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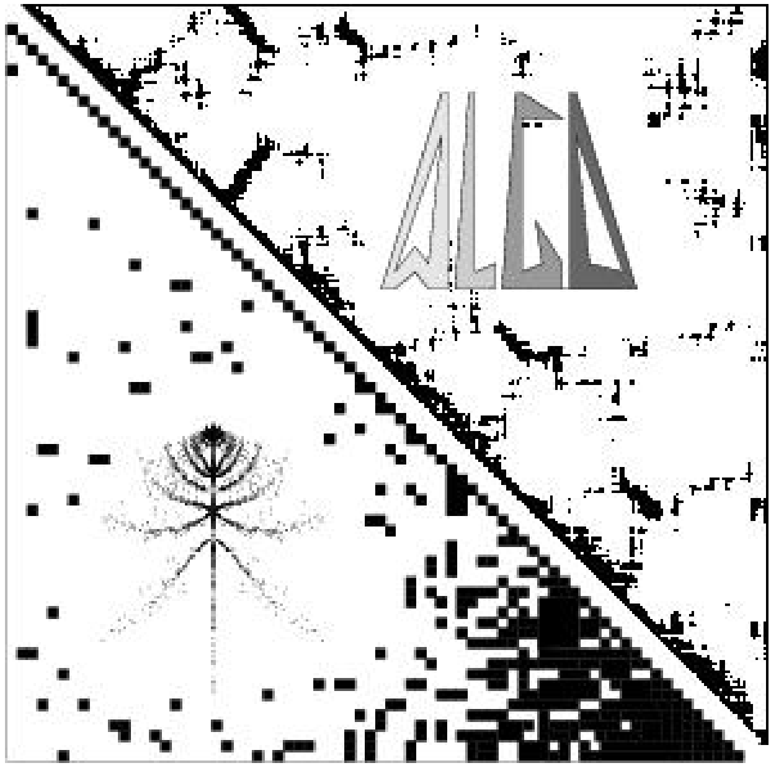

ACTIVITY REPORT of the PARALLEL ALGORITHMS PROJECT at CERFACS

JANUARY 2000 - DECEMBER 2000

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Contents

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.

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 committees such as the CCT of CNES. 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 have recorded more than 6000 hits per month on average. On our publication pages alone we have nearly 900 downloads a month and people have requested no fewer than 379 different reports.

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 code is now very robust and has been downloaded by over 50 researchers from the MUMPS website. Extensive comparisons, conducted with the support of funding from the France-Berkeley Fund have shown that the performance of MUMPS is on a par or better than any similar code from the United States. The MUMPS code has been used extensively within domain decomposition software both at CERFACS and in the DDM code at Parallab in Bergen. It has also been evaluated positively for use by Dassault. The MUMPS Project is also responsible for some secondary or spin-off research, an example being the work on incremental norm estimation which should prove to be very useful in the context of rank revealing factorizations.

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. This project was completed in December and the report on the standard will appear as a special issue of the journal "High Performance Computing Applications". We have been the developer for the Fortran 95 instantiation of the Sparse BLAS from within this project, and the resulting software is available on the CERFACS web and has been downloaded more than 50 times already.

Although iterative methods remove many of the bottlenecks of direct approaches, particularly regarding memory, it is now well established that they can only be used in the solution of really challenging problems if the system is preconditioned to create a new system more amenable to the iterative solver. During this last year we have continued our work on developing such preconditioners, including two-level DDM schemes for solving problems which have discontinuous coefficients. Work has continued on the use of the MUMPS direct solver as a preconditioner within a domain decomposition scheme and the resulting algorithm and code have been used with success in the solution of problems from drift diffusion in semiconductor device modelling in a joint collaboration with INRIA. On a more theoretical but very practical area, the loss of orthogonality when performing a QR factorization using modified Gram Schmidt has been extensively analysed. The GMRES and FGMRES codes that were discussed in last year's report are available through the CERFACS web and have attracted over 300 downloads, some from important establishments including partners of CERFACS. The capability of solving complex problems when the matrix is Hermitian has been added to this package during this reporting period. Our work on developing sparse approximate inverses to precondition a dense matrix in an electromagnetics application from one of our shareholders continues, and we have extended this work to allow for the incorporation of these techniques within a fast multipole code. A prototype is currently being used by EADS. Initial experiments using complex shifts are proving interesting.

The main area of interest for the Qualitative Computing Group concerns the reliability of numerical software in finite-precision arithmetic. One of the major areas studied has been that of inner-outer iteration, two principal and important applications being the use of Krylov solvers (inner iteration) within an eigensystem calculation (outer iteration), and the use of an iterative solver on the Schur complement in a domain decomposition context (outer iteration) where, at each iteration, a subproblem or preconditioner might require a system solution (inner iteration). The major result of this work has shown that, almost counter-intuitively, it is possible to relax the accuracy of the operator or inner iteration in a controlled way without affecting overall convergence. The Group has also collaborated closely with CNES in the context of the Jason project, principally studying the solution of integer least-squares problems. On a more esoteric level, algorithms and theory have been developed for the use of hypercomplex numbers. Other work includes more robust termination criteria for Arnoldi-based methods, the development of more robust eigensolvers using hybrid algorithms in a joint effort with INRIA, and work on the solution of Schrödinger equations and triple-deck boundary layer problems.

Although we have been unable to replace our senior scientist in the optimization area, this remains an important activity of the Team and has been adequately pursued by a resident postdoc and student along with past group members and visitors who were supported by the funds that would have otherwise supported the senior scientist. Current areas of research include major work on an approach for solving ill-posed problems where a regularized solution is obtained after the solution of a subsidiary eigenproblem. Recent work includes the development of efficient preconditioners for the eigenproblem and the use of the algorithm and software in medical tomography and image restoration applications. On the latter application, extensions which respect nonnegativity constraints are being developed. A major research kernel in optimization is the primal-dual trust-region interior point method. This has been extensively analysed and an approach defined that has componentwise fast asymptotic convergence. The work has been extended to the case of parametrized variants of Newton's method. An important requirement of the international community in the development and use of optimization techniques is the existence of a versatile testing environment and set of test examples. Work has been conducted at CERFACS into the expansion and reorganization of the well known and respected CUTE package to produce the forthcoming CUTEr (r for revisited) package. The work on the use of large scale optimization and the use of state-of-the-art techniques in meteorological data assimilation, in conjunction with our shareholders from Météo-France, the PALM and MERCATOR Team has continued, and should accelerate now that a new graduate student has been recruited.

The Parallel Algorithms Team is heavily involved in the Advanced Training aspects of CERFACS' mission. We ran an internal training course for new recruits to all Teams at CERFACS to give them a basic understanding of high performance computing and numerical libraries. This course was also open to the shareholders of CERFACS. Following a specific request of CNES through its CCT "calcul scientifique" we organized a three day training course entitled "Outils de programmation efficace et robuste pour le logiciel scientifique" targeted at CNES engineers. We are also involved in training through the "stagiaire" system and feel that this is both 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. Members of the Team have assisted in many lecture courses at other centres, including ENSICA, INPT, Météo, Toulouse 1 and UPS. We run a regular series of "internal seminars" that are primarily for Team members to learn about each other's work and are also a good forum for young researchers to hone their presentational skills. We run a series of seminars from external people who are visiting the Team that attract a wider audience and this has benefited greatly this year through an extensive visitor programme. Indeed, our list of visitors is a veritable who's who of numerical analysis, including many distinguished scientists from Europe and the United States. We have included a list of the visitors in the following subsection. Team members have participated in many international conferences at both an invited and contributed level, and we have welcomed many visitors to CERFACS for both short and long periods. During this past year, both Valérie Frayssé and Luc Giraud successfully defended their habilitation theses (HDR). Valérie summed up her many activities under the umbrella of the power of backward error analysis and Luc described with great clarity his many contributions to the iterative solution of linear equations. It was a bumper year for theses with no fewer than three other Team members successfully defending their PhD theses. These were Elisabeth Traviesas with a thesis on matrix spectra (and pseudo-spectra), Amina Bouras on the convergence of embedded Krylov solvers in eigensystem or linear system calculation and Ahmed Zaoui on his contributions to eigensolvers and hypercomplex computation.

The most significant meeting hosted by the Parallel Algorithm Team was the Workshop on inner-outer iterations organized at the request of three of our partners and held at CERFACS in September. Gene Golub gave the keynote address, and there were invited presentations from Andreas Griewank and Sven Hammarling. The program was completed by several contributions from CERFACS researchers and the shareholders representatives.

I am very pleased to report that, over the past year, we have continued to increase our involvement in joint research projects with shareholders and with other teams at CERFACS. We have successfully completed a major project on orbitography with CNES. We have two projects with EADS on preconditioning techniques in electromagnetics and a sponsored PhD on iterative solution techniques for multiple right-hand sides. We are involved in the training programme for the Mastere, organized by ENM. One of the two active collaborations with INRIA has been successfully finished by the defence of a PhD and the other on domain decomposition is still fruitful and ongoing. We assist the other Teams at CERFACS on a daily basis but sometimes collaborate on a more substantial level as for instance in the PALM project or the optimal use of our public domain linear solvers with EMC.

