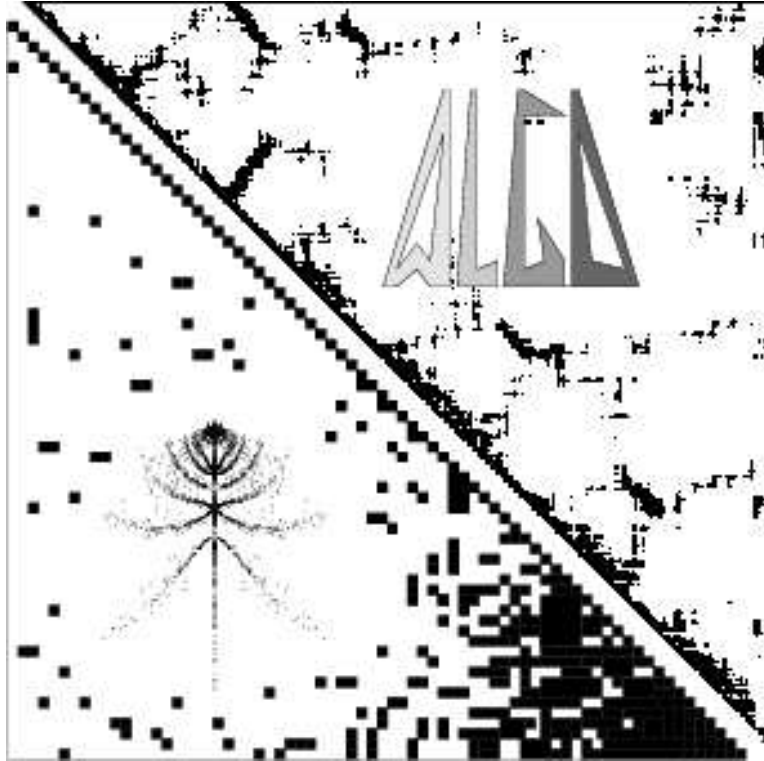


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ACTIVITY REPORT
of the
PARALLEL ALGORITHMS PROJECT
at
CERFACS

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1 Introduction

1.1 Introduction

The research programme conducted by the Parallel Algorithms Project combines the excitement of basic research discoveries with their use in the solution of large-scale problems in science and engineering 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 statistics of accesses to the CERFACS Web pages where a major part 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 symmetric indefinite and general sparse matrices. Some of this work is related to numerical properties of the matrices and methods for obtaining an ordering that respects these properties in an efficient way. Other work concerns the scheduling of the multifrontal factorization in a distributed memory environment and has a very significant impact on the performance of our parallel code. Some of the work on direct solvers has been supported by the bi-lateral Aurora grant that we have with Norway. We also report on the 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. A large part of the work during this past year has been to extend these techniques so that they can be applied to a wide range of problems in different application areas. The work on inner-outer iterations, pioneered by the Team some years ago, has been developed further and extended both computationally and theoretically. The work on matrix partitioning schemes has been developed to provide an efficient block Jacobi preconditioner for use with standard iterative methods such as GMRES. It shows an expected good performance on parallel computers. Since the GMRES and FGMRES routines are widely used and have been downloaded over 1000 times, a future project might involve developing this preconditioner so that it can be used with these packages.

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. Of particular concern are a deeper understanding of the role of nonlinearities and singularities in the context of floating-point arithmetic. A major tool in this work continues to be the use of homotopic deviations, a technique again pioneered at CERFACS by the Qualitative Computing Group. An application of this work gives a theoretical basis to the sometimes unexpected good behaviour of Krylov type methods.

A major focus of our work on nonlinear systems and optimization has been in joint work with the PALM Project and the Climate Modelling Group on data assimilation. This area is becoming one of the main interdisciplinary focus points at CERFACS. 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 investigated several aspects of this including appropriate condition numbers for this problem and further investigation of the relationship of the 4D-Var algorithm and Gauss-Newton iterations. We are also developing software for solving large dense linear least-squares systems that is competitive with ScaLAPACK routines from the point of view of efficiency but requires about half the storage. Better techniques for the storage are also being explored. A new initiative in this area is the innovative combination of multilevel schemes with trust region methods for optimization problems including those arising in the solution of partial differential equations. This work is being done jointly with our colleagues in Belgium.

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. This year we had only two stagiaires: Eline Jonkers from Delft University in the Netherlands and Christophe Oberdorf from Ecole Central d'Electronique in Paris. Members of the Team have assisted in many lecture courses at other centres, including ENSICA, INPT, Toulouse 1 and INSA. Stéphane Pralet completed his PhD thesis on "Constrained orderings and scheduling for parallel sparse linear algebra" in September. The jury included international experts in this area who were so impressed that they have recommended the thesis is awarded a prize. This is even more commendable when we consider that the thesis was completed in just over

two years.

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: Abdellatif El Ghazi (eigenvalue problems), Marielba Rojas (optimization) and Jean Tshimanga (optimization and climate modelling). As always, it was a pleasure to welcome Gene Golub from Stanford who is a great source of inspiration especially to our younger students. 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. Martin Van Gijzen had the responsibility 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 returned to our normal annual formula of a two-day "Sparse Days at CERAFCS" meeting and we present the talks and the list of participants in Section 7.2. We again had a good European and international involvement. Indeed, the continuing success of our June meetings has led us to be invited to host the Second International Workshop on Combinatorial Scientific Computing in June of 2005.

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 and computational electromagnetics. We have a project with EADS on preconditioning techniques in electromagnetics. We have had detailed discussions with EDF on parallel linear solvers and on embedded iterations for multi-phase flow. 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 numerical algorithms with Global Change. We now have a strong and growing collaboration with the Climate Modelling Team on aspects of data assimilation, have co-hosted a visit of a researcher from Belgium with the PALM Project of that Group, and have hosted a visit from Nancy Nichols of Reading University who works partly in numerical analysis and partly with the meteorologists at Reading. 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. Sadly Martin left us at the beginning of November to take up a post on the faculty at the University of Delft in his native Netherlands. Although sorry to see him go, we wish him every success in his new career and note that we will still have close cooperation with him through our Van Gogh programme that has been extended for another year.

Iain S. Duff.

Visitors to Parallel Algorithm Project in 2004

In alphabetical order, our visitors in the year 2004 included:

GUILLAUME ALLÉON (EADS-CCR, France),
PATRICK AMESTOY (ENSEEIH-IRIT, France),
MARIO ARIOLI (RAL, U.K.),
LUIZ CARVALHO (Universidade do Estado do Rio de Janeiro, Brazil),
VICTOR EIJKHKOUT (University of Tennessee, U.S.A.),
ABDELLATIF EL GHAZI (Université Mohammed V, Rabat, Morocco),
GENE GOLUB (Stanford University, U.S.A.),
PASCAL HÉNON (INRIA Futurs, LaBRI, Talence, France),
ELINE JONKERS (Delft University of Technology, The Netherlands),
JEAN-YVES L'EXCELLENT (INRIA-ENS, Lyon, France),
SHANE MULLIGAN (Dublin Institute of Technology, Dublin, Ireland),
FRÉDÉRIC NATAF (CMAP, Palaiseau, France),
NANCY K. NICHOLS (University of Reading, U.K.),
ESMOND NG (Lawrence Berkeley National Laboratory, Berkeley, U.S.A.),
MIKE OSBORNE (Australian National University, Australia),
MICHAEL OVERTON (Courant Institute, U.S.A.),
ALEX POTHEN (Old Dominion University, Norfolk VA, U.S.A.),
THIERRY PRIOL (IRISA-INRIA Rennes, France),
PIERRE RAMET (INRIA Futurs, LaBRI, Talence, France),
MARIELBA ROJAS (Wake Forest University, Winston-Salem, U.S.A.),
JEAN ROMAN (INRIA Futurs, LaBRI, Talence, France),
DANIEL RUIZ (ENSEEIH-IRIT, France),
ANNICK SARTENAER (The University of Namur, Belgium),
JENNIFER SCOTT (Rutherford Appleton Laboratory, U.K.),
MASHA SOSONKINA (AMES Lab., Iowa, U.S.A.),
ARNO SWART (Utrecht University, The Netherlands),
GUILLAUME SYLVAND (EADS-CCR, France),
PHILIPPE TOINT (The University of Namur, Belgium),
JEAN TSHIMANGA (The University of Namur, Belgium),
ANDY WATHEN (Oxford University Computing Laboratory, U.K.) and
JERZY WASNIEWSKI (Technical University of Denmark).

