64 preprocessing with two symmetric multifrontal codes MA47 [4] and MA57 [2] to validate our preprocessing heuristics on real test problems.

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- [1] P. R. Amestoy, T. A. Davis, and I. S. Duff. An approximate minimum degree ordering algorithm. *SIAM J. Matrix Analysis and Applications*, 17(4):886–905, 1996.
 - [2] I. S. Duff. MA57 - a new code for the solution of sparse symmetric definite and indefinite systems. Technical report RAL-TR-2002-024, Rutherford Appleton Laboratory, 2002.
 - [3] I. S. Duff and J. Koster. The design and use of algorithms for permuting large entries to the diagonal of sparse matrices. *SIAM J. Matrix Analysis and Applications*, 20(4):889–901, 1999.
 - [4] I. S. Duff and J. K. Reid. MA47, a Fortran code for direct solution of sparse symmetric indefinite structured systems of linear equations. Technical Report (to appear), Rutherford Appleton Laboratory, 1994.

3.2 Unsymmetric orderings using a constrained Markowitz scheme

P. R. Amestoy: ENSEEIHT, *France*; **X. S. Li:** LAWRENCE BERKELEY NATIONAL LAB *Berkeley, CA*; **S. Pralet:** CERFACS, *France*

We consider the LU factorization of a sparse unsymmetric matrix A based on a three-phase approach (analysis, factorization, solve). The analysis phase transforms A into \tilde{A} with better properties for sparse factorization. It exploits the structural information to reduce the fill-ins in the LU factors and exploits the numerical information to reduce the amount of numerical pivoting needed during factorization. Two separate passes are commonly used for these two objectives. Firstly, scaling and maximum transversal algorithms are used to transform A into A_1 with large entries on the diagonal. Secondly, a symmetric fill-reducing ordering, which preserves the large diagonal, is used to permute

A_1 into A_2 so that the factors of A_2 are sparser than those of A_1 . Note that during factorization, numerical instabilities can still occur and will be handled either by partial pivoting resulting in extra fill-in in the factor matrices or by static pivoting resulting in a potentially less accurate factorization. During analysis, the numerical treatment requires the fill-reducing ordering to be symmetric, and the structural phase does not have numerical information to correct any wrong numerical decisions. To avoid these two drawbacks, we present an approach which mixes the numerical and structural phases. Based on a numerical pre-treatment of the matrix we build at each step k of the elimination a set of numerically acceptable pivots, referred to as matrix C^k that may contain off-diagonal entries. We then compute an unsymmetric ordering taking into account both the structure of A and the numerical information in C^k .

3.3 Adapting a parallel sparse direct solver to architectures with clusters of SMPs

P. R. Amestoy: ENSEEIHT, *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 clusters of SMPs. 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] 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 machine with two-level architecture and we 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 4.3 of MUMPS.

-
- [1] P. R. Amestoy, I. S. Duff, S. Pralet, and C. Vömel. Adapting a parallel sparse direct solver to architectures with clusters of SMPs. *Parallel Computing*, 29(11-12):1645–1668, 2003.
- [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.

3.4 The Grid-TLSE project

P. Amestoy: ENSEEIHT-IRIT, *France*; **M. Buvry:** ENSEEIHT-IRIT, *France*; **M. Daydé:** ENSEEIHT-IRIT, *France*; **I.S. Duff:** CERFACS, *France*; **L. Giraud:** CERFACS, *France*; **J.Y. L'Excellent:** INRIA-ENSL, *France*; **M. Pantel:** ENSEEIHT-IRIT, *France*; **C. Puglisi:** ENSEEIHT-IRIT, *France*

In the context of large sparse calculations, we are involved as one of the leading partners of a ACI-Grid project (funded by the French Ministry of Research from December 2002 until November 2005). This project will use the grid at several levels. It will add new services on the Grid and use the grid capabilities to implement these services. The main services will be mainly twofold:

- provide the users with automatic expertise on sparse direct solvers using matrices either from the data base or provided by the user (a natural follow up step will be to extend this to iterative solvers).
- make available to the scientific community a set of test problems through a data base. The set of examples will grow dynamically as Grid users submit new problems that are integrated within the data set.

A prototype developed in 2003 was opened to the industrial partners that are the end-users (CEA, CNES, EADS, EDF, IFP). The specification phase is still ongoing, it is conducted jointly with ENSEEIHT and involves other academic Labs (LABRI, Bordeaux; INRIA-ENS, Lyon) as well as industrial partners. More information on the project can be found from the URL: <http://www.enseeiht.fr/lima/tlse>

4 Iterative Methods and Preconditioning

4.1 Efficient iterative methods for non-Newtonian fluid flows

D. Loghin: CERFACS, *France*

Discretizations of non-Newtonian flow models lead to large nonlinear block systems of equations the solution of which is usually sought through an iterative approach. Standard techniques suggested and analysed in the literature involve splittings of the block systems which lead to fixed-point iterations which generally are slow to converge. One example is that of the three-fields Stokes problem which arises in the solution of Oldroyd-B models via nonlinear schemes explicit in the nonlinear terms. The slow convergence of the explicit nonlinear scheme is compounded here by the aforementioned sluggish convergence of the splittings employed to solve the resulting linear systems. In this work, we present an approach based on the use of the structure of the underlying system of PDEs to construct a preconditioner for the solution of the global system via a Krylov method. In particular, we use block-triangular preconditioners coupled with GMRES to construct efficient and mesh-independent solution algorithms for mixed finite element discretizations of our problems. While the usual drawback associated with this approach is the need to approximate a Schur complement of the global matrix, in the case of the three-fields Stokes problem this Schur complement is readily available as a scaled mass matrix, not unlike that arising in the solution of the standard Stokes problem for Newtonian flow.

This work was included in the presentation given at the Workshop on Solution Methods for Saddle-Point Problems in Santa Fe. The work is presented in detail in a report which is currently being written [1].

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- [1] D. Loghin. Efficient iterative methods for non-Newtonian fluid flows. Technical Report, CERFACS, Toulouse, France, 2004.

4.2 Stopping criteria in finite element methods

M. Arioli: ATLAS CENTRE, RUTHERFORD APPLETON LABORATORY, OXON OX11 0QX, UK; **D. Loghin:** CERFACS, *France*; **A. J. Wathen:** OXFORD UNIVERSITY COMPUTING LABORATORY, PARKS ROAD, OXFORD, OX1 3QD, UK

This work [2] extends the results of Arioli [1, 3] on stopping criteria for iterative solution methods for linear finite element problems to the case of nonsymmetric positive-definite problems. We show that the residual measured in the norm induced by the symmetric part of the inverse of the system matrix is relevant to convergence in a finite element context. We then use Krylov solvers to provide alternative ways of calculating or estimating this quantity and present numerical experiments which validate our criteria. This work is expected to continue in 2004 with generalizations to the case of finite element discretizations of systems of PDEs.

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- [1] M. Arioli. A stopping criterion for the conjugate gradient algorithm in a finite element method framework. Technical Report IAN-1179, Istituto di Analisi Numerica, Pavia, 2000.
- [2] M. Arioli, D. Loghin, and A. J. Wathen. Stopping criteria for iterations in finite element methods. Technical Report TR/PA/03/21, CERFACS, Toulouse, France, 2003.
- [3] M. Arioli, E. Noulard, and A. Russo. Stopping criteria for iterative methods: applications to PDEs. *Calcolo*, 38:97–112, 2001.

