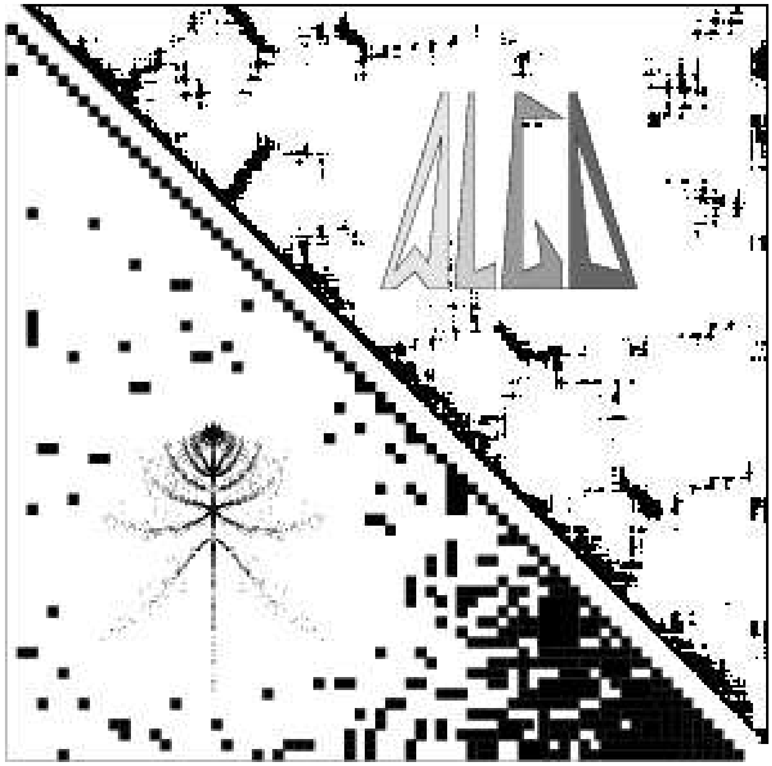

ACTIVITY REPORT
of the
PARALLEL ALGORITHMS PROJECT
at
CERFACS

JANUARY 2005 - DECEMBER 2005

TR/PA/05/110

Contents

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 4.6. 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. Considerable work has been done to understand and develop robust approaches to the case of symmetric indefinite matrices and some of the research work discussed later has been incorporated in `MUMPS`. Other research on examining the out-of-core parallel solution for one or many right-hand sides is still in its infancy but will hopefully also result in future improvements to `MUMPS`. The ACI-GRID Project with ENSEEIHT and others on developing a Grid based expert site for sparse matrices called GRID-Tlse finished in November 2005. This was a great opportunity to develop fruitful collaborations between researchers from different areas ranging from numerical analysis to middleware software. It has enabled some of the partners, namely CERFACS, ENS-Lyon and ENSEEIHT-IRIT, to continue some research in the framework of LEGO, a recently funded ANR project.

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 GMRES and FGMRES routines that are available on our web pages are high on the "google" list, are widely used, and have been downloaded over 3000 times.

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 pioneered at CERFACS by the Qualitative Computing Group.

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 data assimilation algorithms, and we have investigated several aspects of this including appropriate condition numbers for this problem and 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. This work has led CERFACS to be included in a list of major contributors to the ScaLAPACK/LAPACK project. A new initiative in our optimization work 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 and we have recently recruited a PhD student to do a co-tutelle thesis on this topic in conjunction with the University of Namur.

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 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 three stagiaires: Remi Delmas from INSA, Olivier Friedmann from ENSEEIHT, and Xavier Moch from ENS Lyon. Members of the Team have assisted in many lecture courses at other centres, including ENSICA, INPT, Toulouse 1 and INSA. Emeric Martin completed his PhD thesis on "Spectral two-level preconditioners for sequences of linear systems" in July. It also gives us considerable pleasure to record that Serge Gratton successfully defended his HDR thesis presentation on "Fast and Robust Solvers in Scientific Computing Applications in Geosciences" in December.

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. Five of our visitors for this year stayed for a reasonably long period. These were: Gary Howell (matrix factorizations), Nancy Nichols (data assimilation), Marielba Rojas (optimization), Philippe Toint (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. Frank Hülsemann 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 our normal annual formula of a two-day "Sparse Days at CERFACS" meeting was replaced by the Second International Workshop on Combinatorial Scientific Computing in June of 2005. This meeting, which we hosted in the main Météo Conference Centre, was co-sponsored by CERFACS, INRIA, IRIT, Région Midi-Pyrénées and SIAM, and was a great success. We attracted over 80 participants over half from outside France and half again from outside Europe. A number of distinguished scientists who came to this meeting also visited CERFACS and met members of the Team. A list of the speakers at this meeting is given in Section 8.2.

I am very pleased to record that, over the reporting period, we have continued our involvement in joint research projects with shareholders and with other teams at CERFACS.

We have a project with EADS on preconditioning techniques in electromagnetics. We have continued our joint effort with the CERFACS electromagnetics project on the solution of discretized Maxwell equations using the boundary element method in the framework of a DGA/Dassault contract. This has been an occasion for us to use techniques developed for perfect conductors in the more general context of impedance, and to run experiments with the GMRES-DR algorithm in this context.

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 had detailed discussions with EDF on parallel linear solvers. One of our postdocs, Frank Hülsemann, did such an excellent job in studying the use of a direct sparse solver within CODE ASTER, in particular comparing their in-house multifrontal code with `MUMPS`, that he was offered and accepted employment with EDF towards the end of the year. I am pleased that Xavier Vasseur and Serge Gratton were able steer this project through its final stages and Xavier is now looking at null-space computations that are of great interest to EDF.

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 the Climate Modelling and Global Change Group and Météo France. We now have a strong and growing collaboration with the Climate Modelling Team on aspects of data assimilation, and continue to co-host Jean Tshimanga a researcher from Belgium who is doing a PhD at Namur with Annick Sartenaer. In the context of this work, we have also hosted visits from Amos Lawless from the UK MET Office and from Nancy Nichols of the University of Reading who works partly in numerical analysis and partly with the meteorology department. We have also hosted, supervised, and worked with Hervé Le Berre, who was working on the parallelization of the Mocage code in the framework of a contract between CERFACS and 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 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 two seniors, Luc Giraud and Serge Gratton, for doing all the hard work to ensure the smooth running of the Team. It was with very mixed emotions that we learned that Luc had accepted a professorship at INPT. I say “mixed” because, on the one hand, we really will miss his energy and ability as deputy Project Leader in charge of the day to day running of the Team. On the other hand, we are delighted for him that he has such a prestigious post and also that he is not moving far from us so we can continue to welcome him as a senior visitor, thus strengthening even more our strong links with ENSEEIHT-IRIT. It is now Serge who has to bear the many responsibilities of the day-to-day management. I am very pleased to say that he does so in an excellent fashion and is well supported in his efforts by our enthusiastic and talented postdocs.