2 List of Members of the Algo Team

IAIN DUFF - Project Leader
LUC GIRAUD - Deputy Project Leader - Senior Researcher
FRANÇOISE CHAITIN-CHATELIN - Qualitative Computing Group Scientific Advisor
SERGE GRATTON - Senior Researcher
MARTIN VAN GIJZEN - Senior Researcher
BRUNO CARPENTIERI - Post. Doc.
DANIEL LOGHIN - Post. Doc.
CHRISTOPHE HAMMERLING - Engineer
MARC BABOULIN - Ph.D. Student
EMERIC MARTIN - Ph.D. Student
STEPHANE PRALET - Ph.D. Student
SONGKLOD RIYAVONG - Ph.D. Student
MORAD AHMADNASAB - Visitor, University Toulouse I, France
FERMIN BAZAN - Visitor, currently University of S. Catarina in Brazil
NASREDDINE MEGREZ - Visitor, University Toulouse I, France
AHMED TOUHAMI - Visitor, ENSEEIHT-IRIT, France
ELINE JONKER - Trainee
CHRISTOPHE OBERDORF - 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.

Our main contribution is to define a new method for scaling and a way of using an approximation to a symmetric weighted matching to predefine 1×1 and 2×2 pivots prior to the ordering and analysis phase. We also present new classes of orderings called “(relaxed) constrained orderings” that select pivots during the symbolic Gaussian elimination using two graphs: the first one contains information about the structure of the reduced matrix and the second one gives information about the numerical values.

We perform experiments with our symmetric preprocessing in [1] and we validate our heuristics with a symmetric multifrontal code MA57 [2] on real test problems in [3, 4]. Our test sets include both augmented matrices and general indefinite matrices.

-
- [1] I. S. Duff and S. Pralet. Experiments in preprocessing and scaling symmetric problems for multifrontal solutions. Technical Report WN/PA/04/17, CERFACS, Toulouse, France, 2004.
 - [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 S. Pralet. Strategies for scaling and pivoting for sparse symmetric indefinite problems. Technical Report TR/PA/04/59, CERFACS, Toulouse, France, 2004.
 - [4] S. Pralet. *Constrained orderings and scheduling for parallel sparse linear algebra*. Ph.D. dissertation, INPT, September 2004. TH/PA/04/105.

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 unsymmetric sparse matrices using a three-phase approach (analysis, factorization and triangular solution). Usually the analysis phase first determines a set of potentially good pivots and then orders this set of pivots to decrease the fill-in in the factors. We present in [1] a preprocessing algorithm that simultaneously achieves the objectives of selecting numerically good pivots and preserving the sparsity. We describe the algorithmic properties and difficulties in implementation. By mixing the two objectives we show that we can reduce the amount of fill in the factors and can reduce the number of numerical problems during factorization. On a set of large unsymmetric real problems, we obtain average gains of 14% in the factorization time, 12% in the size of the LU factors, and 21% in the number of operations performed in the factorization phase. Full details of our implementation are available in [2].

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- [1] P. R. Amestoy, X. S. Li, and S. Pralet. Constrained Markowitz with local symmetrization. Technical Report TR/PA/04/137, CERFACS, Toulouse, France, 2004.
- [2] S. Pralet. *Constrained orderings and scheduling for parallel sparse linear algebra*. Ph.D. dissertation, INPT, September 2004. TH/PA/04/105.

3.3 Hybrid scheduling for the parallel solution of linear systems

P. R. Amestoy: ENSEEIHT, *France*; **A. Guermouche:** INRIA, *France*;
J.-Y. L'Excellent: INRIA, *France*; **S. Pralet:** CERFACS, *France*

We consider the problem of designing a dynamic scheduling strategy that takes into account both workload and memory information in the context of a parallel multifrontal factorization. The originality of our approach is that we base our estimations (work and memory) on a static optimistic scenario during the analysis phase. This scenario is then used during the factorization phase to constrain the dynamic decisions. The task scheduler has been redesigned to take into account these new features. Moreover, the performance has been improved because the new constraints allow the new scheduler to make optimal decisions that were forbidden or too dangerous in unconstrained formulations. Performance analysis in [1] show that the memory estimation becomes much closer to the memory effectively used and that, even in a constrained memory environment, we decrease the factorization time with respect to the initial approach. The algorithms will be integrated into the next release of MUMPS.

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- [1] P. R. Amestoy, A. Guermouche, J.-Y. L'Excellent, and S. Pralet. Hybrid scheduling for the parallel solution of linear systems. Research report RR-5404, INRIA, December 2004. Also available as LIP report RR2004-53 and as an ENSEEIHT-IRIT technical report.

3.4 The Grid-TLSE project

P. R. Amestoy: ENSEEIHT-IRIT, *France*; **M. Buvry:** ENSEEIHT-IRIT, *France*;
M. Daydé: ENSEEIHT-IRIT, *France*; **I. S. Duff:** CERFACS, *France* and RUTHERFORD APPLETON LABORATORY, *England*; **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 to the Grid and use the Grid capabilities to implement these services. The principal services will be mainly twofold:

- to 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).
- to make available to the scientific community a set of test problems through a data base. The set of examples will grow dynamically as users submit new problems that are integrated within the data set.

In September, a review meeting was organized. All the academic partners were involved as well as some of our colleagues and experts in sparse linear algebra that were visiting CERFACS at that time (E. Ng, A. Pothen and J. Scott). During this year the project has made significant progress and a prototype of the final version of the site will be available early next summer. Experiments on the Grid-5000 platform are also scheduled. Finally the results of the project have been presented at various conferences [1, 2, 3]. More information on the project can be found from the URL:

<http://www.enseeiht.fr/lima/tlse>

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- [1] P. R. Amestoy, I. S. Duff, L. Giraud, J-Y. L'Excellent, and C. Puglisi. GRID-TLSE: A Web Site for Experimenting with Sparse Direct Solvers on a Computational Grid. See <http://www.siam.org/meetings/pp04/>, February 25-27 2004. Conference: SIAM conference on Parallel Processing for Scientific Computing, San Francisco, (USA).
 - [2] M. Daydé, L. Giraud, M. Hernandez, J.-Y. L'Excellent, C. Puglisi, and M. Pantel. An Overview of the Grid-TLSE Project. In *Lecture notes in Sciences*, to appear.
 - [3] M. Pantel, M. Buvry, C. Hamerling, and C. Puglisi. Grid-TLSE project: Meta-data for matrices, computers and solvers, 18-22 October 2004. 3rd International Workshop on Parallel Matrix Algorithms and Applications (PMAA'04), CIRM, Marseille, (France).

4 Iterative Methods and Preconditioning

4.1 Additive and multiplicative two-level spectral preconditioning for general linear systems

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

Multigrid methods are among the fastest techniques for solving linear systems arising from the discretization of partial differential equations. The core of the multigrid algorithms is a two-grid procedure that is applied recursively. A two-grid method can be fully defined by the smoother that is applied on the fine grid, the coarse grid and the grid transfer operators to move between the fine and the coarse grid. With these ingredients both additive and multiplicative procedures can be defined. In this project, we develop preconditioners for general sparse linear systems that exploit ideas from the two-grid methods. They attempt to improve the convergence rate of a prescribed preconditioner M_1 that is viewed as a smoother, the coarse space is spanned by the eigenvectors associated with the smallest eigenvalues of the preconditioned matrix $M_1 A$. We derive both additive and multiplicative variants of the iterated two-level preconditioners for unsymmetric linear systems that can also be adapted for Hermitian positive definite problems. We show that these two-level preconditioners shift the smallest eigenvalues to one and tend to better cluster around one those that M_1 already succeeded to move to the neighbourhood of one. We illustrate the performance of our method through extensive numerical experiments on a set of general linear systems. Finally, we consider two case studies, one from a non-overlapping domain decomposition method in semiconductor device modelling, another one from electromagnetism applications. Results of this study are presented in [1].

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- [1] B. Carpentieri, L. Giraud, and S. Gratton. Additive and multiplicative two-level spectral preconditioning for general linear systems. Technical Report TR/PA/04/38, CERFACS, Toulouse, France, 2004.