1.0.1 Visitors to Parallel Algorithm Team in 2000

In alphabetical order, our visitors in the year 2000 included:

Mario Ahues (St Etienne University), Filomena Dias d'Almeida (Porto University), Nerses Ananikyan (Armenia), Charles Audet (Rice University), Robert Beauwens (ULB, Brussels University), Jean-Claude Bergès (CNES), Mattheus Bollhöfer (Berlin), Tony Chan (UCLA), Edmond Chow (Lawrence Livermore National Laboratory), John Dennis (Rice University), Quang V. Dinh (Dassault Aviation), Jaqueline Fleckinger (Toulouse I), Michael Friedlander (Stanford University), Andreas Frommer (Wuppertal University), Gene Golub (Stanford University), Nick Gould (Rutherford Appleton Laboratory), Serge Gratton (CNES), Andreas Griewank (Dresden University), Andreas Grothey (Edinburgh University), Sven Hammarling (NAG), John Haws (Raleigh), Gary Howell (Florida Tech), Abderrazak Ilahi (Tunisia), Erricos Kontoghiorghes (Neuchatel University), Jacko Koster (Parallab, Bergen), Alain Largillier (St Etienne University), Rasmus Larsen (Stanford University), Sven Leyffer (Dundee University), Mardochee Magolu (ULB, Brussels University), Osni Marques (NERSC, Berkeley), Gérard Meurant (CEA), Jorge Nocedal (Northwestern University), Beresford Parlett (UC Berkeley), Bernard Philippe (IRISA, Rennes), Yousef Saad (Minneapolis

University), Annick Sartenaer (FUNDP, Namur), Masha Sosonkina (Minnesota University), Pierre Spitéri (ENSEEIHT), Daniel Szyld (Temple University), Patrick Le Tallec (Ecole polytechnique), Philippe Toint (FUNDP, Namur), Miroslav Tůma (Academy of Sciences of the Czech Republic), Jean-Louis Vaudescal (EDF), and Steve Wright (Argonne National Laboratory).

2 Dense and Sparse Matrix Computations

2.1 Rank-revealing and incremental norm estimation

I. S. Duff: CERFACS, *France*; **C. Vömel**: CERFACS, *France*.

There are many cases when it is interesting and important to detect the ill-conditioning of a square matrix A from the triangular factors arising in its LU or QR factorization. Applications include the calculation of forward error bounds based on the condition number of A, robust pivot selection criteria and rank-revealing factorizations. When *inverse* factors arise in a factorization, an efficient norm estimator is needed. In [2], we have introduced such a scheme applicable for both dense and sparse matrices.

Our approach is based on the idea of incremental condition estimation for dense matrices which was originally presented in [1]. The advantage of our scheme is its additional applicability to sparse matrices. We have studied its performance on standard dense and sparse test cases. The quality of our results is consistently good and demonstrates the general reliability of our scheme.

[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.

2.2 Development of kernels for sparse numerical linear algebra

I. S. Duff: CERFACS, *France*; **C. Vömel**: CERFACS, *France*.

We have developed basic kernels for sparse matrix operations. Our Fortran 95 implementation of the Basic Linear Algebra Subprograms for sparse matrices (Sparse BLAS) follows the Sparse BLAS standard defined by the Blas Technical Forum [1]. 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. M. Youan, a summer student at CERFACS, participated in the coding. Our work is documented in [2, 1].

[1] I. S. Duff and C. Vömel. Level 2 and Level 3 Basic Linear Algebra Subprograms for Sparse Matrices: A Fortran 95 instantiation. Technical Report TR/PA/00/18, CERFACS, Toulouse, France, 2000.

[2] I. S. Duff, C. Vömel, and M. Youan. Implementing the Sparse BLAS in Fortran 95. Technical Report TR/PA/00/82, CERFACS, Toulouse, France, 2000.

2.3 MUMPS - a MUltifrontal Massively Parallel Solver

P. R. Amestoy: ENSEEIHT, *France*; **I. S. Duff**: CERFACS, *France*; **J.-Y. L'Excellent**: *NAG, UK*; **J. Koster**: *Parallab, Norway.*

The software MUMPS was originally developed in the context of the EU LTR PARASOL Project, which project ended in the middle of 1999. However, since then and during the course of this

[1] `http://www.netlib.org/blas/blast-forum/blast-forum.html`

reporting year, we have continued to develop and enhance this package, disseminate it to a wide number of researchers, and use it in other applications at CERFACS and elsewhere.

Perhaps the most important development is that the code has been made far more robust, as witnessed by the few complaints from people who have downloaded it. We continue to receive comments and requests to the generic email address `mumps@cerfacs.fr` and have made the code available through the web page `www.enseeiht.fr/apo/MUMPS`. To date, the code has been downloaded by about fifty people.

During this reporting period we prepared a major report on the algorithm and software and have recently had it accepted by the journal SIAM Journal of Matrix Analysis and Applications [2]. The work was presented at the PARA 2000 meeting at Bergen in June [1] and in a number of seminars.

Koster is now working at Parallab in Bergen who were one of the other PARASOL partners. As a result, the MUMPS code has been further incorporated within the domain decomposition solvers at Parallab. A later article in this report (see §3.5) discusses the use of MUMPS within domain decomposition work at CERFACS.

[1] P. R. Amestoy, I. S. Duff, J.-Y. L'Excellent, and J. Koster. `MUMPS`: a general purpose distributed memory sparse solver. In A. H. Gebremedhin, F. Manne, R. Moe, and T. Sørevik, editors, *Proceedings of PARA2000, the Fifth International Workshop on Applied Parallel Computing, Bergen, June 18-21*, pages 122–131. Springer-Verlag, 2000. Lecture Notes in Computer Science, 1947.

[2] 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.

2.4 Analysis and comparison of distributed memory sparse solvers

P. R. Amestoy: ENSEEIHT, *France*; **I. S. Duff**: CERFACS, *France*; **J.-Y. L'Excellent**: *NAG, UK*; **X. Li**: *Lawrence Berkeley National Laboratory, USA.*

We were awarded a grant from the France Berkeley fund for teams at ENSEEIHT-IRIT and CERFACS to collaborate with NERSC at Lawrence Berkeley National Laboratory on distributed sparse solvers. This grant started in January 1999 and was extended until May 2000, enabling Duff to visit Berkeley twice for discussions with Li and Amestoy (who was on sabbatical leave for the year).

The main result was an in depth analysis comparing the merits of a supernodal solver (SuperLU) [4] with MUMPS (see §2.3). This showed broadly that MUMPS generally outperformed SuperLU although the latter showed somewhat better scalability and was competitive on a large number of processors. Many ideas for improvements to both codes were generated during this investigation and both will be enhanced as a result.

The main report to the France-Berkeley Fund [2] was accepted and a shorter version has been submitted to the ACM Transactions on Mathematical Software [1]. The work will be presented at the SIAM Parallel Processing Conference in March 2001 [3].

[1] P. R. Amestoy, I. S. Duff, J.-Y. L'Excellent, and X. S. Li. Analysis and comparison of two general sparse solvers for distributed memory computers. Technical Report TR/PA/00/90, CERFACS, Toulouse, France, December 2000. Submitted to *ACM Trans. Math. Softw.*

[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, 2000.

[3] P. R. Amestoy, I. S. Duff, J.-Y. L'Excellent, and X. S. Li. Performance and tuning of two distributed memory sparse solvers. Technical Report TR/PA/00/91, CERFACS, Toulouse, France, December 2000. Accepted for presentation at the Tenth SIAM Conference on Parallel Processing for Scientific Computing that will be held in Norfolk, Virginia from March 12th-14th, 2001.

[4] J. W. Demmel, J. R. Gilbert, and X. S. Li. An asynchronous parallel supernodal algorithm for sparse Gaussian elimination. *SIAM J. Matrix Analysis and Applications*, 20(4):915–952, 1999.

2.5 Study of the effect of matrix orderings on MUMPS and a code from Argonne National Laboratory

I. S. Duff: CERFACS*, France*; **S. Leblond**: CERFACS*, France*; **H. Tufo**: *Argonne National Laboratory, USA.*

In this work, two different solvers for the direct solution of sparse equations on multiprocessor machines were examined. This investigation was conducted by a stagiaire Simon Leblond [1], primarily under the guidance of Duff.

The first part of the investigation deals with the MUMPS multifrontal method for an LU factorization computation. The phases of this approach were described and results on a few large tests made on the supercomputer COMPAQ IXIA were analysed. The main study concerned the effect of the ordering algorithm on the analysis and the performance of the code when an ordering was input by the user. Some suggestions for future improvements to MUMPS are presented.

The second part concerned an approach using an X^TX factorization developed by Tufo and used in a massively parallel environment to obtain factors of the inverse of a large sparse matrix [2]. The findings showed that the current version of the code was rather slow in the factorization phase but very quick for the backsolves. This had been the design intention of Tufo who, partly as a result of this study, is tuning the factorization part of his algorithm.

[1] S. Leblond. Two direct methods for large sparse problems: Multifrontal massively parallel solver (MUMPS) and fast parallel direct solver for coarse grid problems (H. TUFO). Technical Report WN/PA/00/105, CERFACS, 2000.

[2] H. M. Tufo and P. F. Fischer. Fast parallel direct solvers for coarse grid problems. *J. Parallel and Distributed Computing*, 61(2):151–177, 2001.