Iain S. Duff.

Visitors to Parallel Algorithm Project in 2005

In alphabetical order, our visitors in the year 2005 included:
Angelica Bunse-Gerstner (Bremen University, Germany),
Marc Garbey (University of Houston, U.S.A.),
Gene Golub (Stanford University, U.S.A.),
Gary W. Howell (North Carolina State University, U.S.A.),
David R. Kincaid (University of Texas, Austin, U.S.A.),
Julien Langou (The University of Tennessee, U.S.A.),
Amos Lawless (University of Reading, U.K.),
Sherry Li (Lawrence Berkeley National Laboratory, Berkeley, U.S.A.),
Frederic Magoules (Université Henri Poincaré, Nancy, France),
Gerard Meurant (CEA, Bruyères-le-Châtel, France),
Esmond G. Ng (Lawrence Berkeley National Laboratory, Berkeley, U.S.A.),
Nancy Nichols (University of Reading, U.K.),
Marielba Rojas (Wake Forest University, U.S.A.),
Daniel Ruiz (ENSEEIHT-IRIT, France),
Annick Sartenaer (The University of Namur, Belgium),
Gerard L.G. Sleijpen (Utrecht University, The Netherlands),
Masha Sosonkina (University of Minnesota Duluth, U.S.A.),
Ken Stanley (University of Central Florida School, U.S.A.),
Philippe Toint (The University of Namur, Belgium),
Jean Tshimanga (The University of Namur, Belgium),
Robert Van de Geijn (University of Texas, Austin, U.S.A.),
Martin Van Gijzen (Delft University of Technology, The Netherlands),
Christoph Vömel (Lawrence Berkeley National Laboratory, Berkeley, U.S.A.).

2 List of Members of the Algo Team

Iain Duff - Project Leader
Luc Giraud - Deputy Project Leader until August 2005 - Senior Researcher
Françoise Chaitin-Chatelin - Qualitative Computing Group Scientific Advisor
Serge Gratton - Senior Researcher
Fabian Bastin - Post. Doc.
Xavier Vasseur - Post. Doc.
Christophe Hammerling - Engineer
Hervé Le Berre - Engineer
Marc Baboulin - Ph.D. Student
Azzam Haidar - Ph.D. Student
Emeric Martin - Ph.D. Student
Mélodie Mouffe - Ph.D. Student
Tzvetomila Slavova - Ph.D. Student
Morad Ahmadnasab - Visitor, University Toulouse I, France
Patrick Amestoy - Senior Visitor, ENSEEIHT-IRIT, France
Luc Giraud - Senior Visitor from September 2005, ENSEEIHT-IRIT, France
Ahmed Touhami - Visitor, ENSEEIHT-IRIT, France
Rémi Delmas - Trainee
Olivier Friedmann - Trainee
Xavier Moch - Trainee
Brigitte Yzel - Administration

3 Dense and Sparse Matrix Computations

3.1 Pivoting strategies for sparse symmetric indefinite systems

I.S. Duff: CERFACS*, France*; **S. Pralet**: ENSEEIHT*, France*

We consider the direct solution of sparse symmetric indefinite matrices. We develop new pivoting strategies that combine numerical and static pivoting. Then an iterative refinement process uses our approximate factorization to compute a solution. We show that our pivoting strategies are numerically robust, that few steps of iterative refinement are required and that the factorization is significantly faster because of this static/numerical combination. Furthermore, we propose original approaches that are designed for parallel distributed factorization. A key point of our parallel implementation is the cheap and reliable estimation of the growth factor. This estimation is based on an approximation of the off-diagonal entries and does not require any supplementary messages.

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[1] I. S. Duff and S. Pralet. Towards a stable static pivoting strategy for the sequential and parallel solution of sparse symmetric indefinite systems. Technical Report TR/PA/05/26, CERFACS, Toulouse, France, 2005. Also available as RAL Report RAL-TR-2005-007 and IRIT Report RT/TLSE/05/08.

3.2 Integration of the parallel, direct sparse linear solver MUMPS into Code Aster

O. Boiteau: EDF Division R&D*, France*; **F. Hülsemann**: CERFACS*, France*; **X. Vasseur**: CERFACS*, France*

The long term goal of this collaboration is the integration of the parallel, direct sparse linear solver MUMPS into Code Aster, a structural mechanics code developed at EDF. The topic of the short note [1] is the comparison of the linear solver MUMPS with the inbuilt serial multifrontal out-of-core solver of Code Aster for two and three dimensional linear problems arising in structural mechanics. It summarizes the background of this study, explains the main steps of this comparison and presents few results.

A more detailed study was performed on a large number of test cases late in 2005. This comparison was done both in terms of run time performance and stability using backward error estimates. It has been found that MUMPS is an attractive alternative to the current multifrontal solver in Code Aster as its run time behaviour is more predictable and it offers error diagnostic and iterative refinement features that are currently not available in the inbuilt solver. A technical report on this work will be published early in 2006.

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[1] O. Boiteau and F. Hülsemann. Suivi de la collaboration CERFACS/EDF R&D autour de MUMPS et de Code Aster. Technical Report CR-I23/2005/032, EDF R&D, 2005.

3.3 Solving sparse linear systems in an out-of-core environment

P. Amestoy: ENSEEIHT, *France*; **I.S. Duff**: CERFACS, *France*; **T. Slavova**: CERFACS, *France*

In collaboration with INRIA and ENSEEIHT, we are working with MUMPS (Multifrontal Massively Parallel Solver) to solve large-scale equations using direct methods. The aim of our research is to design an out-of-core implementation of the solution phase efficient at reducing memory usage and computing time for both sequential and parallel environments.
Preliminary results indicate that, in a sequential environment, the out-of-core implementation is competitive with respect to the standard in core implementation. Although reasonable performance can be obtained on a moderate number of processors much work still has to be done to improve the parallel behaviour of the algorithms.