4.2 Incremental spectral preconditioners for sequences of linear systems

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

In many scientific applications a set of linear systems with the same coefficient matrix but different right-hand sides have to be solved in sequence. Such a situation exists for instance in the calculation of the radar cross section for electromagnetic calculations or in the calculation of eigenvalues using shift and invert techniques, etc. Efficient methods for tackling this problem attempt to benefit from the previously solved right-hand sides for the solution of the next. This goal can be achieved either by recycling Krylov subspaces (see for instance [6] and references therein) or by building preconditioner updates based on near invariant subspace information (see for instance [1, 2, 3] and references therein). In this work we investigate the use of Krylov linear solvers based on an Arnoldi process, that are variants of GMRES. In particular, because we aim at removing the possible slowdown effect of the smallest eigenvalues, we consider the GMRES-DR solver [5]. The harmonic Ritz vectors computed by this linear solver for a given right-hand side are used to update an incremental spectral low-rank preconditioner [2] that is used for the next right-hand side. We implement several strategies to select

the appropriate spectral information and illustrate their numerical behaviour on some academic problems from the Matrix Market as well as from large computations in industrial electromagnetic applications.

Results of this study are presented in [4].

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- [1] J. Baglama, D. Calvetti, G. H. Golub, and L. Reichel. Adaptively preconditioned GMRES algorithms. *SIAM J. Scientific Computing*, 20(1):243–269, 1999.
 - [2] B. Carpentieri, I. S. Duff, and L. Giraud. A class of spectral two-level preconditioners. *SIAM J. Scientific Computing*, 25(2):749–765, 2003.
 - [3] J. Erhel, K. Burrage, and B. Pohl. Restarted GMRES preconditioned by deflation. *J. Comput. Appl. Math.*, 69:303–318, 1996.
 - [4] L. Giraud, S. Gratton, and E. Martin. Incremental spectral preconditioners for sequences of linear systems. Technical Report in preparation, CERFACS, Toulouse, France, 2005.
 - [5] R. B. Morgan. GMRES with deflated restarting. *SIAM J. Scientific Computing*, 24(1):20–37, 2002.
 - [6] M. L. Parks, E. de Sturler, G. Mackey, D. D. Jhonson, and S. Maiti. Recycling Krylov subspaces for sequences of linear systems. Technical Report UIUCDCS-R-2004-2421 (CS), University of Illinois at Urbana-Champaign, 2004.

4.3 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 $Ax = b$ with the conjugate gradient method, the smallest eigenvalues in the matrix A often slow down the convergence. Consequently if the smallest eigenvalues in A could be somehow “removed”, the convergence may be improved. This observation is of importance even when a preconditioner is used, and some extra techniques might be investigated to further improve the convergence rate of the conjugate gradient on the given preconditioned system. Several techniques have been proposed in the literature that either consist of updating the preconditioner or enforcing the conjugate gradient algorithm to work in the orthogonal complement of an invariant subspace associated with the smallest eigenvalues. Among these approaches we consider first a two-phase algorithm using a deflation-type idea. In a first stage this algorithm computes a partial spectral decomposition simply using matrix-vector products. More precisely it combines Chebyshev iterations with a block Lanczos procedure to accurately compute an orthogonal basis of the invariant subspace associated with the smallest eigenvalues. Then, the solution on this subspace is computed using a projector while the solution in the orthogonal complement is obtained with Chebyshev iterations that benefit from the reduced condition number. For the sake of comparison, this eigen-information is used in combination with other techniques. In particular we consider the deflated version of conjugate gradients. As representative of techniques exploiting the spectral information to update the preconditioner we consider also the approaches that attempt to shift the smallest eigenvalues close to one where most of the eigenvalues of the preconditioned matrix should be located. In this work, we study these various variants as well as the observed numerical behaviour on a set of model problems from the Matrix Market or arising from the discretization of some 2D heterogeneous diffusion PDE problems via finite-element techniques. We discuss their numerical efficiency, computational complexity and sensitivity to the accuracy of the eigencalculation.

For more details on this work we refer to [1].

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- [1] L. Giraud, D. Ruiz, and A. Touhami. A comparative study of iterative solvers exploiting spectral information for SPD systems. Technical Report TR/PA/04/40, CERFACS, Toulouse, France, 2004.

4.4 Convergence in backward error of relaxed GMRES

L. Giraud: CERFACS, *France*; **S. Gratton:** CERFACS, *France*; **J. Langou:** UNIVERSITY OF TENNESSEE, *USA*

This work is the follow up of the experimental study presented in [1]. It is based on and extends some theoretical results in [3, 4]. In a backward error framework, we study the convergence of GMRES when the matrix-vector products are performed inaccurately. This inaccuracy is modelled by a perturbation of the original matrix. We prove the convergence of GMRES when the perturbation size is proportional to the inverse of the computed residual norm; this implies that the accuracy can be relaxed as the method proceeds which gives rise to the terminology relaxed GMRES. As for exact GMRES, we show under proper assumptions that only happy breakdowns can occur. Furthermore, the convergence can be detected using a by-product of the algorithm. We explore the links between relaxed right-preconditioned GMRES and flexible GMRES. In particular this enables us to derive a proof of convergence of FGMRES. Finally we report results on numerical experiments to illustrate the behaviour of the relaxed GMRES monitored by the proposed relaxation strategies.

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4.5 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 accurate the matrix-vector product is approximated, 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, 3]. 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 strategies may yield a significant reduction of the computing time while the target accuracy is still achieved. However, they are far from being well understood theoretically and experimentally. On the theoretical side, some progress has been made by using the theory of Homotopic Deviation, see Section 5.2 for more information on this. We describe below some algorithmic advances which are supported by extensive numerical evidence. The research that we describe has (in part) been carried out in collaboration with the University of Utrecht and was supported through the Van Gogh programme for Dutch-French scientific collaborations.

In [5] we have investigated the possibility of increasing the computational gain that can be obtained by applying a relaxation strategy using a *nested* Krylov method. The advantage of this approach is that the matrix-vector products in the inner loop only have to be computed to a low accuracy. The accurate matrix-vector products in the outer loop ensure that the target accuracy can be achieved. A revised and improved version of [5] has been accepted for publication in JCAM.

In the past year we have progressed in two different ways. Firstly we have studied a suitable strategy to control the error in the matrix-vector multiplications in restarted GMRES. Our first observation is that restarted GMRES is a nested method, with full GMRES in the inner loop (in which only a modest residual reduction has to be achieved) and Richardson's method in the outer loop. We have found that there are two different ways to control the errors, and the appropriate way depends on how the residuals are updated. If the residuals are computed recursively a relaxation strategy should be applied. If the residuals are computed directly from the latest iterand, however, a similar strategy as for Newton's method has to be employed, i.e. in the beginning of the process, the matrix-vector products can be performed with low accuracy, while the accuracy has to be increased when the approximate solution comes closer to the true solution. Our results were presented during a mini-symposium on inner-outer iterative methods (organised by M. van Gijzen) at the NAA'04 conference in Rousse, Bulgaria. [4] has been accepted for publication in a volume of Lecture Notes in Computer Science (Springer).

We have also made progress in the theoretical understanding of the relaxation strategies. In [6] we provide insight into why some iterative methods are more sensitive to errors in the matrix-vector product than others. The key observation is that the sensitivity for errors in the matrix-vector product is determined by the conditioning of the basis vectors to which the matrix-vector product is applied. The paper [6] has been accepted for publication in the proceedings of the Third International Workshop on Numerical Analysis and Lattice QC.

As part of the partnership between EDF and CERFACS, consulting work was carried out with N. Megrez, a visiting post-doc from UT1 (Ceremath), in which we have analysed a nested algorithm for multi-phase flow calculations. One of the main difficulties in the present formulations is that special precautions have to be taken to preserve positive volume fractions. In this work we have suggested alternative formulations of the current algorithm for which we can derive a time-step such that positive volume fractions are always preserved.

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4.6 Bounds on the eigenvalue range and on the field of values of non-Hermitian and indefinite finite element matrices

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In the beginning of the seventies, Fried [1] formulated bounds on the spectrum of assembled Hermitian (semi-)Positive Definite finite-element matrices using the extreme eigenvalues of the element matrices.

Since element matrices are small in size relative to the assembled matrix, these eigenvalue bounds are cheap to compute.

We have generalised the bounds proposed by Fried for non-Hermitian and indefinite matrices. In particular, we have derived bounds on the Field of Values, on the spectrum and on the numerical radius for both the standard and the generalised problem.

We have illustrated our bounds with an example from acoustics that involves a complex, non-Hermitian matrix.

As an application, we have used our estimates in the GMRES algorithm for solving linear systems, to derive an upper bound on the number of iterations that is needed to achieve a residual norm that is smaller than a given tolerance.

We presented our results at the ICCAM 2004 conference in Leuven. The report [2] has been submitted for publication in JCAM.

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4.7 Combining direct and iterative methods for the solution of large systems in different application areas

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We first consider the size of problems that can currently be solved by sparse direct methods. We then discuss the limitations of such methods, where current research is going in moving these limitations, and how far we might expect to go with direct solvers in the near future.