4.3 Parallel algebraic preconditioners for the solution of Schur complement systems

L. Giraud: CERFACS, 42 AV. GASPARD CORIOLIS, 31057 TOULOUSE CEDEX, *France*;
S. Mulligan: SCHOOL OF COMPUTING, DUBLIN INSTITUTE OF TECHNOLOGY, KEVIN STREET,
 DUBLIN 8, *Ireland*

Domain decomposition methods are a natural way to parallelize the numerical solution of elliptic partial differential equations for 2D and 3D problems. In this study we consider the parallel solution of a standard finite element discretisation of 3D elliptic problems. The method used is a preconditioned conjugate-gradient solver following [?] on the Schur complement system for the interface unknowns. An additive Schwarz preconditioner is computed which consists of the local assembled Schur complements for each subdomain. These schur complements are computed using the MUMPS [1] package. We also used a sparsified version of this preconditioner, where elements whose relative magnitudes are below a certain tolerance are dropped; this typically results in Cholesky factors that retain only about 10% of the original dense factors.

The methods were implemented on an IBM SP by assigning each sub-domain to a single process and using MPI for the parallel communication. The numerical results have been obtained for a number of model problems, including problems with variable and discontinuous coefficients. The results indicate a good parallel scalability of these methods for 3D problems, in that the convergence rate is not seriously degraded as the number of domains increases. Further tests are being carried out, including comparisons with a direct solver and results will be documented.

-
- [1] J.-Y. L'Excellent P.R. Amestoy, I.S. Duff and J. Koster. Multifrontal massively parallel solver (mumps version 4.3) users' guide. Tech. Rep., ENSEEIHT-IRIT, France, 2003.

4.4 Two grid spectral preconditioning for general sparse linear systems

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

Multigrid methods are among the fastest techniques to solve a linear system $Ax = b$ arising from the discretization of a partial differential equation. The core of the multigrid algorithms is a two-grid procedure that is applied recursively. The basic idea of the two-grid solver is :

1. given x_0 , perform a few (μ_1) steps of a basic stationary method of the form $x^{(k+1)} = (I - MA)x^{(k)} + g$ to compute x^{μ_1} . This step is referred to as the pre-smoothing.
2. project the residual $r = b - Ax^{\mu_1}$ on a coarse space using a restriction operator R and solve the linear system $RAPe = Rr$, where P is the prolongation operator.
3. prolongate the error in the fine space and update $x = x^{\mu_1} + Pe$.
4. perform few (μ_2) steps of a basic stationary method of the form $x^{(k+1)} = (I - MA)x^{(k)} + g$ to compute x^{μ_2} . This step is referred to as the post-smoothing.
5. If x_2^{μ} is accurate enough stop, else $x_0 = x^{\mu_2}$, go to Step 1.

The smoother iterations aim at reducing the high frequencies of the error (ie the components of the error in the space spanned by the vectors associated with the largest eigenvectors of A). The restriction operator and consequently the coarse space is chosen so that this space contains the low frequency of the error (i.e. the components associated with the smallest eigenvalues). In classical multigrid, the coarse space is not defined explicitly through the knowledge of the eigencomponents

but by the selection of a space that is expected to capture them. The scheme presented above is a multiplicative algorithm [2] but additive variants [3] also exist.

In this work, we exploit the idea of the two-grid method to design additive and multiplicative preconditioners for general linear systems. We explicitly define the coarse space by computing the eigenvectors V associated with the smallest eigenvalues of MA (that is, the components of the error that are not damped efficiently by the smoother). In that context, the prolongation operator is $P = V$. We show that our preconditioners shift the smallest eigenvalues of MA to one and tend to cluster those that were already in the neighbourhood of one closer to one. We illustrate the performance of our method through numerical experiments on a set of general linear systems, both symmetric and positive definite and unsymmetric. Finally, we consider a case study of a non-overlapping domain decomposition method of semiconductor device modelling for the solution of the drift-diffusion equations.

A more detail description of these approaches as well as their numerical behaviour on a range of standard test problems is available in [1]

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- [1] B. Carpentieri, L. Giraud, and S. Gratton. Two-grid spectral preconditioning for general sparse linear systems. Technical Report In preparation, CERFACS, Toulouse, France, 2004.
 - [2] W. Hackbusch. *Multigrid methods and applications*. Springer-Verlag, 1985.
 - [3] R. S. Tuminaro. A highly parallel multigrid-like method for the solution of the Euler equations. *SIAM J. Scientific and Statistical Computing*, 13:88–100, 1992.

4.5 A comparative study of iterative solvers exploiting spectral information for SPD systems

L. Giraud: CERFACS, *France*; D. Ruiz: ENSEEIHT-IRIT, *France*;
A. Touhami: ENSEEIHT-IRIT, *France*

When solving the Symmetric Positive Definite (SPD) linear system $\mathbf{Ax} = \mathbf{b}$ with the Conjugate Gradient (CG) method, the smallest eigenvalues of the matrix A often slow down the convergence. This observation is still of course true when a preconditioner is used and some additional techniques can be investigated to improve the convergence rate of CG on the preconditioned system. Several techniques have been proposed in the literature that either consists of updating the preconditioner or enforcing CG to work in the orthogonal complement to the invariant subspace associated with small eigenvalues. In this work, we compare the numerical efficiency and computational complexity of the techniques presented in [1, 2, 4, 5, 6]. A more detail description of these approaches as well as their numerical behaviour on a range of standard test problems is available in [3].

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4.6 Adaptive preconditioners for Newton-Krylov methods

D. Loghin: CERFACS, *France* ; **D. Ruiz:** INPT-ENSEEIH, *France*; **A. Touhami:** INPT-ENSEEIH, *France*

The use of preconditioned Newton-Krylov methods has become a mandatory choice for the solution of large nonlinear systems of equations. In many situations the available preconditioners are sub-optimal, due to the changing nature of the linearized operator. This the case, for instance, for quasi-Newton methods where the Jacobian (and its preconditioner) are kept fixed at each non-linear iteration, with the rate of convergence usually degraded from quadratic to linear. Updated Jacobians, on the other hand require updated preconditioners, which may not be readily available. In this work, we introduce an adaptive preconditioning technique based on the Krylov subspace information generated at previous steps in the nonlinear iteration. In particular, we use to advantage a deflation technique suggested by Reichel, Calvetti and Golub for restarted GMRES to enhance existing preconditioners with information about (almost) invariant subspaces constructed by GMRES at previous stages in the nonlinear iteration. We provide guidelines on the choice of invariant-subspace bases used in the construction of our preconditioner and demonstrate the improved performance on various test problems. We also describe an efficient implementation of our approach in the case of augmented systems arising from CFD modelling. This work has been contributed to the Copper Mountain Conference on Iterative Methods [1].

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4.7 Using spectral low rank preconditioners for large electromagnetic calculations

I. S. Duff: CERFACS, *France* and RUTHERFORD APPLETON LABORATORY, *England*;
L. Giraud: CERFACS, *France*; **J. Langou:** *University of Tennessee, USA*; **E. Martin:** CERFACS, *France*.

For solving large dense complex linear systems that arise in electromagnetic calculations, we perform experiments using a general purpose spectral low rank update preconditioner [2] in the context of the GMRES method preconditioned by an approximate inverse preconditioner [1]. The goal of the spectral preconditioner is to improve the convergence properties by shifting by one the smallest eigenvalues of the original preconditioned system.

Numerical experiments have been performed on parallel distributed memory computers, using a Fast Multipole code [4], to illustrate the efficiency of this technique on large and challenging real-life industrial problems. More details on this work are available in [3].