[1] E. Agullo, A. Guermouche, and J.-Y. L'Exellent. Preliminary out-of-core extension of a parallel multifrontal solver. Technical Report, INRIA / LIP, 2005. In preparation.

4 Iterative Methods and Preconditioning

4.1 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 [7] 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 [6]. 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 extract 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, 5].

[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 TR/PA/05/17, 2005. Preliminary version of the paper to appear in Applied Numerical Mathematics.

[5] E. Martin. *Spectral two-level preconditioners for sequences of linear systems.* Ph.D. dissertation, INPT, September 2005. TH/PA/05/57.

[6] R. B. Morgan. GMRES with deflated restarting. *SIAM J. Scientific Computing*, 24(1):20–37, 2002.

[7] 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.

4.2 Parallel algebraic preconditioners for the solution of Schur complement systems in 3D

L. Giraud: CERFACS, *France*; **A. Haidar**: CERFACS, *France*; **S. Mulligan**: Dublin Institute of Technology, , *Ireland*

Domain decomposition methods are a natural way to parallelize the numerical solution of elliptic partial differential equations for 2D and 3D problems. In this study we consider the parallel solution of a standard finite element discretisation of 3D elliptic problems. The method used is a preconditioned conjugate-gradient solver following [2, 3] on the Schur complement system for the interface unknowns. An additive Schwarz preconditioner is computed which consists of the local assembled Schur complements for each subdomain. These Schur complements are computed using the MUMPS [1] package. We also used a sparsified version of this preconditioner, where elements whose relative magnitudes are below a certain tolerance are dropped; this typically results in Cholesky factors that retain only about 10% of the original dense factors. The resulting block-preconditioners are compared with an approach that consists in using a sparsified approximation of the complete Schur complement. This latter sparsified Schur complement is factorized in parallel by MUMPS and used as a preconditioner.
The methods were implemented on an IBM SP by assigning each sub-domain to a single process and using MPI for the parallel communication. The numerical results have been obtained for a number of model problems, including problems with variable and discontinuous coefficients [4]. The preliminary results indicate a good parallel scalability of these methods for 3D problems, in that the convergence rate is not seriously degraded as the number of domains increases. Further tests are being carried out, including comparisons with a direct solver and the results will be the subject of a forthcoming report.

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[1] P. R. Amestoy, I. S. Duff, J.-Y. L'Excellent, and J. Koster. A fully asynchronous multifrontal solver using distributed dynamic scheduling. *SIAM J. Matrix Analysis and Applications*, 23(1):15–41, 2001.

[2] 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.

[3] L. Giraud, A. Marrocco, and J.-C. Rioual. Iterative versus direct parallel substructuring methods in semiconductor device modelling. *Numerical Linear Algebra with Applications*, 12(1):33–53, 2005.

[4] L. Giraud, S. Mulligan, and J.C. Rioual. Algebraic preconditioners for the solution of schur complement systems, February 25-27 2004. SIAM Conference on Parallel Processing for Scientific Computng.

4.3 Parallel Distributed Numerical Simulations in Aeronautic Applications

G. Alléon: EADS CRC, *France*; **S. Champagneux**: Cerfacs, *France*; **G. Chevalier**: Cerfacs, *France*; **L. Giraud**: Cerfacs, *France*; **G. Sylvand**: EADS CRC, *France*

Numerical simulation plays a key role in industrial design because it reduces the time and the cost to develop new products. Because of international competition, it is important to have a complete chain of simulation tools to perform efficiently some virtual prototyping. In this paper, we describe two components of large aeronautic numerical simulation chains that are extremely consuming of computer resources. The first concerns computational fluid dynamics for aerodynamic studies. The second is used to study the wave propagation phenomena and concerns acoustics. Because those softwares are used to analyse large and complex case studies in a limited amount of time, they are implemented on parallel distributed computers. We describe the physical problems addressed by

these codes and the main characteristics of their implementation. For the sake of re-usability and interoperability, the software is developed using object-oriented technologies. We illustrate their parallel performance on clusters of symmetric multiprocessors. Finally, we discuss some challenges for the future generations of parallel distributed numerical software that will have to enable the simulation of multi-physics phenomena in the context of virtual organizations also known as the extended enterprise.
Results of this study are presented in [1]

[1] G. Alléon, S. Champagneux, G. Chevalier, L. Giraud, and G. Sylvand. Parallel distributed numerical simulations in aeronautic applications. Technical Report TR/CFD-PA/05/44, CERFACS, Toulouse, France, 2005.

5 Qualitative Computing

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

The work of the 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 algebraic singularities.
Some of these laws are now well understood for Numerical Linear Algebra. 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. Some of these more basic laws can be established by analytic tools (complex variables, matrix algebra). They include:

a) the basic role of *non linearities* 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.

Their common feature is that the analysis of round-off is essentially 2-level (full versus machine precision). This 2-level analysis is sufficient for most matrix algorithms. But it cannot capture essential aspects of nonlinear computation such as chaotic iterations. These phenomena signal strong nonlinearities which are active at more than two levels. We currently explore such multiscale instability phenomena by means of Numerical Nonlinear Algebra.

Our research and understanding has been driven by work on practical numerical software applications in physics and technology, which come from CERFACS partners. In May 2004, Françoise Chaitin-Chatelin was one of the five external experts in charge of the review, for the EDF Scientific Council, of their ambitious programme to turn to "Numerical Simulation only" (Tout numérique) at the 2010 horizon.
We review below the work accomplished with respect to Qualitative Computing.

5.1 Homotopic Deviation in Linear Algebra

It is customary in Numerical Linear Algebra to analyse the robustness of a method/problem involving as data the matrix $A \in \mathbb{C}^{n\times n}$ by considering all (or a subset of) perturbations $\triangle A$ of A. This leads to perturbation theory and is successful when $\|\triangle A\|$ is not too large.
This approach finds its limits in the case of highly nonnormal matrices for example. A fruitful alternative is to consider a structurally fixed family $\triangle A = tE$, where $t \in \mathbb{C}$, $E \in \mathbb{C}^{n\times n}$. This leads to the *linear* coupling $A + tE$.