This leads us to the conclusion that very large systems, by which we mean three dimensional problems in more than a million degrees of freedom, require the assistance of iterative methods in their solution. However, even the strongest advocates and developers of iterative methods recognize their limitations when solving difficult problems, that is problems that are poorly conditioned and/or very unstructured. It is now universally accepted that sophisticated preconditioners must be used in such instances.

A very standard and sometimes successful class of preconditioners are based on incomplete factorizations or sparse approximate inverses, but we very much want to exploit the powerful software that we have developed for sparse direct methods over a period of more than thirty years. We thus discuss various ways in which a symbiotic relationship can be developed between direct and iterative methods in order to solve problems that would be intractable for one class of methods alone. In these approaches, we will use a direct factorization on a “nearby” problem or on a subproblem.

We then look at examples using this paradigm in four quite different application areas; the first solves a subproblem and the others a nearby problem using a direct method.

We presented this work [1] at a conference in Delhi in December 2004.

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4.8 Parallel preconditioners based on partitioning sparse matrices

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

We describe a method for constructing an efficient block diagonal preconditioner for accelerating the iterative solution of general sets of sparse linear equations. Our method uses a hypergraph partitioner on a scaled and sparsified matrix and attempts to ensure that the diagonal blocks are nonsingular and dominant. We illustrate our approach using the partitioner PaToH and the Krylov-based GMRES algorithm. We verify our approach with runs on problems from economic modelling and chemical engineering, traditionally difficult applications for iterative methods. Our approach and the block diagonal preconditioning lends itself to good exploitation of parallelism. This we also demonstrate. We presented the work at the PMAA'04 conference in Marseilles and have submitted it to the Journal Parallel Computing [1].

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4.9 Rounding error analysis of the classical Gram-Schmidt orthogonalization process

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In many applications it is important to compute an orthonormal basis $Q = (q_1, \dots, q_n)$ of $\text{span}(A)$ such that $A = QR$, where R is upper triangular matrix of order n . In this work we focus on the Classical Gram-Schmidt (CGS) orthogonalization process. Due to roundoff errors the set of vectors Q produced by this method can be far from orthogonal and sometimes the orthogonality can even be completely absent. In this work we provide two results on the numerical behaviour of the classical Gram-Schmidt algorithm that enable us to predict the level of orthogonality (*the quality*) obtained after the orthogonalization. Up to now there was no bound available for the loss of orthogonality of vectors computed by the CGS process. In the first part of the work, we derive a new bound for the loss of orthogonality in the CGS process. Provided that the matrix $A^T A$ is numerically nonsingular, we show that the loss orthogonality of the vectors computed by the CGS algorithm can be bounded by a term proportional to the square of the condition number, i.e. $\kappa^2(A)$, times the unit roundoff. We illustrate through an numerical experiment that this bound is indeed tight.

In some other applications it may be important to produce a set of basis vectors for which the orthogonality is close to the machine precision. In this case the orthogonality of the vectors computed by a Gram-Schmidt process can be improved by reorthogonalization, where the orthogonalization step is iterated twice. In the second part of this work we analyse the CGS algorithm with reorthogonalization, where each orthogonalization step is performed exactly twice. The main result of this section is a proof of the fact that, assuming full rank of the matrix A , two iterations are sufficient to guarantee that the level of orthogonality of the computed vectors is close to the unit roundoff level.

These results are important from a theoretical point of view; they fill the last gaps in the understanding of the Classical Gram-Schmidt algorithm. From a computational point of view, these results are very useful; they enable us to choose the fastest algorithm depending on the level of orthogonality needed by the application on a given computing platform.

For more details on this work we refer to [1].

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4.10 On the parallel solution of large industrial wave propagation problems

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G. Sylvand: EADS-CCR, *France*

The use of Fast Multipole Methods (FMM) combined with embedded Krylov solvers preconditioned by a sparse approximate inverse is investigated for the solution of large linear systems arising in industrial acoustic and electromagnetic simulations. We use a boundary elements integral equation method to solve the Helmholtz and the Maxwell equations in the frequency domain. The resulting linear systems are solved by iterative solvers using FMM to accelerate the matrix-vector products. The simulation code is developed in a distributed memory environment using message passing and it has out-of-core capabilities to handle very large calculations. When the calculation involves one incident wave, one linear system has to be solved. In this situation, embedded solvers can be combined with an approximate inverse preconditioner to design extremely robust algorithms. For radar cross section calculations, several linear systems have to be solved. They involve the same coefficient matrix but different right-hand sides. In this case, we propose a block variant of the single right-hand side scheme. The efficiency, robustness and parallel scalability of our approach are illustrated on a set of large academic and industrial test problems.

For more details on this work we refer to [1].

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5 Qualitative Computing

Group members: Françoise Chaitin-Chatelin, Morad Ahmadnasab, CERFACS and Université Toulouse 1.

The work on Qualitative Computing Group is an on-going collaborative effort to assess the validity of computer simulations. The central question is to assess the validity of 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.

These laws for finite-precision computations are derived from underlying laws for mathematical computation. These more basic laws stem mainly from analysis in complex variables and matrix algebra. We are currently focusing on three aspects:

- a) the basic role of *multiplication* and nonlinearities in computer simulations using floating-point arithmetic,
- b) *inexact computing* and the associated homotopic deviation theory as a fruitful framework to understand approximate numerical methods, in exact arithmetic,
- c) the unreasonable robustness of Krylov-type methods to perturbations in the data.

Our research and understanding is driven by work on practical numerical software applications in physics and technology, which come from CERFACS partners. The long established collaboration with the EDF on Numerical Quality continues (Jean-Louis Vaudescal, and Olivier Boiteau). Françoise Chaitin-Chatelin was one of the 5 external experts in charge of the review, for EDF Scientific Council, (May 2004) of their ambitious programme to turn to “Numerical Simulation only” (Tout numérique) by the 2010 horizon.

We review below the work accomplished in 2004 with respect to Numerical Reliability.

5.1 Nonlinearities in computing simulations with floating-point arithmetic

General purpose computers use a floating-point representation for real numbers in a given base β (most often $\beta = 2$). As a consequence, the distribution of the digits in any result of a sequence of arithmetic operations including at least 3 multiplications depends on their rank in the representation in the base β . The trailing digits are uniformly distributed, which allows us to use finite-precision arithmetic. But the leading digits are *not* equally distributed. For $\beta = 10$, the first digit is 1 with a probability more than 6 times that of being 9 (Newcomb, 1881). This result is well explained by a little known central limit theorem of P. Lévy (1939): the addition of random variables mod 1 has a uniform limit distribution [6].

This experimental fact has not received much attention from software developers, despite its crucial consequences for the assessment of the reliability of computer simulations. One reason is that it

contradicts the better-known theorem of E. Borel (1909) according to which *all* digits are equally distributed [6].

The reason behind this apparent contradiction lies in the difference in writing a real number x in *fixed* (i) or in *floating point* (ii) representation [6]. Let $[x]$ (resp. $\{x\}$) denote the integer (resp. fractional) part of $x \in \mathbb{R}$: $\{x\} = x \bmod 1$ in $[0, 1[$. Therefore (i) $x = [x] + \{x\}$, or (ii), in a given base β , $x = \beta^{\log_\beta x} = \beta^{\lfloor \log_\beta x \rfloor} \beta^{\{\log_\beta x\}}$.

The first representation (i) is additive, whereas the second one (ii) is multiplicative: it leads to the floating-point representation in computer arithmetic. The mantissa is $\beta^{\{\log_\beta x\}-1}$ and the exponent is $\lfloor \log_\beta x \rfloor + 1$ in base β [6, 3, 2].

The Newcomb-Borel paradox comes from the *nonlinear* aspect of most computations. It exemplifies one of the formidable difficulties in the assessment of the validity of computer simulations. Should they be assessed against results which are exact in Mathematics (according to Borel)? Or should they be assessed against the reality of Experimental Sciences (according to Newcomb)? The validity of computer simulations realized with the best software strongly depends on the answer to this question which often remains *implicit* [6].

An equally important consequence of Lévy's central limit theorem is concerned with the repeated multiplication of complex numbers. The arguments, which add mod 2π , tend to be uniformly distributed on $[0, 2\pi[$.

The phenomenon can be perceived in the multiplication of numbers which are more than real or complex scalars (that is real vectors of dimension 1 or 2). It can be perceived in hypercomplex multiplication [5, 6]. This has important consequences not only for floating-point computation, but also for fundamental physics in connection with number theory [1, 5, 2].