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4.8 Combining fast multipole techniques and approximate inverse preconditioners for large calculations in electromagnetism

B. Carpentieri: CERFACS, *France*; **I.S. Duff:** CERFACS, *France*; **L. Giraud:** CERFACS, *France*;
G. Sylvand: CERMICS-INRIA, *Sophia Antipolis, France*

The boundary element method has become a popular tool for the solution of Maxwell's equations in electromagnetism. From a linear algebra point of view, this leads to the solution of large dense complex linear systems where the unknowns are associated with the edges of the mesh defined on the surface of the illuminated object. In this paper, we address the iterative solution of these linear systems via preconditioned Krylov solvers. Our primary focus is on the design of an efficient parallelizable preconditioner. In that respect, we consider an approximate inverse method based on the Frobenius-norm minimization. The preconditioner is constructed from a sparse approximation of the dense coefficient matrix, and the patterns both for the preconditioner and for the coefficient matrix are computed *a priori* using geometric information from the mesh. We describe how such a preconditioner can be naturally implemented in a parallel code that implements the multipole technique for the matrix-vector product calculation. We investigate the numerical scalability of our preconditioner on realistic industrial test problems and show that it exhibits some limitations on very large problems of size close to one million unknowns. To improve its robustness on those large problems we propose an embedded iterative scheme that combines nested GMRES solvers with different fast multipole computations. We show through extensive numerical experiments that this new scheme is extremely robust at affordable memory and CPU costs for the solution of very large and challenging problems. More details can be found in [1].

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4.9 Two level parallelism in a stream-function model for global ocean circulation.

M. van Gijzen: CERFACS, *France*

In ocean modelling, it is customary to split the ocean flow into a 2D depth-averaged part, and the 3D deviations from it. The 2D part can be formulated in terms of a stream-function, which simplifies the governing partial differential equations. However, in this formulation additional contour integral conditions around continents are needed. These conditions destroy the structure in the matrix that results after discretisation and pose difficulties to parallelisation. In [1] we describe how the continent boundary conditions can be treated in a parallel setting by taking into account the land points in the calculations. We have implemented our ideas in the model described in [2]. By far the computationally most expensive part of a model calculation is the solution of a linear system of equations. Our iterative solution technique combines loop-level parallelism with a domain decomposition method. The communication between subdomains is implemented with MPI and the loop-level parallelism with OpenMP. Realistic numerical experiments on a cluster of bi-processor PC's using field data show superlinear performance, which can be attributed to a better use of the cache memory. Moreover, the performance of the mixed OpenMP/MPI method is noticeably better than for a pure MPI approach.

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4.10 Efficient CFD calculations on clusters of SMPs

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G. Chevalier: CERFACS, *France*; **L. Giraud:** CERFACS, *France*; **F. Loercher:** CERFACS,
France; **M. Montagnac:** CERFACS, *France*

Based on our experience on high performance scientific platforms and their associated programming techniques [2] we have studied how the code elsA [1] can efficiently exploit clusters of SMPs. In particular, we investigate techniques that avoid some of the penalizing effects of the memory hierarchy (cache or TLB) and also combine MPI and Open-MP in the context of this multi-block solver. The results of this work will be presented at the forthcoming ECCOMAS 2004 conference.

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4.11 Experiments on parallel matrix-vector products

S. Riyavong: CERFACS, *France*

We designed and implemented a data structure appropriate for computing the matrix-vector product efficiently on distributed computing environments using MPI. Experiments with GMRES [2] have been performed with sparse matrices selected from the Rutherford-Boeing Collection [1]. Numerical results on a COMPAQ and a cluster of PCs show a satisfactory performance and scalability. The details are given in the working note [3].

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5 Qualitative Computing

Group members: Françoise Chaitin-Chatelin, Martin van Gijzen.

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 discovering 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 fundamental laws have been discovered, which are the focus of attention for the Group. These laws concern in particular:

- a) *inexact computing* and the associated homotopic deviation theory 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 2003 in five related areas.

5.1 Inner-outer iterations

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There are classes of problems for which the matrix-vector product is a time consuming operation because an expensive approximation method is required to compute it to a given accuracy. Obviously, the more accurately the matrix-vector product is computed the more expensive or time consuming the overall process becomes. The question of how to control the accuracy of the matrix-vector product if the outer loop is a Krylov method has been extensively investigated at CERFACS [1, 2]. This work has led to the development of so called *relaxation strategies* in which the accuracy to which the matrix-vector multiplication is computed is reduced when the process comes closer to the solution. These results have attracted the attention of several other groups [4, 5].

The relaxation strategies have been proved to be an effective tool for various problems, see for example [3] for an industrial application. Typically a reduction in computing time between 20% and 50% can be obtained. In order to obtain a further reduction we have studied, in collaboration with the Numerical Mathematics group at the University of Utrecht, the combination of a relaxation strategy with so called flexible Krylov methods for the solution of linear systems of equations. A flexible Krylov subspace method allows a variable preconditioner. The preconditioning operation can for such a method be performed by applying a Krylov method like GMRES. In the preconditioning operation, GMRES only has to yield an approximate solution of the system, so at this level only a low

accuracy is required. In such a nested Krylov method, a relaxation strategy can be employed both at the outer level (the flexible Krylov method) and at the inner level (the preconditioning operation performed with GMRES).

We have analysed this nested approach for several flexible Krylov methods. We have experimentally verified the efficiency of this computational scheme with a Schur complement system that arises in the modelling of global ocean circulation. If we solve this system with GMRES we gain a factor of two by applying a relaxation strategy. If we combine this with a nested GMRES method (FGMRES or GMRESR) we gain an additional factor of five, thus yielding an overall improvement of performance of a factor of ten. The results are reported in [6].

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5.2 Inexact Computing and Homotopic Deviation

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

To study the robustness of approximation methods to large perturbations, it is useful to consider the linear coupling $\mathbf{A} + t\mathbf{E}$, where $\mathbf{A}, \mathbf{E} \in \mathbb{C}^{n \times n}$ and the parameter $t \in \mathbb{C}$.

The variation of the spectrum of linear operators and matrices under the influence of one or several parameters has long been an active domain of research, giving rise to the elegant analytic/algebraic spectral theory initiated by Puiseux. The case of a linear dependence on a parameter $t \in \mathbb{C}$, of the form $\mathbf{A}(t) = \mathbf{A} + t\mathbf{E}$ has been particularly studied [9, 10, 11]. See also [1, 2, 12].

In the 1990's, there has been a renewed interest for the topic amongst numerical analysts, coming from the widespread availability of graphical tools, as exemplified by Trefethen [13], Simoncini [12], and Chaitin-Chatelin and co-workers [6, 7, 8]. In particular, the easy access to plots of parameterised computed spectra of matrices make it possible to explore computationally the spectral maps $t \rightarrow \lambda(t) \in \sigma(\mathbf{A}(t))$, the spectrum of $\mathbf{A}(t)$, that is the set of eigenvalues of $\mathbf{A}(t)$. They are the singularities of the resolvent field $z \rightarrow \mathbf{R}(t, z) = (\mathbf{A} + t\mathbf{E} - z\mathbf{I})^{-1}$ [9, 10, 11].

For any $t \in \mathbb{C}$, $\mathbf{R}(t, z)$ is defined for all z in the resolvent set $re(\mathbf{A}) = \mathbb{C} \setminus \sigma(\mathbf{A})$, as long as z is not an eigenvalue of $\mathbf{A}(t) = \mathbf{A} + t\mathbf{E}$. The analyticity of $t \rightarrow \mathbf{R}(t, z)$ is guaranteed for $|t| < 1/\rho(\mathbf{E}(\mathbf{A} - z\mathbf{I})^{-1})$, where $\rho(\cdot)$ denotes the spectral radius [9, 10, 11]. What can be said beyond, for $|t| \geq 1/\rho(\mathbf{E}(\mathbf{A} - z\mathbf{I})^{-1})$?