3 Iterative Methods and Preconditioning

3.1 Loss of orthogonality in the modified Gram-Schmidt algorithm

L. Giraud: CERFACS, *France*; **S. Gratton**: *CNES, France*; **J. Langou**: CERFACS, *France*.

We consider the Modified Gram-Schmidt orthogonalization applied to a matrix $\Gamma \in \mathbb{R}^{m \times n}$ with rank $n \leq m$ and singular values $\sigma_1 \geq \ldots \geq \sigma_n > 0$. This gives a QR factorization : $\Gamma = VR$ where $R \in \mathbb{R}^{n \times n}$ is triangular and $V \in \mathbb{R}^{m \times n}$ has orthonormal columns in exact arithmetic. We study this algorithm in finite-precision computation when $\sigma_{n-i+1}/\sigma_1 \sim \mathbf{u}$, $i = 1, \ldots, k$, $\mathbf{u}$ being the machine precision. This subject has already been considered by Björck in 1963 [1], then continued by Björck and Paige in 1992 [2]. They give useful bounds in term of norms. We extend their results to provide bounds on singular values and our results can be viewed in term of numerical rank. In our case,

$$\text{Rank}(\Gamma) = n - k.$$

We show that

$$\text{Rank}(I - V^T V) = k$$

and

$$\exists E \text{ so that } \begin{cases} \text{Rank}(E) = k \\ Q = V - E, \quad Q^T Q = I, \quad \Gamma = QR. \end{cases}$$

At the same time, we have developed an algorithm in exact arithmetic to study the loss of orthogonality in V. This model gives us good results. Both improvements give new perspectives in reorthogonalization issues and permit a better understanding of algorithms based on Modified Gram-Schmidt such as in the solution of Least Squares Problems or the Arnoldi algorithm.

[1] A. Björck. Solving linear least squares problems using Gram-Schmidt orthogonalization. *BIT*, 7:1–21, 1967.

[2] A. Björck and C. Paige. Loss and recapture of orthogonality in the modified Gram-Schmidt Algorithm. *SIAM J. Matrix Analysis and Applications*, 13(1):176–190, January 1992.

3.2 Grid transfer operators for highly variable coefficient problems in two-level non-overlapping domain decomposition methods

L. Giraud: CERFACS, *France*; **F. Guevara Vasquez**: CERFACS, *France*; **R. S. Tuminaro**: *Sandia National Laboratories, USA*.

In the framework of a joint research project with R. S. Tuminaro from Sandia National Laboratory, Livermore, we propose a robust interpolation scheme for non-overlapping two-level domain decomposition methods applied to two-dimensional elliptic problems with discontinuous coefficients. This interpolation is used to design a preconditioner closely related to the BPS scheme proposed in [1]. Through numerical experiments, we show on structured and unstructured finite-element problems that the new preconditioning scheme reduces to the BPS method on smooth problems but outperforms it on problems with discontinuous coefficients. In particular it maintains good scalable convergence behaviour even when the jumps in the coefficients are not aligned with subdomain interfaces. Results related to this work are in particular reported in [2, 3]

[1] J. H. Bramble, J. E. Pasciak, and A. H. Schatz. The construction of preconditioners for elliptic problems by substructuring I. *Math. Comp.*, 47(175):103–134, 1986.

[2] 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. Tech. Rep. TR/PA/01/03, CERFACS, Toulouse, France, 1995. submitted.

[3] F. Guevara Vasquez. Internship report on domain decomposition methods for the solution of partial differential equations. Technical Report TR/PA/00/98, CERFACS, Toulouse, France, 2000.

3.3 A real/complex conjugate gradient package for sequential and parallel computation

V. Frayssé: CERFACS*, France*; **L. Giraud**: CERFACS*, France.*

To complete the GMRES package developed in 1997 [2] (downloaded more than 280 times so far), and the Flexible-GMRES package developed in 1998 [3] (downloaded more than 61 times so far), a set of conjugate gradients solvers for Hermitian linear systems has been developed for both real and complex, single and double precision arithmetic suitable for serial, shared memory and distributed memory computers. For the sake of simplicity, flexibility and efficiency, the conjugate gradient solvers have been implemented in Fortran 77 using the reverse communication mechanism for the matrix-vector product, the preconditioning and the dot product computations. Finally the implemented stopping criterion is based on a normwise backward error.

The source codes and the user's guide [1] can be accessed from the CERFACS Web server at the following URL address:

`http://www.cerfacs.fr/algor/`

This public domain software has received much interest. Amongst the downloaders, we can cite Bell-Lab, CRS4, EDF, INRIA and ONERA.

In some cases, we have provided the downloaders with some support upon request, and this has allowed us to improve the robustness of the code and the clarity of the User's Guide.

[1] V. Frayssé and L. Giraud. A set of conjugate gradient routines for real and complex arithmetics. Technical Report TR/PA/00/47, CERFACS, Toulouse, France, 2000.

[2] V. Frayssé, L. Giraud, and S. Gratton. A set of GMRES routines for real and complex arithmetics. Technical Report TR/PA/97/49, CERFACS, Toulouse, France, 1997.

[3] V. Frayssé, L. Giraud, and S. Gratton. A set of Flexible-GMRES routines for real and complex arithmetics. Technical Report TR/PA/98/20, CERFACS, Toulouse, France, 1998.

3.4 Preconditioning design in electromagnetism

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

In recent years, there has been a significant amount of work on the simulation of electromagnetic wave propagation phenomena, addressing various topics ranging from radar cross section to electromagnetic compatibility, to absorbing materials, and antenna design. To address these problems the Maxwell equations are often solved in the frequency domain leading to singular integral equations of the first kind. The discretization by the boundary element method (BEM) results in linear systems with dense complex matrices which are very challenging to solve. In this project we propose preconditioning strategies for the iterative solution of these systems. In a first study [1] we compare different preconditioners of both implicit and explicit form in connection with Krylov methods. We emphasize in particular sparse approximate inverse techniques based on Frobenius norm minimization that use a static nonzero pattern selection. The novelty of our approach comes from using a different nonzero pattern selection for the original matrix from that for the preconditioner and from exploiting geometric or topological information from the underlying meshes instead of using methods based on the magnitude of the entries. An extract from this work has been accepted for publication in the Proceedings of the *Second Conference on Numerical Analysis and Applications* (Rousse, Bulgaria). The results of our numerical experiments suggest that the new strategies are viable approaches for the solution of large-scale electromagnetic problems using preconditioned Krylov methods. In particular, our strategies are applicable when fast multipole techniques are used for the matrix-vector product on parallel distributed memory computers. A paper [2] related to this research has been accepted for publication. We are currently testing on large problems the numerical scalability of our preconditioner in collaboration with AEDS, implemented in its FMM code. In a second project [3], we consider implicit preconditioners based on incomplete factorization algorithms. Imaginary diagonal perturbations are incorporated, which significantly improves the performance. This project is still ongoing.

[1] B. Carpentieri, I. S. Duff, and L. Giraud. Robust preconditioning of dense problems from electromagnetics. In L. Vulkov, J. Waśniewski, and P. Yalamov, editors, *Numerical Analysis and Its Applications. Lecture Notes in Computer Science 1988*, pages 170–178. Springer-Verlag, 2000.

[2] B. Carpentieri, I. S. Duff, and L. Giraud. Sparse pattern selection strategies for robust frobenius-norm minimization preconditioners in electromagnetism. *Numerical Linear Algebra with Applications*, 7(7-8):667–685, 2000.

[3] B. Carpentieri, I. S. Duff, L. Giraud, and M. Magolu Monga Made. Implicit and explicit preconditionings for dense linear systems arising in electromagnectics scattering problems. Technical Report in preparation, CERFACS, Toulouse, France, 2001.

3.5 Domain decomposition methods in semiconductor device modeling

L. Giraud: CERFACS, *France*; **J. Koster**: *Parallab, Norway*; **J.-C. Rioual**: CERFACS, *France.*

In the framework of a joint research project between INRIA (A. Marrocco), Parallab (J. Koster) and CERFACS (L. Giraud, J. C. Rioual) we are developping a parallel domain decomposition code for the solution of the drift diffusion equation involved in semiconductor device modelling. A nonlinear time dependent problem has to be solved where each nonlinear iteration requires the solution of a linear mixed finite-element problem resulting in a large sparse linear system.

In order to solve these linear systems in a parallel distributed memory environment using message passing we investigate direct and iterative substructuring techniques. These techniques imply the computation of the local Schur complement matrices associated with each subdomain. If we use classical sparse direct solver, the computation of the local Schur complement matrices is usually too time expensive. We used some functionalities of the multifrontal parallel solver MUMPS [1] to compute them efficiently. Having an explicit distributed formulation of the Schur complement we can implement substructuring methods, direct or iterative. Direct substructuring is efficient and numerically stable. Iterative substructuring requires a good preconditioner for the Schur complement system. In collaboration with Parallab from Bergen University, we have tested Balanced a Neumann-Neumann preconditioner [2, 5] and compared it with another two-level preconditioner designed at CERFACS [3, 4]. We also investigate scaling techniques on the Schur complement to improve the numerical stability of the method.

[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. E. Bjørstad, J. Koster, and P. Krzyżanowski. Domain decomposition solvers for large scale industrial finite element problems. In *PARA2000 Workshop on Applied Parallel Computing*. Lecture Notes in Computer Science, Springer-Verlag, 2000. To appear.

[3] L. M. Carvalho, L. Giraud, and G. Meurant. Local preconditioners for two-level non-overlapping domain decomposition methods. Tech. Rep. TR/PA/99/38, CERFACS, Toulouse, France, 1999. Preliminary version of the article published in Numerical Linear Algebra with Applications, vol. 8, nber 4, pp 207-227.