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5.2 Inexact computing and homotopic deviation

To study the robustness of approximation methods to large perturbations, it is useful to consider the linear coupling $A + tE$, where $A, E \in \mathbb{C}^{n \times n}$ 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 linear dependence on a parameter $t \in \mathbb{C}$, of the form $A(t) = A + tE$ has been particularly studied [9, 10, 7].

We consider the resolvent field $z \mapsto R(t, z) = (A + tE - zI)^{-1}$ for $t \in \mathbb{C}$. Its singularities as t varies define the spectral field $t \mapsto \sigma(A(t))$ which denotes the spectrum of $A(t)$. For $z \in \text{re}(A) = \mathbb{C} \setminus \sigma(A)$, we use the *multiplicative* representation

$$(A + tE - zI)^{-1} = (A - zI)^{-1} (I + tE(A - zI)^{-1})^{-1}.$$

For a fixed z in $\text{re}(A)$, the map $t \mapsto R(t, z)$ is analytic for $|t| < 1/\rho(E(A - zI)^{-1})$ [9, 10].

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 $0 \in \sigma(E)$. The rank deficient matrix E is called the *deviation*, and the term “perturbation” covers the case where $|t|||E||$ is limited, E being possibly of full rank. Our work provides an elementary analysis for $z, t \in \widehat{\mathbb{C}} = \mathbb{C} \cup \infty$ of singular perturbation theory for matrices, since E is singular in the case of interest. The elementary approach of Homotopic Deviation is driven by algorithmic considerations arising from the Sherman-Morrison formula. The key role of the structure of $0 \in \sigma(E)$ emerges naturally from a computational perspective [2, 3, 4].

Linearization of quadratic eigenproblems often leads to a situation where $0 \in \sigma(E)$ is semi-simple. [8] treats an example from computational acoustics, where t represents the complex admittance.

The theoretical resolution of the general case ($0 \in \sigma(E)$ is defective) in [3, 4] has led to a fresh look at the important works of Puiseux and Lidskii [5, 6] with respect to the Schur complement of a partitioned matrix.

This uncovers new computational challenges which can be addressed by an appropriate modification of the simple Homotopic Deviation theory [6]. The key point is that when a matrix is partitioned into 4 blocks with 2 invertible diagonal blocks there exist *two* dual Schur complements associated with its inverse, leading to a polynomial and a rational form.

Interaction with F. Bazan was instrumental in directing our attention to matrix polynomials. [1] studies the rational fraction

$$M_z = (\det(zI - A))^{-1} V^H \operatorname{adj}(zI_n - A) U,$$

where $E = UV^H$, $U, V \in \mathbb{C}^{n \times r}$, $r < n$.

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5.3 Robustness of Krylov type methods

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]. To study the dynamics of this 2-level algorithm, we perform a homotopic deviation of the matrix of order $k+1$

$$B = \begin{pmatrix} H_k & u \\ 0 & a \end{pmatrix},$$

such that

$$H_{k+1} = \begin{pmatrix} H_k & u \\ 0 & h_{k+1,k} & a \end{pmatrix}.$$

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

An analysis of $h \mapsto \{(H^+ - zI)^{-1}, \sigma(H^+)\}$ is performed in [2, 3, 1] under specific assumptions which ensure that the generic theory of Lidskii can be applied. The paper [3] is a written version of the *keynote presentation* that Françoise Chaitin-Chatelin was invited to present at NAA 2004 in Rousse, Bulgaria. The talk was actually delivered by M. van Gijzen.

The restrictive conditions placed by the generic approach of Lidskii have been relaxed in [4]. Numerical experiments were performed by M. Ahmadnasab to illustrate how finite-precision affects the mathematical theory.

Preliminary results indicate that finite-precision computation tends, in this case, to reproduce the mathematical reality much more faithfully than we are accustomed to. If this is confirmed, this phenomenon is yet another reason to marvel at the “unreasonable” robustness of Krylov methods to perturbations.

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6 Nonlinear Systems and Optimization

6.1 An investigation of incremental 4D-Var using non-tangent linear models

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We investigate the convergence of incremental four-dimensional variational data assimilation (4DVar) when an approximation to the tangent linear model is used within the inner loop. Using a semi-implicit semi-Lagrangian model of the one-dimensional shallow water equations, we perform data assimilation experiments using an exact tangent linear model and using an inexact linear model (i.e. perturbation forecast model). We find that the two assimilations converge at a similar rate and analysis are also similar, with the difference between them dependent on the amount of noise in the observations. To understand the numerical results we present the incremental 4D-Var algorithm as a Gauss-Newton iteration for solving a least-squares problem and consider its fixed points.

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6.2 Recursive trust-region methods for multiscale nonlinear optimization

S. Gratton: CERFACS, *France*; **A. Sartenaer:** FUNDP, *Belgium*; **Ph. L. Toint:** FUNDP, *Belgium*

A class of trust-region methods is presented for solving unconstrained nonlinear and possibly nonconvex discretized optimization problems, like those arising in systems governed by partial differential equations. The algorithms in this class make use of the discretization level as a means of speeding up the computation of the step. This use is recursive, leading to true multilevel/multiscale optimization methods reminiscent of multigrid methods in linear algebra and the solution of partial-differential equations. Global convergence of the recursive algorithm is proved to first-order stationary points on the fine grid. A new theoretical complexity result is also proved for single- as well as multiscale trust-region algorithms, that gives a bound on the number of iterations that are necessary to reduce the norm of the gradient below a given threshold.

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- [1] S. Gratton, A. Sartenaer, and Ph. L. Toint. Recursive trust-region methods for multiscale nonlinear optimization: Global convergence and complexity. Technical Report, CERFACS, Toulouse, France, 2005. In preparation.

6.3 Partial condition number for linear least-squares problems

M. Arioli: RUTHERFORD APPLETON LABORATORY, *England*; **M. Baboulin:** CERFACS, *France*;
S. Gratton: CERFACS, *France*

We consider here the linear least-squares problem $\min_{y \in \mathbb{R}^n} \|Ay - b\|_2$ where $b \in \mathbb{R}^m$ and $A \in \mathbb{R}^{m \times n}$ is a matrix of full column rank n and we denote its solution by x . We assume that both A and b can be perturbed and that these perturbations are measured using Frobenius norms. In this paper, we are concerned with the condition number of a linear function of x ($L^T x$ where $L \in \mathbb{R}^{n \times k}$) for which we provide an exact formula. This quantity requires the computation of the singular values and the right singular vectors of the matrix A , which can be very expensive in practice. This is why we also propose a statistical method based on [2] that estimates this condition number by using the exact condition numbers in random orthogonal directions. Provided the triangular R factor of A from $A^T A = R^T R$ is available, this statistical approach enables the computation of a condition estimate in $\mathcal{O}(n^2)$. We also address the question of the numerical reliability of this statistical estimate. In the case where the perturbation of A is measured using the spectral norm, though we do not have a closed formula for the condition number, we provide sharp estimates. The theoretical results and numerical experiments related to this study are presented in [1].

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- [1] M. Arioli, M. Baboulin, and S. Gratton. Partial condition number for linear least squares problems. Technical Report TR/PA/04/111, CERFACS, Toulouse, France, 2004.
 - [2] C. S. Kenney, A. J. Laub, and M. S. Reese. Statistical condition estimation for linear least squares. *SIAM J. Matrix Analysis and Applications*, 19:906–923, 1998.

6.4 Sensitivity of some spectral preconditioners

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

It is well known that the convergence of the conjugate gradient method for solving symmetric positive definite linear systems depends to a large extent on the eigenvalue distribution. In many cases, it is observed that “removing” the extreme eigenvalues can greatly improve the convergence. Several preconditioning techniques based on approximate eigenlements have been proposed in the past few years that attempt to tackle this problem. The proposed approaches can be split into two main families depending on whether the extreme eigenvalues are moved exactly to one or are shifted close to one. The first technique is often referred to as the deflating approach, while the latter is referred to as the coarse grid preconditioner by analogy to techniques first used in domain decomposition methods. Many variants exist in the two families that reduce to the same preconditioners if the exact eigenlements are used. In this work, we investigate the behaviour of some of these techniques when the eigenlements are only known approximately. We use the perturbation theory for eigenvalues and eigenvectors to investigate the behaviour of the spectrum of the preconditioned systems using a first order approximation. We illustrate the sharpness of the first order approximation and show the effect of the inexactness of the eigenlements on the behaviour of the resulting preconditioner when applied to accelerate the conjugate gradient method. We show how this analysis can be used to screen spectral information in the case of a sequence of SPD linear systems occurring in a nonlinear process. Such an application can be seen in variational data assimilation [1] where the Gauss-Newton methods consist in solving a sequence of normal equations.