We exclude the degenerate case where $\sigma(\mathbf{A}(t)) = \sigma(\mathbf{A}) \forall t \in \mathbb{C}$. Then there are at most n different matrices $\mathbf{A}(t_i), i = 1, \dots, n$, such that $z \in \sigma(\mathbf{A}(t_i))$ for any z in $re(\mathbf{A})$: $\mathbf{R}(t, z)$ exists for almost all $t \in \mathbb{C}$. The connection between z and t which makes $\mathbf{R}(t, z)$ singular is central in our investigation.

When \mathbf{E} is regular, $\lim_{|t| \rightarrow \infty} \mathbf{R}(t, z) = 0$ and for all n eigenvalues $\lambda(t)$ of $\mathbf{A}(t)$, $|\lambda(t)| \rightarrow \infty$. However, when \mathbf{E} has rank r , $1 \leq r < n$, two new phenomena occur. Firstly, when $\lim_{|t| \rightarrow \infty} \mathbf{R}(t, z) = \mathbf{R}(\infty, z)$ exists, it is *nonzero* and *computable in closed form*. Secondly, certain eigenvalues $\lambda(t)$ may remain at a finite distance in the limit of $|t| \rightarrow \infty$. Among the points in $re(\mathbf{A})$ where $\mathbf{R}(\infty, z)$ does not exist,

there are finitely many *kernel* points which are the limit of $\lambda(t)$ as $|t| \rightarrow \infty$. Moreover, it is possible that among these kernel points there exist *critical* ones for which z cannot be an eigenvalue of $\mathbf{A}(t)$ for any finite t . At a critical point, the resolvent $\mathbf{R}(t, z)$ is a polynomial in t of degree $\delta \leq r$. The properties of $\mathbf{R}(t, z)$ and of $\sigma(\mathbf{A}(t))$ in the limit $|t| \rightarrow \infty$ depend on the Jordan and Frobenius structures of $0 \in \sigma(\mathbf{E})$. An account of the complete theory of Homotopic Deviation is in [3, 4, 5].

Homotopic Deviation is a specialized version of more general problems in Matrix and Linear Operator Theory, usually analysed by analytic spectral theory, which often puts a limit to $|t|\|\mathbf{E}\|$, or by algebraic geometry on the spectral variety $(t, z) \rightarrow \det(\mathbf{A} + t\mathbf{E} - z\mathbf{I}) = 0$, where (t, z) describe \mathbb{C}^2 . A third approach for such problems, stimulated by linear systems theory, consists of the theory of (nonmonic) matrix polynomials.

In Homotopic Deviation theory, we specifically look beyond analyticity in t , for $|t|$ large enough. Our tools are elementary linear algebra, based on the Jordan structure of $0 \in \sigma(\mathbf{E})$. The rank deficient matrix \mathbf{E} is called the *deviation*, and the term "perturbation" covers the case where $|t|\|\mathbf{E}\|$ is limited, \mathbf{E} being possibly of full rank. Our work provides an elementary analysis for $z, t \in \mathbb{C} = \mathbb{C} \cup \infty$ of singular perturbation theory for matrices, since \mathbf{E} is singular in the case of interest. To the best of our knowledge, the study of $\mathbf{R}(t, z)$ and $\lambda(t)$ as $|t| \rightarrow \infty$ has been, so far, scattered in the literature. We believe that the notion of kernel/critical points is new [5].

The elementary approach of Homotopic Deviation is driven by algorithmic considerations arising from the Sherman-Morrison formula. The key role of the structure of $0 \in \sigma(\mathbf{E})$ emerges naturally from the computational perspective; see [5] for an application to Arnoldi's algorithm, where \mathbf{E} is nilpotent (see also 4.4). Homotopic Deviation tries to make the best use of the extreme simplicity of the matrix setting to present results which are specific to the *linear* coupling $\mathbf{A}(t) = \mathbf{A} + t\mathbf{E}$, leading to computational insight for numerical software. The following two articles present two different applications of homotopic deviation.

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5.3 Quadratic eigenproblems, an example in Computational Acoustics

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

In the basic Homotopic Deviation the matrix $\mathbf{A} + t\mathbf{E} - z\mathbf{I}$ depends linearly on the parameters t and z . The analysis can be extended straightforwardly to a polynomial dependence in z . For example, the quadratic case $z^2\mathbf{M} + z\mathbf{C} + \mathbf{K}$, where \mathbf{M} is regular, is treated in [1, 2] for a problem arising in computational acoustics. It concerns the discrete wave equation with an impeding boundary condition controlled by the complex impedance ζ [3]. The condition becomes Neumann (resp. Dirichlet) as $|\zeta| \rightarrow \infty$ (resp 0) [4]. The homotopy parameter t is taken to be $t = 1/\zeta$. The Homotopic Deviation theory, combined with the properties of the continuous wave equation allows us to give the *kernel points* in *closed form* as eigenvalues of the discrete Dirichlet problem. We also specify which of them are *critical*. We are able to prove that the degree δ of the polynomial $\mathbf{R}(t, z)$ is $\delta = 1$ for the critical points. Ample numerical illustrations are provided in [1, 2].

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5.4 Robustness of Krylov type methods

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

We approach this question by considering an iterative Krylov method as an inner–outer iteration. The outer loop modifies the starting vector for the construction of the Krylov basis. The inner loop is a direct method which consists of an incomplete Arnoldi decomposition of size $k \ll n$ [2, 5]. To study the dynamics of this 2-level algorithm, we perform a homotopic deviation of the matrix of order $k + 1$

$$\mathbf{B} = \begin{pmatrix} \mathbf{H}_k & \mathbf{u} \\ 0 & a \end{pmatrix},$$

such that

$$\mathbf{H}_{k+1} = \begin{pmatrix} \mathbf{H}_k & \mathbf{u} \\ 0 & h_{k+1,k} & a \end{pmatrix}.$$

The homotopy parameter is $h = h_{k+1,k} \in \mathbb{C}$ and the deviation matrix is $\mathbf{E} = \mathbf{e}_{k+1}\mathbf{e}_k^T$. \mathbf{E} is nilpotent ($\mathbf{E}^2 = 0$), with $\sigma(\mathbf{E}) = \{(0^1)^{k-1}, (0^2)\}$. For k fixed, $1 < k < n$, we set $\mathbf{H}^- = \mathbf{H}_{k-1}$, $\mathbf{H} = \mathbf{H}_k$, $\mathbf{H}^+ = \mathbf{H}_{k+1}$. The three matrices represent the sections of order $k - 1, k, k + 1$ for the Hessenberg matrix constructed from \mathbf{A} by the iterative Arnoldi process.

A complete analysis of $h \mapsto \{(\mathbf{H}^+ - z\mathbf{I})^{-1}, \sigma(\mathbf{H}^+)\}$ is performed in [1, 3]. This is the first step in our study. The second step will relate the algebraic properties present in the inner loop to the quality of the convergence of the outer loop [4].

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5.5 Geometric aspects of Computing

F. Chaitin-Chatelin: 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 five 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 three imaginary components as space [1, 5].

The first four real hypercomplex algebras A_k , which are isometric, 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 [4, 5, 6]. $B_1 \sim \mathbb{Z}_4$ 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 $\pi/2$ [5].