[4] L. M. Carvalho, L. Giraud, and P. Le Tallec. Algebraic two-level preconditioners for the Schur complement method. Tech. Rep. TR/PA/98/18, CERFACS, France, 1998. Preliminary version of the paper published in SIAM SISC.

[5] J. Mandel. Balancing domain decomposition. *Comm. Numer. Meth. Engrg.*, 9:233–241, 1993.

4 Qualitative Computing

Group members: Françoise Chaitin-Chatelin, Amina Bouras, Sargis Dallakyan, Valérie Frayssé, Tadas Meškauskas, Laurent Plantié, Elisabeth Traviesas and Ahmed Zaoui.

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

This year, a particular focus was on embedded iterative solvers. A Ph.D thesis was defended on this topic (A. Bouras, September 2000). This problem was also addressed in the "habilitation à diriger des recherches" of V. Frayssé devoted to the more general subject of backward error analysis and defended in September 2000. She is now on sabbatical leave in Boston, USA, since October 2000. A workshop on this topic (`http://www.cerfacs.fr/algor/iter2000.html`) was organised at CERFACS, September 11-12, 2000, with the support of SMAI, following a request of our shareholders EADS, EDF and CNES. This brought together several well known researchers in this subject. Two other Ph.D theses were defended successfully this year (E. Traviesas in May and A. Zaoui in December). The JASON contract (S. Dallakyan) also came to end in August 2000 with significant results.

We now discuss some points that have been particularly investigated during the year 2000.

4.1 Embedded iterative solvers

Embedded solvers with iterative methods are more and more used in scientific computing. The problem of the control of the inner accuracy was an important research direction of the group. We have started to explore this problem in the light of backward error analysis, our favourite approach, whose potentialities are described in the manuscript of V. Frayssé for her "habilitation à diriger des recherches" [6] defended in September 2000. This problem is also the core of the Ph.D thesis of A. Bouras [1]. She also presented her thesis results at CANUM 2000. Part of this work was supported by a contract with CNES [2].

Additionally, following the request of our shareholders EADS, EDF and CNES, two industrial days were organised at CERFACS on the topic of inner-outer iterations, on September 11-12, 2000, with the support of SMAI. Two presentations on the work at CERFACS were given by V. Frayssé and F. Chaitin-Chatelin.

The problem we addressed can be stated: *what is the best strategy for stopping the inner iterations to ensure the convergence of the outer iterations while minimising the global computational cost ?* In the late nineties, it was emphasised that the behaviour of embedded solvers involving a Krylov outer process is very different from that of inexact Newton-like methods. Why do Krylov methods behave so differently ? How can we take advantage of their robustness ?

In order to better understand the behaviour of outer Krylov processes, we first studied the Krylov method GMRES with inexact matrix-vector products. By perturbing each matrix-vector product, we are able to control the accuracy of the inner process which consists here in the computation of a new vector in the Krylov basis. We have shown that an interesting and efficient strategy consists in

linking the accuracy of the matrix-vector product to the reciprocal of the outer residual. Therefore, the matrix-vector products become less and less accurate as the outer convergence proceeds. This approach is called the *relaxation strategy.* Its efficiency is supported by a wide range of numerical results, reported in [3].
The robustness of Krylov methods to perturbations of the Krylov basis is a remarkable fact which has many important implications. We have started to explore two applications that we now briefly review.

4.1.1 Inner-outer iterations in Krylov methods

We first applied the *relaxation strategy* to the computation of eigenvalues with shift and invert. In this case, the inner process consists in the solution of a linear system. This work is reported in [4]. We propose two relaxation strategies for the control of the accuracy of the inner loop. Indeed, two backward errors can be considered: the one associated with the computed eigenvalue $\hat{\lambda}$ of A and the other associated with the computed eigenvalue $\hat{\mu}$ of $B = A^{-1}$. We cannot yet propose a definite choice between both viewpoints and this important question remains open for future work [1].

4.1.2 Domain decomposition

Domain decomposition is used to solve discretized partial differential equations and consists in solving a condensed system whose matrix, the Schur complement, involves the local matrices associated with the subdomains. The Schur complement is positive definite when the matrix associated with the whole domain is positive definite. Then, the condensed system can be solved using the conjugate gradient method which is of Krylov type. However, inverse matrices appear in the Schur complement. Then, we have to solve linear systems at each step of the conjugate gradient method. The solution of these systems forms the inner loop and we can apply the *relaxation strategy* exposed above. This work is described in [5]. The numerical experiments show that a significant number of local matrix-vector products can be saved. This work was presented at the 13th International Conference on “Domain Decomposition Methods”, Lyon, October 2000.

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[1] A. Bouras. *Contrôle de convergence des solveurs emboités pour le calcul de valeurs propres avec inversion.* Ph.D. dissertation, Université Toulouse I, TH/PA/00/77, CERFACS, Septembre 2000.

[2] A. Bouras, F. Chaitin-Chatelin, and V. Frayssé. Solveurs itératifs imbriqués. Contract Report FR/PA/00/19, CERFACS, Toulouse, France, 2000.

[3] A. Bouras and V. Frayssé. A relaxation strategy for inexact matrix-vector products for Krylov methods. Technical Report TR/PA/00/15, CERFACS, Toulouse, France, 2000. Submitted to SIAM Journal in Matrix Analysis and Applications.

[4] A. Bouras and V. Frayssé. A relaxation strategy for the Arnoldi method in eigenproblems. Technical Report TR/PA/00/16, CERFACS, Toulouse, France, 2000.

[5] A. Bouras, V. Frayssé, and L. Giraud. A relaxation strategy for inner-outer linear solvers in domain decomposition methods. Technical Report TR/PA/00/17, CERFACS, Toulouse, France, 2000.

[6] V. Frayssé. *The power of backward error analysis.* Habilitation à Diriger des Recherches, Institut National Polytechnique de Toulouse, September 2000. TH/PA/00/65, CERFACS.

4.2 Arnoldi process and happy breakdown

We studied the Arnoldi method in finite precision with three orthogonalization processes. Knowing in advance the theoretical step k_0 of the happy breakdown, we studied the behaviour of each process at and after k_0 [3]. These experiments show the difficulty of detecting theoretical happy breakdown in finite precision ($\tilde{h}_{k+1,k} \neq 0$). A heuristic stopping criterion is proposed and all experiments have been compared with the results given by the software PRECISE. This work together with results

on homotopic pseudospectra is the core of the Ph.D thesis of E. Traviesas [4]. The main part was presented at the "Second Conference on Numerical Analysis and Applications", Rousse, Bulgaria, June 11-15, 2000, in the framework of the invitation of Pr. Chaitin-Chatelin [3]. Another presentation of this work was given at CANUM 2000 by E. Traviesas. She also presented the aspect concerning the homotopic perturbations at SEA 2000, Toulouse. We are now studying the theoretical condition numbers of $h_{k+1,k}$ and v_k associated with a homotopic perturbation of the initial vector v_1 [2]. This is joint work in progress with S. Gratton from CNES.
The software PRECISE has also been updated in order to be compatible with MATLAB 6 and was presented at the 16th IMACS World Congress 2000, Lausanne, Switzerland, August 21-25, 2000 [1].

[1] F. Chaitin-Chatelin and E. Traviesas. PRECISE, a toolbox for assessing the quality of numerical methods and software. Technical Report TR/PA/00/12, August 21-25,2000. to appear in the Proceedings of the 16th IMACS World Congress, Lausanne, Switzerland.

[2] F. Chaitin-Chatelin, E. Traviesas, and S. Gratton. Sensitivity from the initial vector for Krylov based methods, 2001. Work in progress.

[3] F. Chaitin-Chatelin, E. Traviesas, and L. Plantié. Understanding Krylov methods in finite precision, 2000. Also in Proceedings of the Second Conference on Numerical Analysis and Applications, Rousse, Bulgaria, Springer, pp. 187–197.

[4] E. Traviesas. *Sur le déploiement du champ spectral d'une matrice*. Ph.D. dissertation, Université Toulouse I, TH/PA/00/30, CERFACS, May 2000.

4.3 Eigenvalue computations - Collaboration with INRIA

This research concerns the study and the implementation of the software ISABeL: Itérations Simultanées et Arnoldi BLoc. The problem consists in computing the r closest eigenvalues to a given complex value. We use the projection methods of Krylov (Arnoldi) and of subspace iteration. The Arnoldi method is fast but might not yield all the desired eigenvalues. On the other hand, subspace iteration is reliable but slow. The software ISABeL couples both methods and combines their advantages. In this software, the Arnoldi method has a role of a "predictor". Moreover, we use a safety principle (computation of more than r eigenvalues) which enables us to control the separation condition in the subspace iteration method.
This work forms the first part of the Ph.D thesis of A. Zaoui [2], which ends a 3 year collaboration between CERFACS and INRIA: October 1997 - October 2000. It was also presented at the 16th IMACS World Congress 2000 [1].

[1] F. Chaitin-Chatelin and E. Traviesas. PRECISE, a toolbox for assessing the quality of numerical methods and software. Technical Report TR/PA/00/12, August 21-25,2000. to appear in the Proceedings of the 16th IMACS World Congress, Lausanne, Switzerland.

[2] A. N. Zaoui. *Deux Contributions au Calcul Scientifique I-Sur la convergence de la méthode des Itérations Simultanées couplée à l'algorithme d'Arnoldi itératif II-Autour du Calcul Hypercomplexe.* Ph.D. dissertation, Université Toulouse I, TH/PA/00/78, CERFACS and INRIA-IRISA, December 2000.

