**Technical Report**
RAL-TR-2006-006

# Numerical Analysis Group Progress Report January 2004 - December 2005

**Iain S. Duff (Editor)**

March 10, 2006

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**ISSN 1358-6254**

**RAL-TR-2006-006**

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## ABSTRACT

We discuss the research activities of the Numerical Analysis Group in the Computational Science and Engineering Department at the Rutherford Appleton Laboratory of CLRC for the period January 2004 to December 2005. This work was principally supported by EPSRC grant S42170.

**Keywords:** sparse matrices, direct methods, iterative methods, ordering techniques, stopping criteria, numerical linear algebra, large-scale optimization, Harwell Subroutine Library, HSL, GALAHAD, CUTEr

**AMS(MOS) subject classifications:** 65F05, 65F50.

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Computational Science and Engineering Department
Atlas Centre
Rutherford Appleton Laboratory
Oxon OX11 0QX

March 10, 2006.

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Nick Gould.
Optimization and nonlinear equations particularly for large systems.

Jennifer Scott.
Sparse linear systems and sparse eigenvalue problems.

Kath Vann (until 31 January 2005).
Administrative and secretarial support.

Angela Vernon (after 31 January 2005).
Administrative and secretarial support.

## Consultants

Mike Hopper Support for HSL and for TSSD.

John Reid HSL, sparse matrices, automatic differentiation, and Fortran.

## Visitors

Jonathan Boyle (Manchester) Algebraic multigrid methods.

Sue Dollar (Oxford) Linear algebra and preconditioning.

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# 1 Introduction (I. S. Duff)

This report covers the period from January 2004 to December 2005 and describes work performed by the Numerical Analysis Group within the Computational Science and Engineering Department at the CLRC Rutherford Appleton Laboratory. This work was principally supported by EPSRC grant S42170.

The details of our activities are documented in the following pages. These words of introduction are intended merely to provide additional information not appropriate for the detailed reports.

The main news on staff changes is that we recruited two new members for the Group in the summer of 2005 although, because of their existing commitments, neither can join us until the middle of 2006. We thus look forward to welcoming Sue Dollar (presently teaching at Reading) and Coralia Cartis (presently a post doc at Oxford) to the Group. Both are well known to us and we are excited about the prospect of their arrival. Sue recently completed her D Phil at Oxford under the supervision of Andy Wathen on "Iterative Linear Algebra for Constrained Optimization". Cora's thesis was on "On Interior Point Methods for Linear Programming", and she was supervised by Mike Powell at Cambridge. Unfortunately, our secretary Kath Vann was offered a job with more pay and better hours within walking distance of her home and understandably left us early in 2005. Since then we have had an interim arrangement with Angela Vernon from Space Sciences who has done an admirable job with our secretarial and administrative needs.

The support and development of HSL (formerly the Harwell Subroutine Library) continues to be one of our major activities. There was a release of HSL in the autumn of 2004. The HSL marketing effort continues to be supported by Lawrence Daniels and his team from Hyprotech, even though they have now left AEA and are owned by AspenTech Inc. We are still able to employ John Reid as a consultant using HSL funds. We also benefit from the consultancy of Mike Hopper who helps us both in typesetting and the ongoing commitment to higher software standards.

Readers of our Progress Reports will recognize we have adopted a slightly different and more streamlined format than earlier editions. First, the Group members have written their own paragraphs in Section 2. Then the reports on the work performed are far shorter than previously with only an abstract length paragraph or two in the description and a minimal number of references. Finally, we have included more sections on our activities than formerly, viz. lists of conferences attended, seminars presented, and teaching and tutorial activities in Sections 7, 8, and 9, respectively. Lists of seminars (in the joint series with Oxford), technical reports, and publications are given in Sections 10, 11, and 12, respectively. Current information on the activities of the Group and on Group members can be found through page `www.cse.clrc.ac.uk/nag` of the World Wide Web.

## 2 Personal statements

### 2.1 Mario Arioli

Mario Arioli has continued his collaboration with the Academy of Sciences of the Czech Republic, CERFACS (France), IMATI CNR (Italy) and has started a new collaboration with Daniel Loghin who will come to the University of Birmingham as a Lecturer in January 2006. Gianmarco Manzini visited the group during the summer of 2005. Mario and he have collaborated on a new version of the HSL_MI31 package for the conjugate gradient algorithm.