Real hypercomplex algebras A_k are studied in [3] in the light of the dominant role of multiplication over addition, which is experienced in "real life" scientific computing - See the fundamental Borel-Newcomb paradox about the role of the first digit of a number chosen at random [4]. This leads to the study of the hypercomplex exponential on A_k , for $k \geq 2$. The Euler identity $e^{2ik\pi} = 1$ for $k \in \mathbb{Z}$ is extended to Pythagorean triples $(n, m, q) \in \mathbb{N}^*$ such that $n^2 + m^2 = q^2$, in order to insure the commutativity $e^{x+y} = e^x \times e^y = e^y \times e^x$ for a given $x \in \text{Im } A_k, y \in \text{Im } A_k$. For $k \geq 4$, the presence of zero divisors allows us to have commutativity in continuous and finite modes at the same time. By comparison, for $k = 2$ (quaternions) or 3 (octonions) the two modes are mutually exclusive [2, 3].

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6 Nonlinear Systems and Optimization

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

M. Baboulin: CERFACS, *France*; **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 with existing public domain software [2, 3]:

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 $A^T b$, mixing OpenMP and MPI. A sustained Megaflops rate close to the peak performance on each processor has been obtained on various architectures including an IBM Regatta and a quadri-processor Itanium II.

We have also developed a parallel distributed implementation of a linear solver for large-scale applications involving real symmetric or complex symmetric non Hermitian dense systems. The main advantage of this routine is that it performs a Cholesky factorization by requiring half the storage needed by the standard parallel libraries ScaLAPACK or PLAPACK. Our solver uses a left-looking algorithm and a one-dimensional block-cyclic column data distribution but gives similar Megaflops performance when applied to problems that can be solved on moderately parallel computers with up to 32 processors. Experiments and performance comparison with ScaLAPACK on our target applications are presented in [1]. These applications arise from the Earth's gravity field recovery and computational electromagnetics.

However, it is also necessary to assess the normal equation approach and, in this respect, we are investigating the use of a condition number estimate in our Cholesky algorithm.

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6.2 Iterative techniques in variational data assimilation

L. Giraud: CERFACS, *France*; **S. Gratton:** CERFACS, *France*; **A. T. Weaver:** CERFACS, *France*

In this work, we intend to develop and study algorithms for nonlinear least-squares, with a particular focus on large-scale data assimilation problems arising in oceanography. In the framework of an ocean

incremental variational assimilation algorithm [6], we define the nonlinear functional J by

$$J(x_0) = \frac{1}{2}(x_0 - x_b)^T B^{-1}(x_0 - x_b) + \frac{1}{2} \sum_{i=0}^N (\mathcal{H}_i(x(t_i)) - y_i)^T R_i^{-1} (\mathcal{H}_i(x(t_i)) - y_i),$$

where $x(t) = \mathcal{M}(t, t_0)(x_0)$, and the operators \mathcal{H} and $\mathcal{M}(t, t_0)$ are nonlinear. The functional J can be rewritten as a nonlinear least-squares problem $\min_{x_0} \|F(x_0)\|$. This property is exploited in operational data assimilation systems, since J is usually minimized using an inexact Gauss-Newton algorithm named "Incremental 4D-Var algorithm". The target applications are problems for which the size of the unknown vector x_0 is typically several millions : the only viable methods to solve the linear least squares arising in the Gauss-Newton are Conjugate Gradient type iterative method such as CGNE, CGLS, or LSQR [1, 2, 4] algorithm.

A study of the convergence properties of inexact Gauss-Newton is carried out in [3]. We consider the case where the Jacobian of the function F is perturbed. We derive a convergence result for the inexact algorithm, and show the relevance of this analysis in a test case where the data are assimilated in a one-dimensional shallow water system representing the flow of a fluid over an obstacle in the absence of rotation. A key parameter to understand the behaviour of the Inexact Gauss-Newton algorithm is the order of magnitude of F at the optimum, which is also an indicator of the level of noise in the data assimilation system. In the numerical experiments, the exact Jacobian is obtained using an automatic differentiation technique, the inexact one is obtained by solving a linearized shallow water equation using a semi-implicit semi-Lagrangian discretization scheme.

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 [2]. In this work, we have considered an extension of these techniques that improve the convergence of Conjugate Gradient type algorithms when a sequence of slowly varying linear least-squares problems are considered.

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6.3 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 Tikhonov regularization.

We compare three regularization strategies, S_1 , S_2 and S_3 , 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 (Soil Moisture and Ocean Salinity) project. Our formulation leads to an under-determined 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. The third strategy S_3 is based on a truncated singular value decomposition. These strategies 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 and S_3 are superior to S_1 in the sense that the perturbations on the solution resulting from perturbations of the data are smaller for S_2 and S_3 than for S_1 . To confirm these results, we have performed a first order analysis. One of the contributions of this work is the derivation of a first order analysis and of an expected condition number [4, p.136] for the truncated SVD solution.

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 - [2] S. Gratton E. Anterrieu and B. Picard. Inverse problem in remote sensing by aperture synthesis imaging. 2003. Submitted to TS, the french journal of signal processing.
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6.4 Algorithmic and computational techniques for solving large scale sparse linear programming problems using the revised simplex method.

J. Hall: CERFACS, *France*

Based on my experience with asynchronous variants of the revised simplex method, I developed at CERFACS SYNPLEX-MI, a strategy for exploiting parallelism within the revised simplex method when using minor iterations of the standard simplex method. When implemented in parallel on a shared memory multiprocessor, this synchronous algorithm should address the two major drawbacks of the asynchronous algorithms which I have implemented previously. Limited experiments carried out on the CERFACS 32-processor SGI Origin 2000 machine (horus) suggest that one potential limitation of parallel revised simplex algorithms on shared memory machines will not restrict the performance of SYNPLEX-MI.

The phenomenon of hyper-sparsity in the context of linear systems of equations occurs when the solution (for a sparse right-hand-side) is sparse. Given a decomposition of the matrix as a product of elementary (Gauss-Jordan) elimination matrices, in the presence of hyper-sparsity the Gilbert-Peierls algorithm is commonly used to determine which very small subset of these elementary matrices needs to be applied. Whilst at CERFACS, I implemented the Gilbert-Peierls algorithm for use in the context of the revised simplex method for linear programming. This

led to the development of specialist variants of the algorithm which are better adapted to this context.

The branch-and-price algorithm for solving (Mixed)-Integer Programming (MILP) problems requires each of several small MILP sub-problems to be solved (using traditional branch-and-bound) many times. Each instance of a given MILP problem differs only in the coefficients of the objective. The branch-and-bound trees for a given MILP sub-problem are very similar in each instance and, typically, the optimal solution to a node from the previous instance remains optimal. Huge computational savings can be made if the cost of solving each node is reduced to checking optimality of the previous solution and, if necessary, performing the few simplex iterations to obtain the optimal solution. This requires very close integration of the branch-and-bound and LP solvers. I have developed data structure manipulation routines for my revised simplex solver so that this can be achieved. Based on experience so far and expected further efficiency gains, we predict that, for our practical problems of interest, the resulting branch-and-price solver will be orders of magnitude faster than a leading commercial MILP solver.

7 Conferences and Seminars

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

March

Seminar Program in Scientific Computing, University of Uppsala, Sweden, March 26. D. LOGHIN, *Schur complement preconditioning for elliptic systems of partial differential equations*, contributed talk.

April

Colloquium of "Ecole Doctorale Informatique et Télécommunications": EDIT 2003, University Paul Sabatier, Toulouse, France, April 14-15. E. MARTIN, *Efficient solutions of industrial electromagnetism problems on parallel computers*, contributed talk.

35th National Congress of Numerical Analysis: CANUM 2003, University Montpellier 2, Montpellier, France, June 2-6. E. MARTIN, *Efficient solutions of industrial electromagnetism problems on parallel computers*, poster session.

May

Quatrième séminaire sur l'algorithmique numérique appliquée aux problèmes industriels, Calais, France, May 15-16. I. DUFF, *Solving large industrial problems in electromagnetics at CERFACS*, invited plenary speaker.