4.4 Jason contract with CNES

An overview of carrier phase differential GPS has been conducted. The main obstacles for using this technique to achieve centimetre-levels of accuracy are the difficulties related to correct integer ambiguity estimation. The LAMBDA method provides integer least-squares estimates for ambiguities which provides the best unbiased estimates. This method was the main subject of our investigations. Apart from a minor bug (noninteger result) which was fixed, the algorithm for the Z-transformation has been improved.

However, working with the test cases provided by CNES we have found that the LAMBDA method is unable to find correct integer ambiguities in a reasonable time. To overcome this obstacle we modified the search algorithm. Our modified search algorithm allows an *exponential speed-up* which is a considerable achievement. We believe that our modified search algorithm will be used for static/kinematic applications and will allow one to process the data from regional networks of GPS stations as well as the data from Low Earth Orbiting satellites for orbitographic purposes.
This ends the 2 year contract with CNES on which S. Dallakyan worked. He found a postdoc position at ACMS in Tucson, USA, in August 2000.

4.5 Hypercomplex algebras

We carry on our work at different levels. A part of our study focused on the principle of recursive construction of the hypercomplex algebras [2]. This little known construction enables us to recover $\mathbb{C}$ and the quaternion and octonion algebras from $\mathbb{R}$ but can be continued indefinitively yielding algebras of dimension 2^k. It provides more synthetic formulae than the classical ones and highlights the essential role of the geometrical notion of conjugacy. We also applied this recursive construction principle to the binary algebras, the initial algebra being then $B_0 = \{0, 1\}$.
In connection with this first part, we explored the quadratic iteration $x \rightarrow rx(1-x)$ over the quaternions and octonions in finite precision. This work was presented by T. Meškauskas and F. Chaitin-Chatelin at the 3rd World Congress of Nonlinear Analysts (WCNA-2000), Catania, Italy, July 19–26, 2000 [1]. This also forms the second part of the Ph.D thesis of A. Zaoui [4, 3]. He presented these results at CANUM 2000.

[1] F. Chaitin-Chatelin and T. Meškauskas. Computation with hypercomplex numbers. In *Proceedings of WCNA 2000, Catania*, pages ppp–qqq. Journal of Nonlinear Analysis, Elsevier Science, 2001.

[2] F. Chaitin-Chatelin, T. Meškauskas, and A. N. Zaoui. About real and binary algebras: the interplay between geometry and algebra. Technical Report TR/PA/00/74, CERFACS, Toulouse, France, 2000.

[3] F. Chaitin-Chatelin, T. Meškauskas, and A. N. Zaoui. Computation with hypercomplex numbers. Technical Report TR/PA/00/69, CERFACS, Toulouse, France, 2000.

[4] A. N. Zaoui. *Deux Contributions au Calcul Scientifique I-Sur la convergence de la méthode des Itérations Simultanées couplée à l'algorithme d'Arnoldi itératif II-Autour du Calcul Hypercomplexe.* Ph.D. dissertation, Université Toulouse I, TH/PA/00/78, CERFACS and INRIA-IRISA, December 2000.

4.6 Other work

4.6.1 Analysis of the boundary layer problem of triple deck type

We studied the canonical problem of the boundary layers of triple deck type. This problem, introduced in 1969, is close to the classical Prandtl problem but the pressure is unknown. The physical data is the asymptote of the longitudinal velocity, which is a straight line of nonzero slope in these models, and the pressure cannot be deduced from it directly. In [2], we analyse the associated Von Mises problem; we prove the existence of a solution and study the asymptotic behaviours. We use an original method based on a semi-discrete scheme. We also present a non-uniqueness result observed in numerical simulations. Details are given in [3, 4].

4.6.2 Numerical analysis of Schrödinger problems

Numerical analysis of two different initial boundary-value problems for a derivative nonlinear Schrödinger equation was presented in [1, 6]. The boundary conditions were Dirichlet or generalized periodic ones. A two-step algorithm was proposed for the numerical solution of this problem. The method consists of Bäcklund type transformations and difference schemes. The convergence and stability in C and H^1 norms of Crank–Nicholson finite difference scheme for the transformed problem is proved. There are no restrictions between space and time grid steps. For the derivative nonlinear Schrödinger equation, the proposed numerical algorithm converges and is stable in the C^1 norm.

4.6.3 Electrocardiogram processing

A method, based on $1/f$ noise analysis, which measures slopes of spectral functions derived from electrocardiogram (ECG) has been proposed [5]. Statistical tests show that spectral slopes are cardiac indicators, separating *normal* (NRM) subjects from these suffering *idiopathic dilated cardiomyopathy* (IDC).

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[1] F. Ivanauskas and T. Meškauskas. On the numerical algorithms for derivative nonlinear Schrödinger equation. In M. Sapagovas R. Čiegis, A. Samarskii, editor, *Finite difference schemes: theory and applications*, pages 89–98, Vilnius, Lithuania, 2000.

[2] L. Plantié. The boundary layer problem of triple deck type. Technical Report TR/PA/00/61, CERFACS, Toulouse, France, 2000. Also in Proceedings of the Second Conference on Numerical Analysis and Applications, Rousse, Bulgaria, Springer Verlag, pp 675–683.

[3] L. Plantié. A semi-discrete problem for the boundary layer of triple deck type (part 1). Technical Report TR/PA/00/45, CERFACS, Toulouse, France, 2000.

[4] L. Plantié. A semi-discrete problem for the boundary layer of triple deck type (part 2). Technical Report TR/PA/00/46, CERFACS, Toulouse, France, 2000.

[5] T. Meškauskas, P. Caminal, and A. Bayes de Luna. Calculation of 1/ f noise indexes from electrocardiogram data in detection of cardiac illness. Technical Report TR/PA/00/81, CERFACS, Toulouse, France, 2000.

[6] T. Meškauskas and F. Ivanauskas. Initial boundary-value problems for derivative nonlinear schrödinger equation. justification of two-step algorithm. Technical Report TR/PA/00/70, CERFACS, 2000.

5 Nonlinear Systems and Optimization

5.1 Optimization techniques for the regularization of large-scale discrete forms of ill-posed problems

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This research focuses on the development of optimization techniques for the numerical treatment of large-scale discrete forms of ill-posed problems from inverse problems in seismology, medical tomography and image restoration.
In our work with Sorensen, the goal is the development of efficient preconditioners for a special kind of large-scale eigenvalue problem arising in the method LSTRS ([1]). We have successfully used LSTRS for the regularization of ill-posed seismic inversion problems ([2]). However, there is the need to improve the eigenvalue computation which is the main computation in the method. Such improvement will allow the efficient use of the method as an inner iteration of a more sophisticated optimization algorithm for the nonlinear treatment of ill-posed problems. At the present time, we have developed the preconditioners and are testing their performance in practice.
The goal in our work with Noll and Tanoh is the development of a method for the nonlinear treatment of ill-posed problems from medical tomography. The method is a trust-region method that will use LSTRS as an inner iteration to solve the trust-region subproblems. Some of the basic theory and an initial algorithm have already been developed by Tanoh. The next step consists of writing a prototype for the method.
Our work with Steihaug focuses on the solution of norm constrained convex quadratic problems with nonnegativity constraints. These are the kind of problems that arise in image restoration. The goal is to develop a method for large-scale problems. We have already designed a method and are in the process of writing a prototype and testing.
Rojas is also working on image restoration problems. She has already tested the method LSTRS on such problems and obtained some preliminary results.

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[1] M. Rojas, S. A. Santos, and D. C. Sorensen. A new matrix-free method for the large-scale trust-region subproblem. *SIAM J. Optimization*, 11(3):611–646, 2000.

[2] M. Rojas and D. C. Sorensen. A trust-region approach to the regularization of large-scale discrete ill-posed problems. Technical Report TR/PA/00/57, CERFACS, Toulouse, France, 2000.

5.2 High rates of convergence in primal-dual interior point algorithms for nonlinear programming

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We have analysed local convergence properties of the primal-dual trust-region interior point method designed to minimize a nonlinear, possibly nonconvex, objective function subject to linear equality constraints and general inequalities by means of a log-barrier approach. The analysis presented

follows that of [2, 3, 4, 7]. Asymptotically, for each value of the barrier parameter, a single primal-dual linear system is solved, yielding a point that already matches the barrier subproblem stopping tolerances, and Q-superlinear convergence, which can be as close to quadratic as desired, is achieved. Moreover, this fast asymptotic convergence occurs componentwise. Since the inner minimization phase—used in [1] to solve a barrier subproblem—is not required asymptotically, we observe that the conclusions drawn hold independently of the inner minimization procedure [6]. This convergence rate is essentially as fast as that previously obtained for exterior penalty methods [4].
Going further, we examine how fast the rate of convergence may be when the aforementioned extrapolation step is followed by a number of further Newton steps. In two frameworks, we show that a convergence rate that is as fast as desired may be obtained provided one is ready to compute sufficiently many Newton steps. The iterates converge at a Q-rate which can be chosen as close to 2^{q+1} as desired if q Newton steps are taken, and as before, this convergence occurs componentwise. The first framework is that in which the inner iteration is irrelevant in the asymptotics. The second is the trust-region framework of [1]. This work resulted in the report [5].