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

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 $z \in \mathrm{re}(A) = \mathbb{C} \setminus \sigma(A)$, we use the *multiplicative* representation

$$(A + tE - zI)^{-1} \quad = \quad (A - zI)^{-1} \left(I + tE(A - zI)^{-1}\right)^{-1}.$$

For a fixed z in $\mathrm{re}(A)$, the map $t \mapsto R(t,z)$ is analytic for $|t| < \frac{1}{\rho(E(A-zI)^{-1})} = \alpha$ [11, 12].

In Homotopic Deviation theory, we specifically look beyond analyticity in t, for $|t| > \alpha$. 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, with $rankE = r \leq n$. 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 ($r < n$) in the case of interest, where the Sherman-Morrison formula plays a key role.

When $r = n$, $\lim_{|t|\to\infty} R(t,z) = 0$ and $\lim_{|t|\to\infty} \sigma(A(t)) = \infty$. But when $r < n$, a different and more interesting situation prevails, characterized by the spectral properties of the rational matrix:

$$z \rightarrow M_z \quad = \quad (\det(zI_n - A))^{-1} \; V^H \,\mathrm{adj}\,(zI_n - A)\, U \in \mathbb{C}^{r\times r}$$

where $E = UV^H$, $U, V \in \mathbb{C}^{n\times r}$, $r < n$, and z varies in $\mathbb{C}$ outside $\sigma(A)$.

For almost all z in $re(A) = \mathbb{C}\backslash\sigma(A)$, M_z has rank r and $R(t,z)$ is analytic for $|t|$ large enough, $|t| > \beta = \frac{1}{min|\mu_z|}$, $\mu_z \in \sigma(M_z)$, such that $\lim_{|t|\to\infty} R(t,z) \neq 0$. For $\alpha < |t| < \beta$, the resolvent exists almost everywhere in $re(A)$. The spectrum $\sigma(M_z)$ represents the r $finite$ eigenvalues of the pencil $(A - zI) + tE$ for z fixed in $re(A)$, when $0 \notin \sigma(M_z)$.

The points in $re(A)$ such that M_z is singular are the $frontier$ points, where no analyticity at ∞ holds. At any frontier point, the pencil $(A - zI) + tE$ has *less* than r finite eigenvalues. It may have none iff M_z is nilpotent. When $|t| \rightarrow \infty$, we can predict when some of the eigenvalues $\lambda(t) \in \sigma(A(t))$ converge to points in the frontier set, as proved in [4, 5, 6, 7, 8, 3].

Linearization of quadratic eigenproblems often leads to a situation where $0 \in \sigma(E)$ is semi-simple. The paper [10] treats an example from computational Acoustics, where t represents the complex admittance. This joint work with Martin Van Gijzen will appear in NLAA. It consists of a practical application where the homotopy parameter is *complex*. The points where the matrix pencils have *no* finite eigenvalues are given a physical interpretation: they are points where *no resonance* can occur.

An application to the incomplete Arnoldi method (E singular defective of rank 1) has been made.

The paper [6] 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 Martin van Gijzen.

The restrictive conditions placed by the generic approach of Lidskii have been relaxed in [8]. Numerical experiments were performed by Morad 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 have been used to. If this is confirmed, this phenomenon is yet another reason to marvel at the "unreasonable" robustness of Krylov methods to perturbations.

The homotopic backward analysis of eigenvalues has been presented by Morad Ahmadnasab at the 2nd SMAI conference (Evian, May 2005) [2] and at the University of Versaille Saint-Quentin (July 2005) [1].

[1] M. Ahmadnasab. Homotopic backward analysis for matrix eigenvalues. Presentation in CERFACS, and Université Versailles Saint-Quentin en Yvelines. 5 July 2005 .

[2] M. Ahmadnasab and F. Chaitin-Chatelin. Backward analysis for matrix eigenvalues. 2éme Congrés National de Mathématiques Appliquées et Industrielles, Evian - France 23 - 27 May 2005, Evian - France, Poster.

[3] M. Ahmadnasab, F. Chatin-Chatelin, and N. Megrez. Homotopic deviation in the light of algebra. Technical Report TR/PA/05/05, CERFACS, Toulouse, France, 2005.

[4] F. Chaitin-Chatelin. About Singularities in Inexact Computing. Technical Report TR/PA/02/106, CERFACS, Toulouse, France, 2002. Erratum : p.2, line 14, read 'associated with eigenvalues non equal to lambda'.

[5] F. Chaitin-Chatelin. Computing beyond analyticity. Matrix algorithms in Inexact and Uncertain computing. Technical Report TR/PA/03/110, CERFACS, Toulouse, France, 2003.

[6] F. Chaitin-Chatelin. The dynamics of matrix coupling with an application to Krylov methods. Technical Report TR/PA/04/29, CERFACS, Toulouse, France, 2004. Preliminary version of the article published in Z. Li et al. (eds), Proceedings of NAA 2004, pp. 14-24, Springer Verlag LNCS, vol. 3401, 2005.

[7] 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.

[8] F. Chaitin-Chatelin. On Lidskii's algorithm to quantify the first order terms in the asymptotics of a defective eigenvalue. Part II. Technical Report TR/PA/05/04, CERFACS, Toulouse, France, 2005.

[9] F. Chaitin-Chatelin and V. Frayssé. *Lectures on Finite Precision Computations.* SIAM, Philadelphia, 1996.

[10] F. Chaitin-Chatelin and M. B. van Gijzen. Analysis of parameterised quadratic eigenvalue problems in Computational Acoustics with Homotopic Deviation, to appear in NLAA 2006.

[11] F. Chatelin. *Spectral Approximation of Linear Operators.* Academic Press, New York, 1983.

[12] F. Chatelin. *Eigenvalues of matrices.* Enlarged Translation, J. Wiley and Sons edition, 1993.