Quatrième séminaire sur l'algorithmique numérique appliquée aux problèmes industriels, Calais, France, May 15-16. S. GRATTON, *Iterative techniques in variational data assimilation*, contributed talk.

Quatrième séminaire sur l'algorithmique numérique appliquée aux problèmes industriels, Calais, France, May 15-16. M. VAN GIJZEN, *Relaxation strategies for nested Krylov methods*, contributed talk.

June

35th National Congress of Numerical Analysis: CANUM 2003, University Montpellier 2, Montpellier, France. June 2-6. E. MARTIN, *Efficient solutions of industrial electromagnetism problems on parallel computers*, poster session.

2003 SIAM Annual Meeting, Montreal, QC, Canada, June 16-20. S. PRALET *Adapting a parallel sparse direct solver to SMP architectures*, contributed talk.

July

Visiting Lecturer in the Suranaree University of Technology, Nakhon Ratchasima, Thailand. July 2-4. I. DUFF, *Solving Large Industrial Problems in Electromagnetics at CERFACS*, seminar.

ICIAM 2003, Sydney, Australia, July 7-11. I. DUFF, *Novel pivoting strategies for sparse indefinite matrices*, invited minisymposium speaker.

ICIAM 2003, Sydney, Australia, July 7-11. I. DUFF, *The HSL Library*, invited minisymposium speaker.

ICIAM 2003, Sydney, Australia, July 7-11. I. DUFF, *The use of direct methods as a preconditioner for the solution of augmented systems in optimization*, invited minisymposium speaker.

Minisymposium on New Approaches to preconditioning, ICIAM-2003, Sydney, July 7-11. L. GIRAUD, *Some recent investigations on parallel iterative solvers for dense linear systems in electromagnetic applications*, joint effort with G. Alléon, B. Carpentieri, I.S. Duff, J. Langou, E. Martin and G. Sylvand, invited talk.

Visiting Lecturer in the Centre for Mathematics and its Applications (CMA), School of Mathematical Sciences, ANU, Canberra, Australia, July 13-20. I. DUFF.

Mini-symposium speaker at the SIAM Conference on Applied Linear Algebra, Williamsburg, Virginia, USA, July 15-19. D. LOGHIN, *Analysis of preconditioners for saddle-point problems*, invited talk.

Conference on Computational Mathematics, Australian National University, Canberra, July 16-18. I. DUFF, *The symbiosis of direct and iterative methods for solving large sparse systems*, invited speaker.

Queensland University of Technology, Brisbane, Australia, July 28. I. DUFF, *Solving Large Industrial Problems in Electromagnetics at CERFACS*, seminar.

August

Workshop on Numerical Linear Algebra, University of British Columbia, Vancouver, Canada, August 6-9. I. DUFF, *The symbiosis of direct and iterative methods for solving large sparse systems*, invited speaker.

Workshop on Numerical Linear Algebra, University of British Columbia, Vancouver, Canada, August 6-9. I. DUFF, *Solving Large Industrial Problems in Electromagnetics at CERFACS*, invited speaker.

Euro-Par 2003, Klagenfurt, Austria, August 26-29. M. VAN GIJZEN, *Two Level Parallelism in a Stream-Function Model for Global Ocean Circulation*, contributed talk.

September

Bath-RAL Numerical Analysis Day, Rutherford Appleton Laboratory, Oxfordshire, England, September 26. I. DUFF, *The symbiosis of direct and iterative methods for solving large sparse systems*, invited speaker.

PPAM 2003, Fifth International Conference on Parallel Processing and Applied Mathematics, Czestochowa, Poland, September 7-10. B. CARPENTIERI, *An embedded iterative scheme in electromagnetism*, joint work with I.S. Duff, L. Giraud and G. Sylvand, contributed talk.

NLAA 2003 Numerical Linear Algebra and its Applications XXI International Workshop Monopoli, Bari, Italy, September 22-24. B. CARPENTIERI, *Two-grid spectral preconditioning for general linear systems*, joint work with L. Giraud and S. Gratton, contributed talk.

International Conference on Supercomputing in Nuclear Applications, Paris, September 22-24. L. GIRAUD, *Efficient parallel iterative solvers for the solution of large dense linear systems arising from the boundary element method in electromagnetism*, contributed talk.

October

International Conference on Preconditioning Techniques for Large Sparse Matrix Problems, Napa, California, USA, October 26-29. I. DUFF, program committee, chairman, and attendee.

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

2003 International conference on preconditioning techniques for large sparse matrix problems in scientific and industrial applications, 2003 Embassy Suites Napa Valley Napa, California, October 27-29. L. GIRAUD, *Some recent developments on iterative techniques for solving large industrial problems in electromagnetics*, invited talk.

NIST Seminar, Maryland, USA, October 31. L. GIRAUD, *Sparse iterative techniques for the solution of the 3D Maxwell equations in boundary element formulation*, invited talk.

December

Workshop on Solution Methods for Saddle-Point Problems in Santa Fe, New Mexico, USA, December 3-6. D. LOGHIN, *Schur complement preconditioning for elliptic systems of partial differential equations*, invited talk.

7.2 Conferences and seminars organized by the Parallel Algorithms Project

June

Sparse Days and Grid Computing at St. Girons, June 10-13.

Recent developments in iterative solvers, G. GOLUB (Stanford, USA).

The norm of the error in the conjugate gradient algorithm, G. MEURANT (CEA, France).

Parallel iterative and direct methods: a comparison, M. SOSONKINA (Duluth, USA).

Inexact Krylov subspace methods: theory and applications, V. SIMONCINI (Bologna, Italy).

Recent advances in inverse-based preconditioning techniques, M. BOLLHOEFER (Berlin, Germany).

- A parallel deflated Krylov solver for finite element problems*, K. VUIK (Delft, The Netherlands).
- Thesis defence: Solving large linear systems with multiple right-hand sides*, J. LANGOU (Cerfacs).
- External Memory Algorithms for a Sparse Direct Solver*, A. POTHEN (Old Dominion, USA).
- An efficient hybrid MPI/Thread implementation on a network of SMP nodes for the parallel sparse direct solver PaStix: ordering / scheduling / memory management / out-of-core issues, and application to preconditioning*, P. HENON, F. PELLEGRINI, P. RAMET AND J. ROMAN (Bordeaux, France).
- A column pre-ordering strategy for the unsymmetric-pattern multifrontal method*, T. DAVIS (Florida, USA).
- Some Memory Issues in the Multifrontal Method*, A. GUERMOUCHE (Lyon, France).
- Use of parallel SuperLU in large-scale scientific calculations*, S. LI (NERSC, USA).
- On direct and iterative solvers for semiconductor device simulation problems*, O. SCHENK (Basel, Switzerland).
- Model Reduction of Passive Systems through Interpolation of Spectral Zeros*, D. SORENSEN (Rice, USA).
- Multilevel preconditioners for solving eigenvalue problems occurring in the design of resonant cavities*, P. ARBENZ (Zurich, Switzerland).
- Preconditioning techniques based on a Parallel Hierarchical Interface Decomposition (PHIDAL)*, P. HENON AND Y. SAAD.
- Grid computing in Framework 6*, R. TIRLER (European Commission).
- The EUROGRID project*, C. AUDERLIK (University of Bergen, Norway).
- Grid computing at IBM*, J. P. PROST (IBM, France).
- Grid computing at SGI*, O. MULTON (SGI, France).
- High Performance Computing, Computational Grids, and Numerical Libraries*, J. DONGARRA (University of Tennessee, USA).
- Getting to know the Grid to use it better*, M. QUINSON (ENS Lyon, France).
- Programming the Grid with parallel software components*, C. PEREZ (INRIA/IRISA, Rennes, France).
- Grid-TLSE: A Web expertise site for sparse linear algebra*, P. Amestoy and M. Pantel (ENSEEIH-IRIT).
- Property G and Large Interior Eigenproblems*, Y. SUN, G. GOLUB AND M. SAUNDERS (Stanford, USA).
- Variational data assimilation for numerical weather forecasting*, N. NICHOLS (Reading, UK).