[1] A. R. Conn, N. I. M. Gould, D. Orban, and Ph. L. Toint. A Primal-Dual Trust-Region Algorithm for Non-Convex Nonlinear Programming. Technical Report TR/PA/99/27, CERFACS, Toulouse, France, 1999. Published in Mathematical Programming "Davidon Festschrift" Online First, DOI 10.1007/s101070000144, March 15, 2000.

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

[3] J.-P. Dussault. Numerical stability and efficiency of penalty algorithms. *SIAM Journal on Numerical Analysis*, 32(1):296–317, 1995.

[4] N. I. M. Gould. On the convergence of a sequential penalty function method for constrained minimization. *SIAM Journal on Numerical Analysis*, 26(1):107–126, 1989.

[5] N. I. M. Gould, D. Orban, A. Sartenaer, and Ph. L. Toint. High Rates of Convergence of Primal-Dual Interior Point Algorithms for Nonlinear Programming. Technical Report TR/PA/00/63, CERFACS, Toulouse, France, 2000. Submitted to the proceedings of "High Performance Algorithms and Software for Nonlinear Optimization", Erice, Italy.

[6] N. I. M. Gould, D. Orban, A. Sartenaer, and Ph. L. Toint. Superlinear convergence of primal-dual interior point algorithms for nonlinear programming. Technical Report TR/PA/00/20, CERFACS, Toulouse, France, 2000. Preliminary version of the article published in SIOPT, vol. 11, nber 4, pp 974-1002.

[7] S. J. Wright and D. Orban. Properties of the log-barrier function on degenerate nonlinear programs. Technical Report TR/PA/99/36, CERFACS, Toulouse, France, 1999. Submitted for publication to Mathematics of Operations Research.

5.3 CUTEr: a Constrained and Unconstrained Testing Environment revisited

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The Constrained and Unconstrained Testing Environment (CUTE) [1] is a versatile environment for testing small to large-scale nonlinear programming problems arising from both real practical applications and from academic circles. It provides Fortran tools for computing function values, gradients, Hessians, matrix-vector products and handles both dense and sparse problems. It has been designed with multi-platform environments in mind and the test problems are written using the SIF (Standard Input Format) description language, formerly used by LANCELOT [2]. CUTE also provides tools to help the users build their own interface to their optimization package, as well as ready-to-use interfaces to famous existing packages like MINOS and OSL.

The purpose of this research is to build CUTEr, the new version of CUTE, and make it available on more platforms, including the quickly growing Linux platforms, and possibly to install it on heterogeneous local networks. Its installation phase is faster, easier, more efficient and makes better use of disk space and memory as architecture-dependent parts have been carefully isolated. CUTEr provides more tools, with enhanced capabilities that implement recent developments in dense and sparse linear algebra and interfaces to more recent optimization packages like NITRO and filterSQP.

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[1] I. Bongartz, A. R. Conn, N. I. M. Gould, and Ph. L. Toint. CUTE: Constrained and Unconstrained Testing Environment. *Transactions of the ACM on Mathematical Software*, 21(1):123–160, 1995.

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

5.4 Componentwise fast convergence in the solution of full-rank systems of nonlinear equations

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Following the good local convergence properties of primal-dual interior point methods for nonlinear programming [2], the asymptotic convergence of parameterized variants of Newton's method for the solution of nonlinear systems of equations is considered. The original system is perturbed by a term involving the variables and a scalar parameter which is driven to zero as the iteration proceeds. The exact local solutions to the perturbed systems then form a differentiable path leading to a solution of the original system, the scalar parameter determining the progress along the path. A homotopy-type algorithm, which involves an inner iteration in which the perturbed systems are approximately solved, is outlined. It is shown that asymptotically a single linear system is solved per update of the scalar parameter.
It turns out that a *componentwise* Q-superlinear rate may be attained under standard assumptions, and that this rate may be made arbitrarily close to quadratic. Numerical experiments illustrate the results and we discuss the relationships that this method shares with interior methods in constrained optimization. This work resulted in report [1].

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[1] 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. Technical Report TR/PA/00/56, CERFACS, Toulouse, France, 2000.

[2] N. I. M. Gould, D. Orban, A. Sartenaer, and Ph. L. Toint. Superlinear convergence of primal-dual interior point algorithms for nonlinear programming. Technical Report TR/PA/00/20, CERFACS, Toulouse, France, 2000. Preliminary version of the article published in SIOPT, vol. 11, nber 4, pp 974-1002.

5.5 Numerical optimization techniques for data assimilation

A. Piacentini: CERFACS*, France*; **A. Sartenaer**: CERFACS*, France*; **A. Weaver**: CERFACS*, France.*

Variational data assimilation methods (as used in meteorology or oceanography for instance) rely on optimization solvers. In collaboration with the Climate Modelling and Global Change team (more precisely the PALM project and the "ocean data assimilation" project), we have started to settle a framework whose goal is twofold. The first is to select existing numerical optimization techniques (such as limited memory methods, conjugate gradient methods, etc) adapted to data assimilation, and to compare their numerical behaviour and performance when embedded in the PALM software. The second goal is to investigate the possibility to enrich these exisiting optimization techniques, knowing that important issues are for instance the development of good preconditioners to accelerate the conjugate gradient method, multi-level resolution techniques, and (weakly) non-quadratic formulations of the data assimilation problem.

6 Conferences and Seminars

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

January

NERSC, Lawrence Berkeley National Laboratory, California, January 27, I.S. Duff, *Sparse pattern selection strategies for robust Frobenius norm minimization preconditioners in electromagnetism,* seminar.

Stanford University, California, January 28, I.S. Duff, *Sparse pattern selection strategies for robust Frobenius norm minimization preconditioners in electromagnetism,* seminar.

March

University of Strathclyde, Glasgow, Scotland, March 3, I.S. Duff, *Sparse pattern selection strategies for robust Frobenius norm minimization preconditioners in electromagnetism,* seminar.

April

Copper Mountain Meeting on Iterative Methods, Colorado, April 1–10. I.S. Duff, organizing committee, chairman, judge for student papers, editing proceedings. J. Langou, attendee.

European Geophysical Society XXV General Assembly, Nice, France, April 25–29, 2000. S. Dallakyan, attendee.

May

Lawrence Livermore National Laboratory, California, May 9, I.S. Duff, *Sparse pattern selection strategies for robust Frobenius norm minimization preconditioners in electromagnetism,* seminar.

Annual meeting of Committee for International Conferences on Applied and Industrial Mathematics (ICIAM), Paris, May 27–28, I.S. Duff, committee member.

June

CANUM'2000, Port-d'Albret, France, June 5–9. E. Traviesas, *The spectrum of a matrix and homotopic perturbations,* Poster Session. A. Zaoui, *Calcul hypercomplexe : quaternions et octonions,* Poster Session. A. Bouras, *Solveurs itératifs emboités,* talk.

Workshop SEA 2000, Toulouse, France, June 14–16. E. Traviesas, *Homotopic perturbations and Arnoldi Method,* talk. J. Langou, *Happy Breakdowns exist in Block GMRES Algorithm too!*, talk.

Second Conference on Numerical Analysis and Applications, Rousse, Bulgaria, June 11–15. B. Carpentieri, *Sparse pattern selection strategies for robust Frobenius norm minimization preconditioners in electromagnetism,* talk. L. Plantié, *Understanding Krylov methods in finite precision,* talk. L. Plantié, *The boundary layer problem of triple deck type,* talk.

Oxford Supercomputing Centre (OSC), University of Oxford, June 14. I.S. Duff, *Analysis and tuning of two general sparse solvers for distributed memory computers,* seminar.

VECPAR 2000, Porto, Portugal, June 19-22. I.S. Duff, *Sparse direct methods and software for systems of equations,* invited tutorial talk, programme committee, chairman.

July

3rd World Congress of Nonlinear Analysts (WCNA-2000), Catania, Italy, July 19–26, 2000. F. Chaitin-Chatelin, *Qualitative computing in Arnoldi process and happy breakdown,* talk, invited speaker. T. Meškauskas, *Computation with hypercomplex numbers,* talk.

August

ISMP2000 — 17th International Symposium on Mathematical Programming, Atlanta, GE., USA, August 7–11. M. Rojas, *Optimization techniques for image restoration problems*, talk. D. Orban, *Superlinear convergence of primal-dual interior-point algorithms for nonlinear programming*, talk.

BIT 40th Anniversary, Lund, Sweden, August 10–13. I.S. Duff, attendee.

16th IMACS World Congress 2000, Lausanne, Switzerland, August 21–25. E. Traviesas, *The hybrid eigensolver ISA to compute the r eigenvalues closest to a given complex point: a qualitative study,* talk. E. Traviesas, *PRECISE, a toolbox for assessing the quality of numerical methods and software,* talk.

EuroPar 2000, Munich, Germany, August 28–31. I.S. Duff, *Sparse direct methods and software for systems of equations,* invited tutorial talk.

September

Boundary Integral Methods: Theory and Applications, Bath, UK, September 12–16. B. Carpentieri, *Sparse pattern selection strategies for robust Frobenius norm minimization preconditioners in electromagnetism,* talk.

Preconditioning Workshop, Oxford, September 18. I.S. Duff, *Sparse pattern selection strategies for robust Frobenius norm minimization preconditioners in electromagnetism,* invited talk. B. Carpentieri, attendee.

IFIP Working Group 2.5 Working on Numerical Softwares, Conference 8, Ottawa, Canada, September 30–October 4, 2000. L. Plantié, attendee.