5.2 Numerical Nonlinear Algebra

Nonlinear Algebra is the required framework to deal with matrix computations which are strongly nonlinear and which do not lend themselves to a computationally reliable linearization. To exploit the algorithmic dynamics created by the nonlinearities (arising from multiplication), one is led to make full use of the inductive complex structure of multiplication which is a characteristic of (possibly non associative) Dickson algebras [4, 2, 3]. By doing so, one goes beyond the classical framework of (associative) Clifford algebras which is used so succesfully in Algebraic Geometry and Theoretical Physics to describe phenomena where multiplication is inherently non commutative, but remains associative.
Associativity puts an arbitrary limit to the type of nonlinearities which can be considered: they cannot be chaotic. The possibility to go beyond this limit is numerically very important to assess the validity of computer simulations in the chaotic regime. This ambitious goal implies going even beyond the framework of Dickson algebras where multiplication is neither associative nor isometric, but remains quadratic and flexible. A quadratic algebra is such that x^2 is a real linear combination of x itself and $\|x\|^2$, where $\|.\|$ denotes the Euclidean norm. This property can be related to the logistic equation (in real variables and under additive form) $x = x^2 + c$, making a significant connection between Dickson algebras and the quadratic polynomial iterations which can display chaos [9, 10]. A body of theory is developing [11, 6, 7, 8, 9, 1, 5] together with experiments [10], which connect various aspects of Computation (Analysis, Algebra, Geometry and Arithmetics) in new *algorithmic* ways. The first item in our agenda is to determine the number of hierachical levels to be taken into

account in very unstable phenomena (leading to chaos), in order to adjust the targeted accuracy to the inherent instability, therefore minimizing the overall computing time.

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[1] F. Chaitin-Chatelin. Calcul matriciel: entre algébre et geométrie. Séminaire Université Montpellier 2, 27 January 2004, talk.

[2] F. Chaitin-Chatelin. Le rôle de la multiplication en calcul scientifique. Séminaire du Dpt. de Physique Théorique, Université Paul Sabatier, Toulouse, 11 January 2005, talk.

[3] F. Chaitin-Chatelin. Le sens des nombres. Grand Séminaire d'Ouverture, Université Paul Sabatier, Toulouse, 5 February 2004, talk.

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

[5] F. Chaitin-Chatelin. The Arnoldi method in the light of Homotopic Deviation theory. Technical Report TR/PA/03/15, CERFACS, Toulouse, France, 2003.

[6] F. Chaitin-Chatelin. Elements of Hypercomputations on $\mathbb{R}$ and $\mathbb{Z}_2$ with the Dickson-Albert inductive process. Technical Report TR/PA/03/34, CERFACS, Toulouse, France, 2003.

[7] F. Chaitin-Chatelin. Beyond ideals in the Dickson ring of integral octonions. Technical Report TR/PA/04/96, CERFACS, Toulouse, France, 2004.

[8] F. Chaitin-Chatelin. Inductive multiplication in Dickson algebras. Technical Report TR/PA/05/56, CERFACS, Toulouse, France, 2005.

[9] F. Chaitin-Chatelin. Computing lessons from the logistic iteration. Working Notes December 2005, to appear as Cerfacs Technical Report.

[10] F. Chaitin-Chatelin and M. Ahmadnasab. The logistics of Feigenbaum and Mandelbrot in real variables revisited. Work in progress to appear as Cerfacs Technical Report, January 2006.

[11] F. Chaitin-Chatelin and E. Traviésas-Cassan. Qualitative Computing, Chapter 5 in B. Einarsson (ed.), *Accuracy and Reliability in Scientific Computing,* SIAM, Philadelphia, 2005, pp. 77-92.

6 Nonlinear Systems and Optimization

6.1 Convergence properties of trust-region methods with application to multigrid optimization

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

Following recent work on the convergence properties of a new recursive multiscale trust-region algorithm for unconstrained optimization [3], we present in [2] the numerical experience gained so far with a particular implementation of the considered algorithm applied to a few significant test problems. We illustrate the strength of methods of this type.
Convergence properties of trust-region methods for unconstrained nonconvex optimization is also considered in the case where information on the objective function's local curvature is incomplete, in the sense that it may be restricted to a fixed set of "test directions" and may not be available at every iteration [1]. It is shown that convergence to local "weak" minimizers can still be obtained under some additional but algorithmically realistic conditions. These theoretical results are then applied to recursive multigrid trust-region methods, which suggests a new class of algorithms with guaranteed second-order convergence properties.

[1] S. Gratton, A. Sartenaer, and Ph. L. Toint. Recursive trust-region methods for multiscale nonlinear optimization: Preliminary numerical experience. Technical Report in preparation, CERFACS, Toulouse, France, 2005.

[2] S. Gratton, A. Sartenaer, and Ph. L. Toint. Second-order convergence properties of trust-region methods using incomplete curvature information. Technical Report in preparation, CERFACS, Toulouse, France, 2005.

[3] S. Gratton, A. Sartenaer, and Ph.L. Toint. A numerical exploration of recursive multiscale unconstrained optimization. In J. Zowei F. Jarre, C. Lemarchal, editor, *In Oberwolfach Reports: Optimization and Applications*. To appear.

6.2 Partial condition number for linear least-squares problems

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

We consider 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 the Frobenius or the spectral norm for A and the Euclidean norm for b. 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 a sharp estimate that lies within a factor $\sqrt{3}$ of the true condition number. Provided the triangular R factor of A from $A^T A = R^T R$ is available, this estimate can be computed in $2kn^2$ flops. We also propose a statistical method based on [2] that estimates the partial condition number by using the exact condition numbers in random orthogonal directions. If R is available, this statistical approach enables us to obtain a condition estimate at a lower computational cost. In the case of the Frobenius norm, we derive a closed formula for the

partial condition number that is based on the singular values and the right singular vectors of the matrix A.
The theoretical results and numerical experiments related to this study are presented in [1].

[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] T. Gudmundsson, C. S. Kenney, and A. J. Laub. Small-sample statistical estimates for matrix norms. *SIAM J. Matrix Analysis and Applications*, 16:776–792, 1995.

6.3 Distributed packed storage for large parallel calculations

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

We propose in [2] a distributed packed storage format that exploits the symmetry or the triangular structure of a matrix. This format stores only half of the matrix while maintaining most of the efficiency compared to full storage for a wide range of operations. This work has been motivated by the fact that, contrary to sequential linear algebra libraries (e.g. LAPACK [1]), there is no routine that handles packed matrices in the currently available parallel distributed libraries. The proposed algorithms exclusively use the existing ScaLAPACK [3] computational kernels which proves the generality of the approach, provides easy portability of the code, efficient re-use of existing software and good load balance of the application even for high processor counts. We present performance results for the Cholesky factorization and for the updating of the R factor of a QR factorization.

[1] E. Anderson, Z. Bai, C. Bischof, S. Blackford, J. Demmel, J. Dongarra, J. Du Croz, A. Greenbaum, S. Hammarling, A. McKenney, and D. Sorensen. *LAPACK User's Guide*. SIAM, 1999. Third edition.