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- [1] M. Fisher. Minimization algorithms for variational data assimilation. In *Recent Developments in Numerical Methods for Atmospheric Modelling*, pages 364–385. ECMWF, 1998.
 - [2] L. Giraud and S. Gratton. On the sensitivity of some spectral preconditioners. Technical Report TR/PA/04/108, CERFACS, Toulouse, France, 2004.

6.5 A parallel packed storage scheme for large dense symmetric calculations

M. Baboulin: CERFACS, France; L. Giraud: CERFACS, France; S. Gratton: CERFACS, France

Large symmetric matrices appear in many scientific applications notably in the area of geodesy and electromagnetics. Considering that the standard parallel libraries ScaLAPACK [2] and PLAPACK [3] do not provide packed storage for symmetric matrices, we investigate a ScaLAPACK-based implementation that exploits the symmetry of the matrix for the Cholesky factorization and the computation of the R factor in the QR factorization. We discuss in [1] the choice of the data structure in terms of optimizing the storage (nearly half that of the whole matrix) and obtaining an implementation that is as scalable and as efficient as ScaLAPACK and PLAPACK for any processor count.

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- [1] M. Baboulin, L. Giraud, and S. Gratton. A packed storage scheme for large dense symmetric calculations. Technical report, CERFACS, Toulouse, France. In preparation.
 - [2] L. S. Blackford, J. Choi, A. Cleary, E. D’Azevedo, J. Demmel, I. Dhillon, J. Dongarra, S. Hammarling, G. Henry, A. Petitet, K. Stanley, D. Walker, and R. C. Whaley. *ScaLAPACK Users’ Guide*. SIAM, 1997.
 - [3] R. A. Van de Geijn. *Using PLAPACK*. The MIT Press, 1997.

6.6 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 handle very large problems on distributed memory computers. A first step has been achieved by developing a parallel distributed implementation of an out-of-core least-squares solver based on the normal equations method. This parallel code computes the upper-triangular part of the normal equations matrix $A^T A$ and the right-hand side $A^T b$ by mixing OpenMP and MPI, and the performance obtained is close to the peak performance of the computer on a matrix-matrix multiply. It also performs a Cholesky factorization requiring only half the storage needed by the standard parallel libraries ScaLAPACK [3] and PLAPACK [4]. Our solver uses a J-variant Cholesky algorithm [1, 5] 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 comparisons with ScaLAPACK and PLAPACK on our target applications are presented in [2]. These applications arise from the Earth’s gravity field calculation and computational electromagnetics. The next step of this work will consist in using orthogonal transformations in order to improve the numerical robustness.

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- [1] E. Anderson and J. Dongarra. Evaluating block algorithm variants in LAPACK. Lapack working note 19, University of Tennessee, 1990. SIAM Conference on Parallel Processing for Scientific Computing.
 - [2] M. Baboulin, L. Giraud, and S. Gratton. A parallel distributed solver for large dense symmetric systems: applications to geodesy and electromagnetism problems. Technical Report TR/PA/04/16, CERFACS, Toulouse, France, 2004.
 - [3] L. S. Blackford, J. Choi, A. Cleary, E. D’Azevedo, J. Demmel, I. Dhillon, J. Dongarra, S. Hammarling, G. Henry, A. Petitet, K. Stanley, D. Walker, and R. C. Whaley. *ScaLAPACK Users’ Guide*. SIAM, 1997.
 - [4] R. A. Van de Geijn. *Using PLAPACK*. The MIT Press, 1997.
 - [5] J.M. Ortega and C. H. Romine. The ijk forms of factorization methods II. Parallel systems. *Parallel Computing*, 7:149–162, 1988.

7 Conferences and Seminars

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

January

SVG Meeting, Stanford, California, 9-10 January, 2004. I. S. DUFF, *Jim Varah, Alan George, and Mike Saunders*, Keynote (after dinner) talk.

North Carolina A&T University seminar, January 15, 2004. M. B. VAN GIJZEN, *Two-level parallelism in a Stream-Function model for Global Ocean Circulation*, invited talk.

Séminaire Université Montpellier 2, 27 January 2004. F. CHAITIN-CHATELIN, *Calcul Matriciel: entre Algèbre et Géométrie*, invited talk.

February

Grand Séminaire d'Ouverture, Université Paul Sabatier, Toulouse, 5 February 2004. F. CHAITIN-CHATELIN, *Le Sens des Nombres*, invited talk.

Utrecht University seminar, February 18, 2004. M. B. VAN GIJZEN, *Solution methods for block systems from oceanography*, joint work with Daniel Loghin, invited talk.

Sandia National Lab. seminar, Livermore, California, February 23, 2004. L. GIRAUD, *Are two-level spectral preconditioners related to two-grid cycles?*, joint work with B. Carpentieri and S. Gratton, invited talk.

Delft University of Technology seminar, February 24, 2004. M. B. VAN GIJZEN, *Two-level parallelism in a Stream-Function model for Global Ocean Circulation*, invited talk.

SIAM Conference on Parallel Processing, San Francisco, California, U.S.A. 24-27 February, 2004. I. S. DUFF, Organizing Committee.

SIAM Conference on Parallel Processing for Scientific Computing, San Francisco, U.S.A., February 25-27, 2004. P. A. AMESTOY, *GRID-TLSE: a web site for experimenting with sparse direct solvers on a computational grid*, joint work with I. S. Duff, L. Giraud, J.-Y. L'Excellent and C. Puglisi, invited minisymposium.

SIAM Conference on Parallel Processing, San Francisco, U.S.A., February 25-27, 2004. M. BABOULIN, *Parallel distributed Cholesky factorization for in-core large dense problems*, joint work with L. Giraud and S. Gratton, contributed talk.

SIAM Conference on Parallel Processing for Scientific Computing, San Francisco, U.S.A., February 25-27, 2004. T.A. DRUMMOND, *Partitioning strategies for the block Cimmino algorithm*, joint work with I. S. Duff and D. Ruiz, invited minisymposium.

SIAM Conference on Parallel Processing, San Francisco, California, U.S.A. 24-27 February, 2004. L. GIRAUD, *Parallel Algebraic Preconditioners for the Solution of Schur Complement Systems*, joint work with J. C. Rioual and S. Mulligan, invited minisymposium.

Combinatorial Scientific Computing Worksop, San Francisco, California, U.S.A. 27-28 February, 2004. P. R. AMESTOY, *Unsymmetric Orderings Using A Constrained Markowitz Scheme*, joint work with X. S. Li and S. Pralet, contributed talk.

Combinatorial Scientific Computing Worksop, San Francisco, California, U.S.A. 27-28 February, 2004. S. PRALET, *Symmetric weighted matching and applications to indefinite multifrontal solvers*, joint work with I. S. Duff, contributed talk.

March

8th Copper Mountain Conference on Iterative Methods, Colorado, U.S.A., March 28–April 2, 2004. I. S. DUFF, Organizing committee, Workshop chair.

8th Copper Mountain Conference on Iterative Methods, Colorado, U.S.A., March 28–April 2, 2004. B. CARPENTIERI, *Two grid spectral preconditioning for general sparse linear systems*, joint work with L. Giraud and S. Gratton, contributed talk.

April

NERSC seminar, Lawrence Berkeley National Laboratory, California, U.S.A., April 5, 2004. B. CARPENTIERI, *Matrix-free preconditionings of dense linear systems from electromagnetics*, joint work with I. S. Duff, L. Giraud and G. Sylvand, invited talk.

May

Helmholtz Review Meeting, Cologne and Jülich, Germany. 3-5 May, 2004. I. S. DUFF, Member of review committee.

Review of CMUP (Mathematics Department), Porto, Portugal. 10-14 May, 2004. I. S. DUFF, Member of review committee.

June

ICCS 04 Conference, Karkow, Poland. 6-10 June, 2004. I. S. DUFF, *Combining direct and iterative methods for the solution of large sparse systems in different application areas*, keynote lecture.

Oxford/RAL Computational Mathematics and Applications Seminar, Rutherford Appleton Laboratory, UK, June 10. S. GRATTON, *Practical implementation of an inexact GMRES method*, joint work with L. Giraud and J. Langou, invited talk.

PARA04 Conference, Copenhagen, Denmark. 20-23 June, 2004. I. S. DUFF, *Partitioning and parallelism in the solution of large sparse systems*, invited speaker.