October

13th International conference in Domain decomposition methods, Lyon, October 9–12. J.C. Rioual. *Two-level preconditioners for the Schur complement: an application to semi-conductor device.* talk. L. Giraud, *A relaxation strategy for inner-outer linear solvers in domain decomposition methods.* talk.

University of Cambridge, October 12. I.S. Duff, *Analysis and tuning of two general sparse solvers for distributed memory computers,* seminar.

Commemoration of Pete Stewart's 60th Birthday, University of Maryland, Washington DC, October 20–21. I.S. Duff, *Bells and Whistles,* invited talk.

SIAM Linear Algebra Meeting, Raleigh, North Carolina, USA, October 22–26. I.S. Duff, *Performance analysis of general sparse solvers for distributed memory computers,* invited minisymposium talk.

November

SC 2000, Dallas, Texas, November 4–10. I.S. Duff, *Sparse direct methods and software for systems of equations,* invited tutorial talk.

6.2 Conferences and seminars organized by the Parallel Algorithms Project

May

Orthogonal Eigenvectors without Gram-Schmidt (for symmetric tridiagonal matrices). May 12. Beresford N. Parlett (University of California at Berkley).

A rigorous framework for optimization using surrogate objectives (joint work with Charles Audet and Doug Moore). May 25. John Dennis (RICE University).

Analysis of Generalized Pattern Search (joint work with Charles Audet). May 30. John Dennis (RICE University).

June

Informal workshop on preconditioning techniques for the iterative solution of linear systems. June 7.
Rational approximation preconditiong techniques. Masha Sosonkina (Minneapolis),
Sparse preconditioning techniques in Electromagnetism. Bruno Carpentieri (CERFACS),
ILUs and factorized approximates inverses. Matthias Bollhöfer (Berlin),
Deflations in Block GMRES. Julien Langou (CERFACS).

Pattern Search Algorithms for Mixed Variable Programming (joint work with John Dennis). June 8. Charles Audet (RICE University).

July

Efficient and stable minimal residual methods for complex symmetric linear systems and least squares problems with multiple right-hand sides. July 3. Rasmus Munk Larsen (Stanford University).

Large-scale nonlinear optimization via sequential linearized constraints (joint work with M.A. Saunders). July 4. Michael P. Friedlander (Stanford University).

Singular values/vectors for all occasions: from Seismology to Information Retrieval. July 12. Osni Marques (NERSC, Lawrence Berkeley National Laboratory, California).

Algebraic Theory of Additive and Multiplicative Schwarz. July 19. Daniel B. Szyld (Temple University).

September

Sparse Approximate Inverse Preconditioning. September 1. Edmond Chow (Lawrence Livermore National Laboratory).

ELMRES: an oblique projection solver for sparse systems of linear equations (joint work with Desmond Stephens). September 1. Gary Howell (Florida Tech).

From PDE's & CFD to Image Processing. September 2. Tony Chan (University of California at Los Angeles).

Industrial days at CERFACS on Inner-Outer iterations and numerical quality of software coupling. September 11–12.

6.3 Internal seminars organized within the Parallel Algorithms Project

Februrary

Asymptotic Complexity for Superlinear Convergence in a Primal-Dual Interior Point Algorithm for Constrained Nonlinear Programming. Februrary 16. Dominique Orban.

Large-Scale Eigenvalue Problems, Trust Regions and the Regularization of Discrete Ill-Posed Problems. Februrary 23. Marielba Rojas.

March

Sparse pattern selection strategies for robust Frobenius norm minimization preconditioners in electromagnetism. March 8. Bruno Carpentieri.

A two-level preconditioner for the Schur complement and application to semi-conductor device modeling. March 15. Jean-Christophe Rioual.

April

Carrier phase ambiguity resolution in Global Positioning System (GPS). April 5. Sargis Dallakyan.

Singular and nearly-singular linear systems. April 12. Christof Vömel.

June

Méthodes de décomposition de domaines pour la résolution d'équations aux dérivées partielles. June 20. Fernando Guevara.

7 Publications

7.1 Journal Publications

[PUB1] P. R. Amestoy, I. S. Duff, and J.-Y. L'Excellent. Multifrontal parallel distributed symmetric and unsymmetric solvers. *Comput. Methods in Appl. Mech. Engrg.*, 184:501–520, 2000.

[PUB2] B. Carpentieri, I. S. Duff, and L. Giraud. Sparse pattern selection strategies for robust frobenius-norm minimization preconditioners in electromagnetism. *Numerical Linear Algebra with Applications*, 7(7-8):667–685, 2000.

[PUB3] F. Chaitin-Chatelin. The computing power of Geometry. *Numerical Analysis*, pages 83–92, 2000.

[PUB4] F. Chaitin-Chatelin and S. Gratton. On the condition number associated with the polar factorization of a rectangular matrix. *Numerical Linear Algebra with Applications*, (7):337–354, 2000.

[PUB5] F. Chaitin-Chatelin, A. Harrabi, and A. Ilahi. About Hölder Condition Numbers and the Stratification diagram for Defective Eigenvalues. *IMACS Journal on Mathematics and Computers in Simulation*, 1800:1–6, 2000.

[PUB6] F. Chaitin-Chatelin, V. Toumazou, and E. Traviesas. Accuracy assessment for eigencomputations : variety of backward errors and pseudospectra. *J. Linear Algebra Appl.*, 309:73–83, 2000.

[PUB7] A. R. Conn, N. I. M. Gould, D. Orban, and Ph. L. Toint. A primal-dual trust-region algorithm for non-convex nonlinear programming. *Mathematical Programming B*, 87(2):215–249, 2000. also appeared on Mathematical Programming B, Online First, DOI 10.1007/s101070000144, March 2000.

[PUB8] S. Dallakyan. A note on the visualization of multiparametric bifurcations. *Computers And Graphics*, 24:269–270, 2000.

[PUB9] V. Frayssé, S. Gratton, and V. Toumazou. Structured backward error and condition number for linear systems of the type $A^*Ax = b$. *BIT*, 40:74–83, 2000.

[PUB10] Y. Saad, O. Axelsson, I. S. Duff, W.-P. Tang, H. van der Vorst, and A. Wathen, editors. *Special Issue: Preconditioning Techniques for Large Sparse Matrix Problems in Industrial Applications, SPARSE'99*, volume 7, 2000.

7.2 Conference Proceedings and Book Chapters

[PRO1] P. R. Amestoy, I. S. Duff, J.-Y. L'Excellent, and J. Koster. `MUMPS`: a general purpose distributed memory sparse solver. In A. H. Gebremedhin, F. Manne, R. Moe, and T. Sørevik, editors, *Proceedings of PARA2000, the Fifth International Workshop on Applied Parallel Computing, Bergen, June 18-21*, pages 122–131. Springer-Verlag, 2000. Lecture Notes in Computer Science, 1947.

[PRO2] F. Chaitin-Chatelin. The computing power of Geometry. In D. F. Griffiths and G. A. Watson, editors, *Numerical Analysis 1999*, pages 83–92. CRC Press LLC, 2000.

[PRO3] F. Chaitin-Chatelin, A. Harrabi, and A. Ilahi. About Hölder Condition Numbers and the Stratification diagram for Defective Eigenvalues. In Elsevier, editor, *Mathematics and Computers in Simulation*, volume 54, pages 397–402, 2000.

[PRO4] F. Ivanauskas and T. Meškauskas. On the numerical algorithms for derivative nonlinear schrödinger equation. In A. Samarskii R. Ciegis and M. Sapagovas, editors, *Finite difference schemes: theory and applications*, IMI, Vilnius, pages 89–98, 2000. 3rd International Conference FDS2000, Palanga, Lithuania.

7.3 Theses

[THS1] A. Bouras. *Contrôle de convergence des solveurs emboités pour le calcul de valeurs propres avec inversion*. Ph.D. dissertation, Université Toulouse I, TH/PA/00/77, CERFACS, Septembre 2000.

[THS2] V. Frayssé. *The power of backward error analysis*. Habilitation à Diriger des Recherches, Institut National Polytechnique de Toulouse, September 2000. TH/PA/00/65, CERFACS.

[THS3] L. Giraud. *On the Numerical Solution of Partial Differential Equations: Iterative Solvers for Parallel Computers*. Habilitation à Diriger des Recherches, Institut National Polytechnique de Toulouse, September 2000. TH/PA/00/64, CERFACS.

[THS4] E. Traviesas. *Sur le déploiement du champ spectral d'une matrice*. Ph.D. dissertation, Université Toulouse I, TH/PA/00/30, CERFACS, Mai 2000.

[THS5] A. N. Zaoui. *Deux Contributions au Calcul Scientifique I-Sur la convergence de la méthode des Itérations Simultanées couplée à l'algorithme d'Arnoldi itératif II-Autour du Calcul Hypercomplexe*. Ph.D. dissertation, Université Toulouse I, TH/PA/00/78, CERFACS and INRIA-IRISA, Décembre 2000.

7.4 Technical Reports

[TRP1] P. R. Amestoy, I. S. Duff, J.-Y. L'Excellent, and X. S. Li. Analysis and comparison of two general sparse solvers for distributed memory computers. Technical Report TR/PA/00/90, CERFACS, Toulouse, France, December 2000. Submitted to *ACM Trans. Math. Softw.*

[TRP2] 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, 2000.