[2] M. Baboulin, L. Giraud, S. Gratton, and J. Langou. A distributed packed storage for large parallel calculations. Technical Report TR/PA/05/30, CERFACS, Toulouse, France, 2005.

[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.

6.4 Trust-region methods with dynamic accuracy and nonlinear least-squares

F. Bastin: CERFACS*, France*; **S. Gratton**: CERFACS*, France*; **C. Cirillo**: UNIVERSITY OF NAMUR*, Belgium*; **Ph. L. Toint**: UNIVERSITY OF NAMUR*, Belgium*

We consider trust-region techniques with adaptive strategies for stochastic programming. We have constructed a convergent method designed for stochastic programs based on expected values [2], and have applied it for mixed logit models, a class of problems encountered in discrete choice theory. We have however identified problems arising when using some popular classes of Hessian approximations, especially the BHHH one [1]. Such difficulties are similar to those that can be encountered with nonlinear least-square problems for the Gauss-Newton method. These similarities are at the origin of a project where we consider these problems inside an unified framework. We have identified the origins of the poor numerical performance and we consider hybrid strategies such as that developed by Dennis et al. [3], which can be shown to be convergent. The next step will be to complete the implementation that has been initiated in order to numerically validate the theoretical developments.

[1] F. Bastin, C. Cirillo, and Ph. L. Toint. Application of an adaptive monte carlo algorithm to mixed logit estimation. *Transportation Research Part B*, 2006. In press.

[2] Fabian Bastin. An adaptive trust-region approach for nonlinear stochastic optimisation with an application in discrete choice theory. In Susanne Albers, Rolf H. Möhring, Georg Ch. Pflug, and Rüdiger Schultz, editors, *Algorithms for Optimization with Incomplete Information*, number 05031 in Dagstuhl Seminar Proceedings. Internationales Begegnungs- und Forschungszentrum (IBFI), Schloss Dagstuhl, Germany, 2005.

[3] J. E. Dennis, D. Gay, and R. E. Welsch. An adaptive nonlinear least-squares algorithm. *ACM Transactions on Mathematical Software*, 7(3):348–368, 1981.

6.5 Trust-Region algorithms applied to discrete choice modelling

Dick Ettema: University of Utrecht, *The Netherlands*; **Fabian Bastin**: CERFACS, *France*; **John Polak**: Imperial College, *United Kingdom*; **Olu Ahiru**: Imperial College, *United Kingdom*

In this research, we have considered the application of trust-region methods to discrete choice models involving random parameters, so that the problem can be viewed as a stochastic program. We have more specifically studied a model of activity and trip scheduling that combines three elements that have previously been investigated in isolation: the duration of activities, the time-of-day preference for activity participation and the effect of schedule delays on the valuation of activities. The model was tested using a 2001 data set from the Netherlands and results are presented in [2]. The method is convergent, and error components included in the model suggest that there is considerable unobserved heterogeneity with respect to mode preferences and schedule delay.

[1] Fabian Bastin. An adaptive trust-region approach for nonlinear stochastic optimisation with an application in discrete choice theory. In Susanne Albers, Rolf H. Möhring, Georg Ch. Pflug, and Rüdiger Schultz, editors, *Algorithms for Optimization with Incomplete Information*, number 05031 in Dagstuhl Seminar Proceedings. Internationales Begegnungs- und Forschungszentrum (IBFI), Schloss Dagstuhl, Germany, 2005.

[2] D. Ettema, F. Bastin, J. Polak, and O. Ashiru. An error-components framework for joint choice models of activity timing and duration. Technical Report TR/PA/06/2, CERFACS, Toulouse, France, 2006.

7 Signal processing

7.1 Phase Closure Imaging and Differential GPS

A. Lannes: CERFACS, *France*

The nearest lattice-point problems arising in Phase Closure Imaging (PCI) and in Differential GPS (DGPS) share a common feature. Their statement appeals to elementary notions of algebraic graph theory. In both cases, the original data are defined on the edges of the graph to be considered, the calibration graph in PCI, and the GPS graph in Global Navigation Satellite Systems (GNSS).

These data are biased by differences between unknown terms defined on the vertices of the graph: phase shifts in PCI and clock offsets in GNNS. The effective data are then closure terms in the sense of Kirchhoff: the sums of the original data on the directed edges of the n cycles defined by the choice of a spanning tree. By construction, these data are no longer biased. The original phase data are defined modulo 2π in interferometry, or modulo the carrier wavelengths in GPS. The "closure integers" involved in the related nearest lattice-point problems are associated with these cycles.

As summarized below, the studies performed at CERFACS in 2004-2005 have shown that the notion of spanning tree of maximal weight plays an essential part in the applications concerned by this approach. (Further details are to be found in [1] for PCI, and in [2] for DGPS.)

[1] A. Lannes. A global analysis of the phase calibration operation. *J. Opt. Soc. Am.*, 22:697–707, 2005.

[2] A. Lannes. On new data validation criteria in differential gps. *J. of Geod.*, 79:280–287, 2005.

7.2 Phase Closure Imaging

A. Lannes: CERFACS, *France*

The edges of the calibration graph correspond to the baselines for which the phase Ψ_{s} of the Fourier transform of the calibration source can be regarded as relatively well known. On each connected component of this graph, the main entries of the problem are the closure phases $\Psi^{(i)} := \Psi_{\mathrm{d}}^{(i)} - \Psi_{\mathrm{s}}^{(i)}$; subscripts d and s stand for data and source, respectively. These closure phases are relative to the cycles defined by the selected spanning tree.

The calibration functional to be minimized is defined by a relation of the form $f(\Phi) := \| \operatorname{arc}(\Psi - \Phi) \|$ where Φ is an Optical Path Difference (OPD), a phase function which takes its values on the edges of the graph. At the end of the initialization step, the baseline phase function Ψ involved in the definition of f is of the form $\sum_{i=1}^{n} \Psi^{(i)} \xi_i$ with $\Psi^{(i)} \leftarrow \operatorname{arc}(\Psi^{(i)})$. Here, $\{\xi_i\}_{i=1}^{n}$ is the standard basis of cycle-entry phase space. The complexity of the correction step depends on the size of the residual closure phases $\Psi^{(i)}$.