Conference on Numerical Analysis and Applications, Bulgaria, June 30, 2004. F. CHAITIN-CHATELIN, *The dynamics of matrix coupling with an application to Krylov methods*, keynote lecture.

Conference on Numerical Analysis and Applications, Bulgaria, June 30, 2004. M. B. VAN GIJZEN, *Restarted GMRES with inexact matrix-vector products*, joint work with J. van den Eshof and G. Sleijpen, invited minisymposium.

July

ICCAM 2004, International Congress on Computational and Applied Mathematics, Katholieke Universiteit Leuven, Belgium, July 26-30, 2004. M. BABOULIN, *Partial condition number for linear least squares problems*, joint work with M. Arioli and S. Gratton, contributed talk.

ICCAM 2004, International Congress on Computational and Applied Mathematics, Katholieke Universiteit Leuven, Belgium, July 26-30, 2004. M. B. VAN GIJZEN, *Bounds on the eigenvalue range and on the field of values of non-Hermitian and indefinite finite element matrices*, joint work with D. Loghin and E. Jonkers, contributed talk.

Thesis defence of Abdou Guermoche, Lyon, France. 28 July, 2004. I.S. DUFF, Rapporteur and member of jury.

August

Karl-Franzens Universität seminar, Graz, Austria, August 23, 2004. B. CARPENTIERI, *High-performance algorithms for solving large dense systems in electromagnetism*, joint work with G. Alléon, I. S. Duff, L. Giraud, E. Martin and G. Sylvand, invited talk

September

IMA Anniversary Meeting, Manchester, England, 2 September, 2004. I. S. DUFF, Attendee.

Conference in Chalkis, Greece, 11-14 September, 2004. I. S. DUFF, *Partitioning and parallelism in the solution of large sparse systems*, invited speaker

Interdisciplinary Workshop on Developments in Boundary Element Methods for Acoustics and Electromagnetics, University of Reading, Reading, U.K., September 15-18, 2004. B. CARPENTIERI, *High-performance iterative solution of large dense systems from electromagnetics*, joint work with G. Alléon, I. S. Duff, L. Giraud, E. Martin and G. Sylvand, contributed talk.

Wake Forest University seminar, September 30, 2004. M. B. VAN GIJZEN, *Bounds on the eigenvalue range and on the field of values of non-Hermitian and indefinite finite element matrices*, joint work with D. Loghin and E. Jonkers, invited talk.

October

Bath-RAL NA Day, Bath, England. 1 October, 2004. I. S. DUFF, Attendee.

Parallel Matrix Algorithms and Applications (PMAA'04), CIRM, Marseille, 20-22 October, 2004. S. GRATTON, *Convergence of an inexact GMRES method*, joint work with L. Giraud and J. Langou, contributed talk.

Parallel Matrix Algorithms and Applications (PMAA'04), CIRM, Marseille, 20-22 October, 2004.
L. GIRAUD, *Algebraic two-level spectral preconditioners for general linear systems*, joint work with B. Carpentieri and S. Gratton, contributed talk.

Parallel Matrix Algorithms and Applications (PMAA'04), CIRM, Marseille, 20-22 October, 2004.
A. GUERMOUCHE, *Hybrid scheduling strategies for the parallel multifrontal method*, joint work with P. R. Amestoy and J.-Y. L'Excellent and S. Pralet, contributed talk.

Lecturing to Institute of Mathematics, Cybernetics and Physics (ICIMAF) of the Ministry of Science, Technology and Environment, Havana, Cuba. 23 October - 1 November, 2004. I. S. DUFF, invited visitor.

December

International Conference on Industrial and Applied Mathematics, New Delhi, India. 4-6 December, 2004. I. S. DUFF, *Combining direct and iterative methods for the solution of large systems in different application areas*, invited talk.

7.2 Conferences and seminars organized by the Parallel Algorithms Project

February

SIAM Conference on Parallel Processing, San Francisco, California, U.S.A. 24-27 February, 2004
I. S. DUFF AND L. GIRAUD, Minisymposium organizers, *Hybrid direct/iterative techniques for the solution of large linear systems:*

Parallel Algebraic Preconditioners for the Solution of Schur Complement Systems,

L. GIRAUD (CERFACS, France).

Combining Direct and Iterative Methods to Solve Partitioned Linear Systems,

F. KWOK (Stanford University, U.S.A.).

Partitioning Strategies for the Block Cimmino Algorithm

L. A. DRUMMOND (NERSC, U.S.A.).

SIAM Conference on Parallel Processing, San Francisco, California, U.S.A. 24-27 February, 2004
I. S. DUFF AND S. LI, Minisymposium organizers, *Parallel sparse direct methods and preconditioning:*

GRID-TLSE: A Web site for experimenting with sparse direct solvers on a computational grid,

P. R. AMESTOY (ENSEEIH-IRIT, France).

SBBB orderings and parallel direct solvers,

J. SCOTT (RAL, U.K.)

Performance evaluation of the recent developments in parallel SuperLU,

L. GRIGORI (INRIA-Lorraine, France).

Recent advances in sparse linear solver technology for semiconductor device simulation matrices,

O. SCHENK (University of Basel, Switzerland).

Parallel multifrontal method with improved memory usage,

A. GUERMOUCHE (LIP-ENS Lyon, France).

Data mapping techniques for parallel sparse factorization,

K. MALKOWSKI (Pennsylvania State University, U.S.A.).

PHIDAL: a parallel multilevel linear system solver based on a hierarchical,

P. HÉNON (INRIA-Futurs, France).

High performance complete and incomplete block factorizations based on Scotch and PaStiX,

J. ROMAN (INRIA-Futurs, France).

June

Sparse Days Meeting at CERFACS, June 2-3, 2004,

Complete pivoting ILU: a multilevel framework,

Y. SAAD (University of Minnesota, U.S.A.).

Inexact Gauss-Newton methods with applications in numerical weather and ocean prediction,

N. NICHOLS (Reading University, U.K.).

Preconditioning Lanczos approximations to the matrix exponential,

J. VAN DEN ESHOF (Heinrich Heine University, Germany)

Augmented Lagrangian techniques for solving saddle point linear systems,

C. GREIF (University of British Columbia, Canada).

Symmetric weighted matchings for LDL^T preconditioning of symmetric indefinite matrices,

M. HAGEMANN (University of Basel, Switzerland).

Adaptive methods for updating/downdating page ranks,

G. GOLUB (Stanford, U.S.A.).

Stiff systems of ODEs and sparse matrix techniques,

S. SKELBOE (University of Copenhagen, Denmark).

V-invariant methods, generalised least squares problems, and the Kalman filter,

M. OSBORNE (Australian National University, Canberra).

Sparse Gaussian elimination as a computational paradigm,

E. LOUTE (Universit Catholique de Louvain, Belgium).

A new sparse out-of-core symmetric indefinite factorization algorithm,

O. MESHAR (Tel-Aviv University, Israel).

A numerical evaluation of sparse direct solvers for the solution of large, sparse, symmetric linear systems of equations,

J. SCOTT (RAL, U.K.).

The snap-back pivoting method for symmetric banded indefinite matrices,

D. IRONY (Tel-Aviv University, Israel).

List of participants.

M. AHMADNASAB (Universit Toulouse 1, France), P. AMESTOY (ENSEEIH-IRIT, France), M. BABOULIN (CERFACS, France), F. BAZAN (Universidade Federal de Santa Catarina, Brazil), B. CARPENTIERI (CERFACS, France), I. S. DUFF (CERFACS, France), V. EIJKHOUT (University of Tennessee, U.S.A), L. GIRAUD (CERFACS, France), G. GOLUB (Stanford University, U.S.A), S. GRATTON (CERFACS, France), C. GREIF (The University of British Columbia, Canada), R. GUIVARCH (ENSEEIH-IRIT, France), M. HAGEMANN (Universitt Basel, Switzerland), C. HAMERLING (CERFACS, France), D. IRONY (Tel-Aviv University, Isral), E. JONKERS (Delft University, The Netherlands), D. LOGHIN (CERFACS, France), E. LOUTE (CORE & POMS/IAG, Belgium), E. MARTIN (CERFACS, France), N. MEGREZ (Universit Toulouse 1, France), O. MESHAR (Tel-Aviv University, Isral), E. NG (Lawrence Berkeley National Lab., U.S.A), N. NICHOLS (The University of Reading, U.K.), M. OSBORNE (Australian National University, Australia), S. PRALET (CERFACS, France), C. PUGLISI (ENSEEIH-IRIT, France), S. RIYAVONG (CERFACS, France), M. ROJAS (Wake Forest University, U.S.A), D. RUIZ (ENSEEIH-IRIT, France), Y. SAAD (University of Minnesota, U.S.A), J. SCOTT (RAL, U.K.), S. SKELBOE (University of Copenhagen, Denmark), A. SWART (Utrecht University, The Netherlands), A. TOUHAMI (ENSEEIH-IRIT, France), J. VAN DEN ESHOF (Heinrich Heine University Düsseldorf, Germany), and M. VAN GIJZEN (CERFACS, France).