[TRP3] P. R. Amestoy, I. S. Duff, J.-Y. L'Excellent, and X. S. Li. Performance and tuning of two distributed memory sparse solvers. Technical Report TR/PA/00/91, CERFACS, Toulouse, France, December 2000. Accepted for presentation at the Tenth SIAM Conference on Parallel Processing for Scientific Computing that will be held in Norfolk, Virginia from March 12th-14th, 2001.

[TRP4] A. Bouras, F. Chaitin-Chatelin, and V. Frayssé. Solveurs itératifs imbriqués. Contract Report FR/PA/00/19, CERFACS, Toulouse, France, 2000.

[TRP5] A. Bouras and V. Frayssé. A relaxation strategy for inexact matrix-vector products for Krylov methods. Technical Report TR/PA/00/15, CERFACS, Toulouse, France, 2000. Submitted to Numerical Linear Algebra with Applications.

[TRP6] A. Bouras and V. Frayssé. A relaxation strategy for the Arnoldi method in eigenproblems. Technical Report TR/PA/00/16, CERFACS, Toulouse, France, 2000.

[TRP7] A. Bouras, V. Frayssé, and L. Giraud. A relaxation strategy for inner-outer linear solvers in domain decomposition methods. Technical Report TR/PA/00/17, CERFACS, Toulouse, France, 2000.

[TRP8] F. Chaitin-Chatelin. Comprendre les méthodes de Krylov en précision finie : le programme du Groupe Qualitative Computing au CERFACS. Technical Report TR/PA/00/11, CERFACS, 2000.

[TRP9] F. Chaitin-Chatelin, S. Dallakyan, and V. Frayssé. GPS Carrier Phase Ambiguity Resolution with the LAMBDA method: 1. a stability analysis 2. an exponential speed-up. Contract Report CR/PA/00/52, CERFACS, Toulouse, France, 2000.

[TRP10] F. Chaitin-Chatelin, T. Meškauskas, and A. N. Zaoui. About real and binary algebras: the interplay between geometry and algebra. Technical Report TR/PA/00/74, CERFACS, Toulouse, France, 2000.

[TRP11] F. Chaitin-Chatelin, T. Meškauskas, and A. N. Zaoui. Computation with hypercomplex numbers. Technical Report TR/PA/00/69, CERFACS, Toulouse, France, 2000.

[TRP12] F. Chaitin-Chatelin and E. Traviesas. PRECISE, a toolbox for assessing the quality of numerical methods and software. Technical Report TR/PA/00/12, August 21-25,2000.

[TRP13] F. Chaitin-Chatelin, E. Traviesas, and L. Plantié. Understanding Krylov methods in finite precision. Technical Report TR/PA/00/40, CERFACS, Toulouse, France, 2000.

[TRP14] I. S. Duff and C. Vömel. Incremental Norm Estimation for Dense and Sparse Matrices. Technical Report TR/PA/00/83, CERFACS, Toulouse, France, 2000.

[TRP15] I. S. Duff and C. Vömel. Level 2 and Level 3 Basic Linear Algebra Subprograms for Sparse Matrices: A Fortran 95 instantiation. Technical Report TR/PA/00/18, CERFACS, Toulouse, France, 2000.

[TRP16] I. S. Duff, C. Vömel, and M. Youan. Implementing the Sparse BLAS in Fortran 95. Technical Report TR/PA/00/82, CERFACS, Toulouse, France, 2000.

[TRP17] V. Frayssé and L. Giraud. A set of conjugate gradient routines for real and complex arithmetics. Technical Report TR/PA/00/47, CERFACS, Toulouse, France, 2000.

[TRP18] 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. Technical Report TR/PA/00/56, CERFACS, Toulouse, France, 2000.

[TRP19] N. I. M. Gould, D. Orban, A. Sartenaer, and Ph. L. Toint. High Rates of Convergence of Primal-Dual Interior Point Algorithms for Nonlinear Programming. Technical Report TR/PA/00/63, CERFACS, Toulouse, France, 2000. Submitted to the proceedings of "High Performance Algorithms and Software for Nonlinear Optimization", Erice, Italy.

[TRP20] N. I. M. Gould, D. Orban, A. Sartenaer, and Ph. L. Toint. Superlinear convergence of primal-dual interior point algorithms for nonlinear programming. Technical Report TR/PA/00/20, CERFACS, Toulouse, France, 2000.

[TRP21] S. Leblond. Two direct methods for large sparse problems: Multifrontal massively parallel solver (MUMPS) and fast parallel direct solver for coarse grid problems (H. TUFO). Technical Report WN/PA/00/105, CERFACS, 2000.

[TRP22] T. Meškauskas, P. Caminal, and A. Bayes de Luna. Calculation of $1/f$ noise indexes from electrocardiogram data in detection of cardias illness. Technical Report TR/PA/00/81, CERFACS, Toulouse, France, 2000.

[TRP23] T. Meškauskas and F. Ivanauskas. Initial boundary-value problems for derivative nonlinear schrodinger equation. justification of two-step algorithm. Technical Report TR/PA/00/70, CERFACS, 2000.

[TRP24] L. Plantié. The boundary layer problem of triple deck type. Technical Report TR/PA/00/61, CERFACS, Toulouse, France, 2000.

[TRP25] L. Plantié. A semi-discrete problem for the boundary layer of triple deck type (part 1). Technical Report TR/PA/00/45, CERFACS, Toulouse, France, 2000.

[TRP26] L. Plantié. A semi-discrete problem for the boundary layer of triple deck type (part 2). Technical Report TR/PA/00/46, CERFACS, Toulouse, France, 2000.

[TRP27] M. Rojas and D. C. Sorensen. A trust-region approach to the regularization of large-scale discrete ill-posed problems from electromagnetic applications. Technical Report TR/PA/00/57, CERFACS, Toulouse, France, 2000.

[TRP28] F. Guevara Vasquez. Internship report on domain decomposition methods for the solution of partial differential equations. Technical Report TR/PA/00/98, CERFACS, Toulouse, France, 2000.

[TRP29] A. Zaoui and E. Traviesas. Sur la fiabilité et la robustesse du code isabel. Technical Report TR/PA/00/76, CERFACS, Toulouse, France, 2000.

[TRP30] A. Zaoui and E. Traviesas. The hybrid eigensolver ISA to compute the r eigenvalues closest to a given complex point : A qualitative study. Technical Report TR/PA/00/13, August 21-25,2000. 16th IMACS World Congress, Lausanne, Switzerland.

7.5 To appear

[APP1] 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.

[APP2] Z.-Z. Bai, I. S. Duff, and A. J. Wathen. A class of incomplete orthogonal factorization methods. I: Methods and theories. *BIT*, 41(1):53–70, 2001.

[APP3] B. Carpentieri, I. S. Duff, and L. Giraud. Robust preconditioning of dense problems from electromagnetics. In L. Vulkov, J. Waśniewski, and P. Yalamov, editors, *Numerical Analysis and Its Applications. Lecture Notes in Computer Science 1988*, pages 170–178. Springer-Verlag, 2000.

[APP4] L. M. Carvalho, L. Giraud, and G. Meurant. Local preconditioners for two-level non-overlapping domain decomposition methods. *Numerical Linear Algebra with Applications*, 8(4):207–227, 2001.

[APP5] L. M. Carvalho, L. Giraud, and P. Le Tallec. Algebraic two-level preconditioners for the Schur complement method. *SIAM J. Scientific Computing*, 22(6), 2001.

[APP6] F. Chaitin-Chatelin and T. Meškauskas. Computation with hypercomplex numbers. In *Proceedings of WCNA 2000, Catania*, pages ppp–qqq. Journal of Nonlinear Analysis, Elsevier Science, 2001.

[APP7] F. Chaitin-Chatelin and E. Traviesas. PRECISE, a toolbox for assessing the quality of numerical methods and software. In E, editor, *Proceedings of the 16th IMACS World Congress, Lausanne, Switzerland*, volume v, pages ppp–qqq, August 21–25,2000. Technical Report TR/PA/00/12.

[APP8] F. Chaitin-Chatelin, E. Traviesas, and L. Plantié. Understanding Krylov methods in finite precision. In L. Vulkov, J. Waśniewski, and P. Yalamov, editors, *Numerical Analysis and Its Applications. Lecture Notes in Computer Science 1988*, pages 187–197. Springer-Verlag, 2000.

[APP9] I. S. Duff and J. Koster. On algorithms for permuting large entries to the diagonal of a sparse matrix. *SIAM J. Matrix Analysis and Applications*, 22(n):ppp–qqq, 2001.

[APP10] L. Giraud, R. Guivarch, and J. Stein. Parallel distributed fast 3D Poisson solver for meso-scale atmospheric simulations. *Int J. of High Performance Computing Applications*, 15(1):36–46, 2001.

[APP11] N .I .M. Gould, D. Orban, A. Sartenaer, and Ph. L. Toint. Superlinear convergence of primal-dual interior point algorithms for nonlinear programming. *SIAM J. Optimization*, 11(4):974–1002, 2001.

[APP12] L. Plantié. The boundary layer problem of triple deck type. In E, editor, *Proceedings of the Second Conference on Numerical Analysis and Applications, Rousse, Bulgaria*, volume v, pages ppp–qqq, 2000. Technical Report TR/PA/00/61.

[APP13] A. N. Zaoui and E. Traviesas. The hybrid eigensolver ISA to compute the r eigenvalues closest to a given complex point : A qualitative study. Technical Report TR/PA/00/13, CERFACS, Toulouse, France, 2001. To appear in the Proceedings of the 16th IMACS World Congress, Lausanne, Switzerland.