As shown in [1] , the minima of f correspond to particular points of $\mathbf{Z}^n$:

$a_\star \equiv (a_\star^{[1]}, \ldots, a_\star^{[n]})$ for the global minimum;
$a_{\star\star} \equiv (a_{\star\star}^{[1]}, \ldots, a_{\star\star}^{[n]})$ for the nearest secondary minimum (if any);
etc.

These points lie in a convex set of $\mathbf{R}^n$ centered on the closure point $\widehat{a} \leftarrow (\psi^{(1)}, \ldots, \psi^{(n)})$ where $\psi^{(i)} \leftarrow \Psi^{(i)}/(2\pi)$; $a_\star$ is the point of $\mathbf{Z}^n$ closest to the float solution $\widehat{a}$, the distance being that induced by a given quadratic form q. The matrix of q is the inverse of the variance-covariance matrix of the closure phases.
When the residual closure phases are relatively large, say between $\pi/3$ and $2\pi/3$ (in absolute value), the correction step is delicate. The situations where $f(\Phi_{\star\star})$ is of the order of $f(\Phi_\star)$ with $\mathrm{arc}(\Psi - \Phi_{\star\star})$ very different from $\mathrm{arc}(\Psi - \Phi_\star)$ must be discarded. The calibration graph must then be truncated by removing the cycle-entry edges for which the residual closure phases are too large. The spanning tree to be selected is therefore the spanning tree of maximal weight.
The applications of this analysis concern, in particular, the situations where the self-calibration procedures must be conducted with much care. The delicate situations can be diagnosed and dealt with. It is thus possible to find a good compromise between the coverage of the calibration graph (which must be as complete as possible), and the quality of the solution (which must of course be reliable).

[1] A. Lannes. A global analysis of the phase calibration operation. *J. Opt. Soc. Am.*, 22:697–707, 2005.

7.3 Differential GPS

A. Lannes: CERFACS, *France*

Once the observations have been screened for strong biases such as cycle slips, multipath, etc., the statistical modelling of the problem may still be unsatisfactory for some receiver-satellite pairs at certain epochs. The data validation tests developed at CERFACS are aimed at detecting these failures [1].
In the process of finding a reliable solution for the DGPS integer ambiguity a, it is important to identify the epochs for which the reference physical modelling is not acceptable. Recursive testing procedures have already been developed for this purpose. One thus gets a first estimate $\widetilde{a}$ of the global float solution $\widehat{a}$. The next step is to find the integer ambiguity solution corresponding to this float estimate. The input for this last step must therefore be very reliable. The data validation tests developed at CERFACS refine the recursive procedures in question. The time to fix the optimal integer ambiguity $\check{a}$ should thereby be reduced.
Relying on the current estimate $\widetilde{a}$ of $\widehat{a}$, one tests, with regard to the model under consideration, the quality of the data obtained at some given epoch. The corresponding phase residual discrepancy is a function $\delta^{(\widetilde{a})}(r,s)$ whose values can easily be computed. Denoting by ℓ a relaxation parameter of the order of the standard deviation of the carrier-phase information, let us now assume that, for a given epoch, the phase discrepancy condition —$\delta^{(\widetilde{a})}(r,s)| \leq \ell$ is satisfied on all the edges of the GPS graph. Clearly, the corresponding data are then physically reliable. Evidently, the smaller ℓ, the more severe the criterion.
The phase residual discrepancy is obtained via the pseudo-inverse of the phase closure operator. The closure operation, which generalizes that of double differencing, depends on the selected spanning tree. The results (of course) do not depend on that choice. To identify the edges on which the GPS data are not reliable, it is however preferable to choose the spanning tree of maximal weight. This crucial point is clarified in [1].

[1] A. Lannes. On new data validation criteria in differential gps. *J. of Geod.*, 79:280–287, 2005.

8 Conferences and Seminars

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

January

Algorithms for Optimization with Incomplete Information, January 16–21, 2005, Dagstuhl, Germany. F. Bastin, *An adaptive trust-region approach for nonlinear stochastic optimisation with an application in discrete choice theory*, Invited Talk.

February

SIAM CSE 2005 Meeting, Orlando, Florida, USA. 9-12 February, 2005. I.S. Duff, Organizing Committee.

SIAM CSE 2005 Meeting, Orlando, Florida, USA. 9-12 February, 2005. L. Giraud, *Solving large wave propagation problems using Krylov techniques*, joint work with S. Gratton, J. Langou, E. Martin and S. Sylvand, Invited Talk.

April

University of Strathclyde, Glasgow, Scotland. 12 April, 2005. I.S. Duff, *Combining direct and iterative methods for the solution of large systems in different application areas,* Seminar.

Twelfth Copper Mountain conference on multigrid methods, Avril 2005. S. Gratton,*On Recursive Multiscale Trust-Region Algorithms for Unconstrained Minimization,* Talk.

May

SIAM Conference on Optimization, Stockholm, Sweden, May 15-19, 2005. F. Bastin, *On Interior Point Methods using a Suitable Decomposition for Multistage Stochastic Programming*, joint work with Annick Sartenaer and Jie Sun, Invited Minisymposium.

Meeting of ICIAM Board, Florence, Italy. 20-21 May 2005. I.S. Duff, Board Member.

Householder Symposium, Seven Springs, Pennsylvannia, USA. 22-27 May, 2005. I.S. Duff, *Talk.*

Seminar at Old Dominion University, Virginia, USA. 30 May, 2005. I.S. Duff, *Combining direct and iterative methods for the solution of large systems in different application areas,* Seminar.

2005 International conference on preconditioning techniques for large sparse matrix problems in scientific and industrial applications, Atlanta, USA, 19-21 May 2005. L. Giraud, *On the sensitivity of some SPD spectral preconditioners*, joint work with S. Gratton, Talk.

2005 International conference on preconditioning techniques for large sparse matrix problems in scientific and industrial applications, Atlanta, USA, 19-21 May 2005. S. GRATTON, *Incremental spectral preconditionner for linear systems with multiple right-hand sides*, joint work with Luc Giraud and Emeric Martin, Talk.

XVI Householder Meeting on Numerical Linear Algebra, Pennsylvania, USA, May 2005. L. GIRAUD, *Two-level spectral preconditioners for general linear systems*, joint work with B. Carpentieri and S. Gratton, Talk.

XVI Householder Meeting on Numerical Linear Algebra, Pennsylvania, USA, May 2005. S. GRATTON, *On the sensitivity of some spectral preconditioners*, joint work with Luc Giraud, Talk.