Conference on Numerical Analysis and Applications, Bulgaria, June 30, 2004, M. B. VAN GIJZEN, Minisymposium organizer, *Inner-outer iterations:*

Restarted GMRES with inexact matrix-vector products,

M. B. GIJZEN, (CERFACS, France).

Preconditioned methods for the matrix exponential,

J. VAN DEN ESHOF, (Heinrich Heine University Düsseldorf, Germany).

Nested iterations and strengthened Cauchy-Bunyakowski-Schwarz inequalities,

J. BRANDTS, (Universiteit van Amsterdam, The Netherlands).

Relaxation techniques for nested iterations in finite element method,

D. LOGHIN, (CERFACS, France).

7.3 Internal seminars organized within the Parallel Algorithms Project

January

Matrix-free preconditionings of dense linear systems from electromagnetics. January 7, 2004.

B. CARPENTIERI.

March

Error energy norm estimations for CG, March 3, 2004. M. ARIOLI.

April

Optimizing matrix stability and controllability, April 14, 2004. M. OVERTON.

June

Internal waves in enclosed geometries, June 2, 2004. A. SWART.

Adaptative methods for updating/downdating page ranks, June 3, 2004. G. GOLUB.

September

Constrained orderings and scheduling for parallel sparse linear algebra, September 21, 2004.

S. PRALET (PH.D THESIS DEFENSE).

Optimized interface conditions in domain decomposition methods in the case of extreme contrasts in the coefficients, September 23, 2004. F. NATAF.

October

Parallel preconditioners based on partitioning sparse matrices, October 5, 2004. S. RIYAVONG.

A hybrid format for blocked Cholesky, October 25, 2004. J. WASNIEWSKI.

Bounds on the eigenvalue range and on the field of values of non-Hermitian and indefinite finite element matrices, October 27, 2004. M. B. VAN GIJZEN.

8 Publications

8.1 Journal Publications

- [PUB1] P. R. Amestoy, T. A. Davis, and I. S. Duff. Algorithm 837: AMD, an approximate minimum degree ordering algorithm. *ACM Trans. Math. Softw.*, 30(3):381–388, 2004.
- [PUB2] E. Anterrieu, S. Gratton, and B. Picard. Inverse problem in remote sensing by aperture synthesis imaging. *Traitement du Signal*, 21(1):1–16, 2004.
- [PUB3] B. Carpentieri, I. S. Duff, L. Giraud, and M. Magolu monga Made. Sparse symmetric preconditioners for dense linear systems in electromagnetism. *Numerical Linear Algebra with Applications*, 11(8-9):753–771, 2004.
- [PUB4] I. S. Duff. MA57 – A code for the solution of sparse symmetric indefinite systems. *ACM Trans. Math. Softw.*, 30(2):118–144, 2004.
- [PUB5] I. S. Duff and J. A. Scott. A parallel direct solver for large highly unsymmetric linear systems. *ACM Trans. Math. Softw.*, 30(2):95–117, 2004.
- [PUB6] L. Giraud, S. Gratton, and J. Langou. A rank- k update procedure for reorthogonalizing the orthogonal factor from modified Gram–Schmidt. *SIAM J. Matrix Analysis and Applications*, 25(4):1163–1177, 2004.
- [PUB7] D. Loghin and A. J. Wathen. Analysis of preconditioners for saddle-point problems. *SIAM J. Scientific Computing*, 25(6):2029–2049, 2004.

8.2 Theses

- [THS1] S. Pralet. *Constrained orderings and scheduling for parallel sparse linear algebra*. Ph.D. dissertation. Jury: P. R. Amestoy, I. S. Duff, J. Y. L’Excellent, E. Ng (rapporteur), A. Pothén (rapporteur), and J. Roman (Président), INPT, September 2004. TH/PA/04/105.

8.3 Technical Reports

- [TRP1] P. Amestoy, A. Guermouche, J. Y. L’Excellent, and S. Pralet. Hybrid scheduling for the parallel solution of linear systems. Technical Report TR/PA/04/140, CERFACS, Toulouse, France, 2004.
- [TRP2] P. R. Amestoy, X. S. Li, and S. Pralet. Constrained Markowitz with local symmetrization. Technical Report TR/PA/04/137, CERFACS, Toulouse, France, 2004.
- [TRP3] M. Arioli, M. Baboulin, and S. Gratton. Partial condition number for linear least squares problems. Technical Report TR/PA/04/111, CERFACS, Toulouse, France, 2004.
- [TRP4] M. Baboulin, L. Giraud, and S. Gratton. A parallel distributed solver for large dense symmetric systems: applications to geodesy and electromagnetism problems. Technical Report TR/PA/04/16, CERFACS, Toulouse, France, 2004.

- [TRP5] F. S. V. Bazan. Matrix polynomials with partially prescribed eigenstructure. Technical Report TR/PA/04/64, CERFACS, Toulouse, France, 2004.
- [TRP6] B. Carpentieri, L. Giraud, and S. Gratton. Additive and multiplicative two-level spectral preconditioning for general linear systems. Technical Report TR/PA/04/38, CERFACS, Toulouse, France, 2004.
- [TRP7] F. Chaitin-Chatelin. Beyond ideals in the rings of hypercomplex integers. Technical Report TR/PA/04/96, CERFACS, Toulouse, France, 2004. In Z. Li et al. (eds), Proceedings of NAA2004, Rousse Bulgaria, LNCS 3401, pp. 14-24.
- [TRP8] F. Chaitin-Chatelin. The dynamics of matrix coupling with an application to Krylov methods. Technical Report TR/PA/04/29, CERFACS, Toulouse, France, 2004.
- [TRP9] F. Chaitin-Chatelin. On Lidskii's algorithm to quantify the first order terms in the asymptotics of a defective eigenvalue. Part I. Technical Report TR/PA/04/129, CERFACS, Toulouse, France, 2004.
- [TRP10] I. S. Duff and S. Pralet. Experiments in preprocessing and scaling symmetric problems for multifrontal solutions. Technical Report WN/PA/04/17, CERFACS, Toulouse, France, 2004.
- [TRP11] I. S. Duff. Combining direct and iterative methods for the solution of large systems in different application areas. Technical Report TR/PA/04/128, CERFACS, Toulouse, France, 2004.
- [TRP12] I. S. Duff and S. Pralet. Strategies for scaling and pivoting for sparse symmetric indefinite problems. Technical Report TR/PA/04/59, CERFACS, Toulouse, France, 2004.
- [TRP13] I. S. Duff, S. Riyavong, and M. B. van Gijzen. Parallel preconditioners based on partitioning sparse matrices. Technical Report TR/PA/04/114, CERFACS, Toulouse, France, 2004.
- [TRP14] L. Giraud and S. Gratton. On the sensitivity of some spectral preconditioners. Technical Report TR/PA/04/108, CERFACS, Toulouse, France, 2004.
- [TRP15] L. Giraud, S. Gratton, and J. Langou. Convergence in backward error of relaxed GMRES. Technical Report TR/PA/04/132, CERFACS, Toulouse, France, 2004.
- [TRP16] L. Giraud, S. Gratton, and J. Langou. A note on relaxed and flexible GMRES. Technical Report TR/PA/04/41, CERFACS, Toulouse, France, 2004.
- [TRP17] L. Giraud, J. Langou, M. Rozložník, and J. van den Eshof. Rounding error analysis of the classical Gram-Schmidt orthogonalization process. Technical Report TR/PA/04/77, CERFACS, Toulouse, France, 2004.
- [TRP18] L. Giraud, J. Langou, and G. Sylvand. On the parallel solution of large industrial wave propagation problems. Technical Report TR/PA/04/52, CERFACS, Toulouse, France, 2004. Preliminary version of a paper to appear in Journal of Computational Acoustic.
- [TRP19] L. Giraud, D. Ruiz, and A. Touhami. A comparative study of iterative solvers exploiting spectral information for SPD systems. Technical Report TR/PA/04/40, CERFACS, Toulouse, France, 2004.
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