List of participants.

- G. ALEFELD (University of Karlsruhe, Germany).
G. ALLEON (EADS-CCR, France).
P. AMESTOY (ENSEEIH-IRIT, France).
C. ANDERLIK (University of Bergen, Norway).

P. ARBENZ (ETH Zurich, Switzerland).
M. ARIOLI (CLRC-Rutherford Appleton Laboratory RAL, UK).
M. BABOULIN (CERFACS, France).
C. BALSÀ (FEUP - Porto/ENSEEIH, France).
A. BJÖRCK (Linköping University, Sweden).
M. BOLLHOEFER (TU Berlin, Germany).
R. BOUCHOIRBAT (Université de Pau, France).
R. BRU (Univ. Politecnica de Valencia, Spain).
B. CARPENTIERI (CERFACS, France).
P. COQUENTIN (Enseeiht, France).
P.-H. CROS (CERFACS, France).
I. D'AST (CERFACS, France).
T. DAVIS (Univ. of Florida, Stanford Univ, and Lawrence Berkeley National Lab SCCM Program, USA).
M. DAYDÈ (ENSEEIH-IRIT, France).
D. DECLAS (CERFACS, France).
L. DELMAS (CERFACS, France).
J. DONGARRA (University of Tennessee, USA).
I. DUFF (CERFACS/RAL, France).
O. FOTI (LIMA, France).
J. GILBERT (University of California, USA).
L. GIRAUD (CERFACS, France).
G. GOLUB (Stanford University, USA).
E. GONDET (MERCATOR-OCEAN, France).
S. GRATTON (CERFACS, France).
A. GUERMOUCHE (LIP,ENS-Lyon, France).
P. GUILLAUME (INSA Toulouse, France).
R. GUIVARCH (IRIT-LIMA, France).
M. GUTKNECHT (ETH Zurich, Switzerland).
F. GUYOMAR'CH (France).
M. GUYON (EDF R&D, France).
P. HÉNON (INRIA Futurs - LaBRI, France).
A. HUARD (INSA Toulouse, France).
J.-Y. L'EXCELLENT (INRIA / LIP-ENS Lyon, France).
C. LACOURT (CERFACS, France).
J. LANGOU (CERFACS, France).
I. LENHARDT (University of Karlsruhe, Germany).
E. MARTIN (CERFACS, France).
K. MER-NKONGA (CEA CESTA, France).
G. MEURANT (CEA DCSA/ED, France).
S. MULLIGAN (CERFACS, France).
O. MULTON (SGI Espace Technology BatB, France).
E. NG (Lawrence Berkeley National Laboratory, USA).
N. K. NICHOLS (The University of Reading, UK).
H. OBERMAIER (University of Karlsruhe, Germany).
M. PANTEL (ENSEEIH IRIT/INPT projet TLSE, France).
P. PASCAL (LAAS-CNRS RST Group, France).
F. PELLEGRINI (INRIA Futurs - LaBRI, Université Bordeaux I, France).
C. PEREZ (IRISA/INRIA, France).
A. POTHEN (Old Dominion University, USA).
S. PRALET (CERFACS, France).
J.-P. PROST (IBM France, France).
C. PUGLISI (INP/ENSEEIH, France).
M. QUINSON (ENS-Lyon LIP, France).
P. RAMET (INRIA Futurs - LaBRI, France).
P. RICHARD (CNES, France).
S. RIYAVONG (CERFACS, France).

M. ROJAS (Wake Forest University, USA).
 J. ROMAN (INRIA Futurs - LaBRI, France).
 D. RUIZ (ENSEEIH-IRIT LIMA-IRIT, France).
 Y. SAAD (Univ. of Minnesota, USA).
 M. SAUNDERS (Stanford University, USA).
 O. SCHENK (University of Basel, Switzerland).
 J. SCOTT (RAL Atlas Centre, UK).
 X. SHERRY LI (Lawrence Berkeley National Laboratory, USA).
 J.-P. SILVAIN (CICT Université Paul Sabatier, France).
 V. SIMONCINI (Università di Bologna and IMATI-CNR, Italy).
 D. SORENSEN (Rice University, USA).
 M. SOSONKINA (University of Minnesota, USA).
 P. SPITERI (ENSEEIH, France).
 R. TIRLER (European Commission DG Information Society, Belgium).
 A. TOUHAMI (ENSEEIH-INPT LIMA-IRIT, France).
 V. TRUONG (LIMA, France).
 M. TŮMA (Academy of Sciences of the Czech Republic, Czech Republic).
 G. UTARD (INRIA Rhone Alpes LIP/ENS Lyon, France).
 J. VAN DEN ESHOF (Utrecht University, The Netherlands).
 M. VAN GIJZEN (CERFACS, France).
 T. VAN NOORDEN (Utrecht University, The Netherlands).
 C. VÖEMEL CERFACS, FRANCE).
 K. VUIK (DELFT UNIVERSITY OF TECHNOLOGY, THE NETHERLANDS).

7.3 Internal seminars organized within the Parallel Algorithms Project

March

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

January

Stopping criteria for iterations in finite element methods. January 23. D. LOGHIN.

February

Numerical methods for semiconductor device modelling. February 5. S. MULLIGAN.

Similitude simultanée des matrices carrées. February 7. A. EL GHAZI.

March

Contributions à la recherche en calcul scientifique haute performance pour les matrices creuses. March 20.
Ph.D Thesis defense. C.VÖMEL.

May

Two-dimensional semiconductor device simulation. May 7. S. RIYAVONG.

Filter techniques and the nonlinear feasibility problem. May 20. P. TOINT.

Contribution of the numerical linear algebra techniques for solving the monostatic radar cross section calculation, an electromagnetism problem where a large linear system with multiple right-hand sides is involved. May 27. J. LANGOU.

July

Using spectral information for accelerating the convergence of Gmres for large electromagnetic calculations. July 1. E. MARTIN.

August

Accurate conjugate gradient methods for families of shifted systems. August 6. G. SLEIJPEN.

September

Two-level parallelism in a stream-function model for global ocean circulation. September 11. M. VAN GIJZEN.

October

Hyper-sparsity in the revised simplex method and how to exploit it. October 9. J. HALL.

Inverse acoustic problems: sound source reconstruction. October 14. C. HANSEN.

Parallel distributed cholesky factorization for in-core large dense problems. October 15. M. BABOULIN.

November

LSTRS: Matlab software for large-scale trust-region subproblems and regularization. November 13. M. ROJAS.

Optimisation: méthodes sans dérivée. November 24. P. TOINT.