June

GS05, Siam Conference on Mathematical and Computational Issues in the Geosciences, Avignon, France, June 7-10. M. BABOULIN, *Parallel distributed solvers for accurate and efficient gravity field computation*, joint work with G. Balmino, L. Giraud and S. Gratton, Contributed Talk.

July

SIAM Annual Meeting, New Orleans, Louisiana, USA. 11-15 July, 2005. I.S. DUFF, Board of Trustees.

Thesis defence of Emeric Martin, CERFACS, Toulouse, France. 26 July, 2005. I.S. DUFF, L. GIRAUD, Member of Jury.

August

ERSA 2005, 45th Congress of the European Regional Science Association, Augustus 23-27, 2005, Amsterdam, The Netherlands. F. BASTIN, *Taste Heterogeneity and Substitution Patterns in Models of the Simultaneous Choice of Activity Timing and Duration*, joint work with O. Ashiru, D. Ettema, and J. Polak, Contributed Talk.

ERSA 2005, 45th Congress of the European Regional Science Association, Augustus 23-27, 2005, Amsterdam, The Netherlands. F. BASTIN, *Dynamic discrete choice aith an inter-temporal resource constraint: the case of door-to-door concessionary traval in London*, joint work with J. Polak, J.-D. Schmoecker, Contributed Talk.

September

RAL-Bath Numerical Analysis Day, Rutherford Appleton Laboratory, Oxfordshire, UK. 27 September, 2005. I.S. DUFF, Attendee.

October

University of Kaiserslautern, Germany. 27 October, 2005. I.S. DUFF, *Direct methods for sparse linear systems,* Seminar.

Institut für Techno- und Wirtschaftsmathematik (ITWM), Kaiserslautern, Germany. 28 October, 2005. I.S. Duff, *The HSL Library,* Seminar.

December

Thesis defence of Ahmed Touhami, ENSEEIHT, Toulouse, France. 25 November, 2005. I.S. Duff, L. Giraud, Member of jury.

SIAM Board of Trustees, Philadelphia, Pennsylvannia, USA. 9-10 December, 2005. I.S. Duff, Member of Board.

HDR defence of Serge Gratton. 13 December, 2005. I.S. Duff, L. Giraud, Member of Jury.

8.2 Conferences and seminars organized by the Parallel Algorithms Project

June

Second International Workshop on Combinatorial Scientific Computing (CSC05) June 21–23th, 2005 at CERFACS, Toulouse, France. The conference was co-sponsored by ENSEEIHT-IRIT, INRIA, CERFACS, 71 attendees.

Invited speakers :

S.C. Eisenstat, (Yale University, U.S.A.),
D. Halperin, (Tel Aviv University, Tel Aviv, Israel),
D. Trystram, (IMAG, Grenoble, France),
V. D. Cung, (INPG, France),
G. Allon, (EADS-CCR, France),
D. Trystram, (IMAG, France).

Speakers :
C. Aykanat, (LBNL, Berkeley, U.S.A.),
S. Bhowmick, (Argonne National Laboratory, U.S.A),
E. Boman, (Sandia National Laboratories, U.S.A.),
D. Goudin, (CEA - CESTA, France),
M. Goyal, (University of Lethbridge, Canada),
L. Grigori, (IRISA / INRIA Rennes, France),
A. Guermouche, (INRIA / ENSEEIHT- IRIT, France),
M. Halappanavar, (Old Dominion University, U.S.A.),
J. Hall, (University of Edinburgh, U.K.),
S. Li, (Lawrence Berkeley National Laboratory, U.S.A.),
S. Oliveira, (The University of Iowa, U.S.A.),
C. Phillips, (Sandia National Laboratories, U.S.A.),
A. Pinar, (Lawrence Berkeley National Laboratory, U.S.A.),
S. Pralet, (CNRS - IRIT, France),
R. Preis, (University of Paderborn, Germany),
D. Ruiz, (ENSEEIHT- IRIT, France),
I. Safro, (Weizmann Institute of Science, Israel),

J. Scott, (RAL, U.K.),
S. H. Teng, (Boston University, U.S.A.),
S. Toledo, (Tel-Aviv University, Israel),
M. Tuma, (Czech Academy of Sciences, Czech Republic),
J. Utke, (Argonne National Laboratory, U.S.A).

8.3 Internal seminars organized within the Parallel Algorithms Project

February

Trust-region approaches for nonlinear stochastic programming and mixed logit models, February 2, 2005. F. Bastin.

March

Towards the Final Generation of Dense Linear Algebra Libraries, March 7, 2005. R.A. van de Geijn (Univ. of Texas, U.S.A). Also CERFACS wide interest seminar.

May

Homotopic backward analysis for matrix eigenvalues, May 12, 2005. M. Ahmadnasab.

June

A few challenging problems in computational sciences, June 28, 2005. M. Garbey (University of Houston, U.S.A.). Also CERFACS wide interest seminar.

July

Spectral two-level preconditioners for sequences of linear systems, July 26, 2005. Ph.D. thesis defence. E. Martin.

September

Pushing geometric multigrid to its limits, September 20, 2005. F. Hulsemann.

October

Mathematical analysis and numerical methods for the parallel solution of some partial differential equations, October 18, 2005. Fréderic Magoules (Universite Henri Poincaré, Nancy, France).

November

On the integration of Code ASTER and Mumps or it is always more complicated than expected, November 7th, 2005. F. Hulsemann.
Parallelization of an atmospheric model and an introduction to physics in the (mathematical) algo world, November 21, 2005. H. Le Berre.

December

Fast and robust solvers in Scientific Computing Applications in Geosciences, December 13, 2005. Accreditation to supervise research defence. S. Gratton.

9 Publications

9.1 Journal Publications

[PUB1] P.R. Amestoy, I.S. Duff, and C. Vömel. Task scheduling in an asynchronous distributed memory multifrontal solver. *SIAM J. Matrix Analysis and Applications*, 26:544–565, 2005.

[PUB2] M. Arioli, D. Loghin, and A. Wathen. Stopping criteria for iterations in finite-element methods. *Numerische Mathematik*, 99:381–410, 2005.

[PUB3] M. Baboulin, L. Giraud, and S. Gratton. A parallel distributed solver for large dense symmetric systems: applications to geodesy and electromagnetism problems. *Int. J. High Speed Computing*, 19(04):353–363, 2005.

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