8 Publications

8.1 Journal Publications

- [PUB1] P. R. Amestoy, I. S. Duff, J.-Y. L'Excellent, and X. S. Li. Impact of the implementation of MPI point-to-point communications on the performance of two general sparse solvers. *Parallel Computing*, 29(7):833–847, 2003.
- [PUB2] P. R. Amestoy, I. S. Duff, S. Pralet, and C. Vömel. Adapting a parallel sparse direct solver to architectures with clusters of s mps. *Parallel Computing*, 29(11-12):1645–1668, 2003.
- [PUB3] B. Carpentieri, I. S. Duff, and L. Giraud. A class of spectral two-level preconditioners. *SIAM J. Scientific Computing*, 25(2):749–765, 2003.
- [PUB4] H. C. Elman, D. Loghin, and A. J. Wathen. Preconditioning techniques for newton's method for the incompressible navier–stokes equations. *BIT*, in press, 2003.
- [PUB5] L. Giraud and J. Langou. Robust selective Gram-Schmidt reorthogonalization. *SIAM J. Scientific Computing*, 25(2):417–441, 2003.
- [PUB6] L. Giraud, F. Guevara Vasquez, and R. S. Tuminaro. Grid transfer operators for highly variable coefficient problems in two-level non-overlapping domain decomposition methods. *Numerical Linear Algebra with Applications*, 10:467–484, 2003.
- [PUB7] N. I. M. Gould, D. Orban, and Ph. L. Toint. CUTeR, a constrained and unconstrained testing environment, revisited. *ACM Transactions on Mathematical Software*, vol. 29(4), 2003.
- [PUB8] D. Laurichesse, S. Gratton, F. Mercier, T. Tournier, and J.P. Berthias. Use of gnss-based pseudo-acceleration measurements and orbital constraints to initialize spaceborne receiver orbit solutions. *Navigation Journal*, 36:455–469, Summer 2003.
- [PUB9] D. Loghin and A. J. Wathen. Schur complement preconditioning for elliptic systems of partial differential equations. *Numerical Linear Algebra with Applications*, 10:423–443, 2003.
- [PUB10] S. Tissari and J. Rahola. Error analysis of a new Galerkin method to solve the forward problem in MEG and EEG using the boundary element method. *Computer Methods and Programs in Biomedicine*, 72:209–222, 2003.

8.2 Theses

- [THS1] J. Langou. *Iterative methods for solving linear systems with multiple right hand sides*. Ph.D. dissertation, INSA Toulouse, June 2003. TH/PA/03/24.
- [THS2] C. Vömel. *Contributions to research in high performance scientific computing for sparse matrices*. Ph.D. dissertation, INPT, March 2003. TH/PA/03/26.

8.3 Technical Reports

- [TRP1] G. Alléon, B. Carpentieri, I. S. Duff, L. Giraud, J. Langou, E. Martin, and G. Sylvand. Efficient parallel iterative solvers for the solution of large dense linear systems arising from the boundary element method in electromagnetism. Technical Report TR/PA/03/65, CERFACS, Toulouse, France, 2003. Preliminary version of the paper published electronically in the proceedings of the international conference on supercomputing in nuclear application, Paris, 2003.

- [TRP2] P. Amestoy, I. S. Duff, S. Pralet, and C. Vömel. Adapting a parallel sparse direct solver to SMP architectures. Technical Report TR/PA/03/05, CERFACS, Toulouse, France, 2003. Preliminary version of the article published in *Parallel Computing*, special issue on Parallel and Distributed Scientific and Engineering Computing, vol. 29, nber 11-12, pp 1645-1668, 2003.
- [TRP3] P. R. Amestoy, I. S. Duff, J. Y. L'Excellent, and X. S. Li. Impact of the implementation of MPI point-to-point communications on the performance of two general sparse solvers. Technical Report TR/PA/03/14, CERFACS, Toulouse, France, 2003. Various versions have appeared as technical reports RT/APO/01/4 from ENSEEIHT-IRIT, Toulouse, RR-4372 from INRIA, Lyon, and LBNL-48968 from Lawrence Berkeley National Laboratory, California. Preliminary version of the article published in *Parallel Computing*, vol. 29, nber 7, pp 833-847, 2003.
- [TRP4] M. Arioli, D. Loghin, and A. J. Wathen. Stopping criteria for iterations in finite element methods. Technical Report TR/PA/03/21, CERFACS, Toulouse, France, 2003.
- [TRP5] B. Carpentieri, I. S. Duff, L. Giraud, and G. Sylvand. Combining fast multipole techniques and an approximate inverse preconditioner for large parallel electromagnetics calculations. Technical Report TR/PA/03/77, CERFACS, Toulouse, France, 2003.
- [TRP6] F. Chaitin-Chatelin. The Arnoldi method in the light of Homotopic Deviation theory. Technical Report TR/PA/03/15, CERFACS, Toulouse, France, 2003.
- [TRP7] F. Chaitin-Chatelin. Computing beyond analyticity. Matrix algorithms in Inexact and Uncertain computing. Technical Report TR/PA/03/110, CERFACS, Toulouse, France, 2003.
- [TRP8] F. Chaitin-Chatelin. Elements of Hypercomputations on \mathbb{R} and \mathbb{Z}_2 with the Dickson-Albert inductive process. Technical Report TR/PA/03/34, CERFACS, Toulouse, France, 2003.
- [TRP9] F. Chaitin-Chatelin. On a recursive hierarchy for numbers algorithmically emerging from processing binary sequences. Technical Report TR/PA/03/08, CERFACS, Toulouse, France, 2003.
- [TRP10] F. Chaitin-Chatelin and M. B. van Gijzen. Homotopic deviation: an example in acoustics. Technical Report TR/PA/03/04, CERFACS, Toulouse, France, 2003. Submitted to LAAP.
- [TRP11] I. S. Duff, L. Giraud, J. Langou, and E. Martin. Using spectral low rank preconditioners for large electromagnetic calculations. Technical Report TR/PA/03/95, CERFACS, Toulouse, France, 2003.
- [TRP12] H. C. Elman, D. Loghin, and A. J. Wathen. Preconditioning techniques for Newton's method for the incompressible Navier–Stokes equations. Technical Report TR/PA/03/31, CERFACS, Toulouse, France, 2003. Preliminary version of the paper to appear in BIT.
- [TRP13] V. Frayssé, L. Giraud, S. Gratton, and J. Langou. A set of GMRES routines for real and complex arithmetics on high performance computers. Technical Report TR/PA/03/03, CERFACS, Toulouse, France, 2003.
- [TRP14] L. Giraud, S. Gratton, and J. Langou. A reorthogonalization procedure for modified Gram–Schmidt algorithm based on a rank- k update. Technical Report TR/PA/03/11, CERFACS, Toulouse, France, 2003. Preliminary version of the paper to appear in SIAM SIMAX.
- [TRP15] L. Giraud, J. Langou, and M. Rozložník. On the loss of orthogonality in the Gram-Schmidt orthogonalization process. Technical Report TR/PA/03/25, CERFACS, Toulouse, France, 2003. Preliminary version of the paper to appear in *Computer and Mathematics with Applications*.
- [TRP16] S. Riyavong. Experiments on parallel matrix-vector product. Working Notes WN/PA/03/127, CERFACS, Toulouse, France, 2003.
- [TRP17] S. Riyavong. Experiments on sparse matrix partitioning. Working Notes WN/PA/03/32, CERFACS, Toulouse, France, 2003.
- [TRP18] J. van den Eshof, G. L. G. Sleijpen, and M. B. van Gijzen. Relaxation strategies for nested Krylov methods. Technical Report TR/PA/03/27, CERFACS, Toulouse, France, 2003.
- [TRP19] M. B. van Gijzen. Two level parallelism in a stream-function model for global ocean circulation. Technical Report TR/PA/03/09, CERFACS, Toulouse, France, 2003. Preliminary version of the paper published in the proceedings of Euro-Par2003, *Lecture Notes in Computer Science* 2790, pp. 820-829, 2003.

8.4 Conference Proceedings

[CPR1] M. B. van Gijzen. Two level parallelism in a stream-function model for global ocean circulation. In H. Hellwagner, editor, *Euro-Par 2003 Parallel Processing*, pages 820–829, Berlin, 2003. Springer-Verlag.