Mario has contributed to the HSL library through the HSL_MI31 package and by developing new Matlab interfaces for some of the sparse solvers in HSL. In particular, the Matlab interface for MA57 is in beta test and has been successfully used by Nick, Sue Dollar, and Andy Wathen in their work "On iterative methods and implicit-factorization preconditioners for regularized saddle-point systems", RAL-TR-2005-011. Mario and Iain are planning to have the Matlab interface for MA48 available for beta test by next spring.

Finally, Mario has continued his activity as chairman of the ERCIM Working Group "Applications of Numerical Mathematics in Science". In particular, he has coordinated the preparation of "ARTDECO" a Marie-Curie Research and Training Network (RTN) proposal for the EU involving 12 partners around Europe.

### 2.2 Iain Duff

Iain still leads a project at the European Centre for Research and Advanced Training in Scientific Computation (CERFACS) at Toulouse in France. In this context, he supervises PhD students, organizes a regular conference "Sparse Days at CERFACS" in June each year, and has served on the jury for four PhD theses and one Habilitation. One of his recent students, Stéphane Pralet, received a top prize for his thesis. Iain also continues to visit Glasgow regularly in his capacity as a Visiting Professor at Strathclyde. He has presented, jointly with Jennifer, MSc lectures on sparse direct methods at Oxford in the Hilary term of both 2004 and 2005. His research interests continue to be in all aspects of sparse matrices, including more recently iterative methods as well as direct methods, and in the exploitation of parallel computers. One of his current interests is in developing robust and efficient pivoting strategies for symmetric indefinite systems, including the block structured matrices from saddle point problems. This is work that he has been doing jointly with John Gilbert from Santa Barbara and Stéphane. He is extending this work in several directions, notably in examining the use of direct factorizations with iterative schemes like GMRES and FGMRES, jointly with Mario, Stéphane, and Serge Gratton from CERFACS, and in developing HSL software for the direct solution of skew symmetric matrices.

He is a Chief Editor of the IMA Journal of Numerical Analysis, the Vice-President of the IMA for Learned Society affairs, editor of the IMANA Newsletter, and IMA representative on the International Committee that oversees the ICIAM international conferences on applied mathematics. He was reelected to the Board of Trustees by the SIAM members in 2005 and was elected as Chairman of the Board in December 2005, the first non-US resident to hold that position. He was interviewed for the SIAM History Project that is recording the history of numerical analysis and computational mathematics. In addition to his many invited talks at international meetings, he has developed a new speciality of after-dinner speaking giving two talks at the SVG meeting in Stanford and the biennial Dundee Conference. He has served on evaluation committees for the Helmholtz Centres in Germany and the Mathematics Department at the University of Porto. He has been on the Programme and Organizing Committee for several international meetings. He has given invited talks at meetings in Chalkis (Greece), Copenhagen, Krakow, and New Delhi and has presented seminars in Havana, Kaiserslautern, Old Dominion, and Strathclyde.

### 2.3 Nick Gould

As always, Nick's work has centered around optimization and the linear-algebraic requirements that surround it. There has been much unpublished development of the next generation of nonlinear optimization solvers within GALAHAD. In particular, an evolving sequential linear-quadratic programming method is being developed jointly with Sven Leyffer, Jorge Moré and Todd Munson from Argonne National Laboratory, and Michael Friedlander from the University of British Columbia. Nick has also been working with Coralia Cartis from Oxford on finding well-centered points within polytopes (regions defined by systems of linear equations and inequalities). This is required by the interior-point nonlinear optimization solver that Nick is developing with Dominique Orban from the Polytechnique de Montreal and Philippe Toint from the University of Namur. Other GALAHAD developments have concerned preconditioners for the vital (indefinite) linear systems that arise in optimization and has involved much work with Sue Dollar and Andy Wathen from Oxford and Wil Schilders from Philips in Eindhoven. The latest official release of GALAHAD includes graphical user-interface to its core solvers. Nick's optimization testing environment CUTEr has also advanced by porting it to Windows and Apple OS X platforms, and by including interfaces to a variety of new solvers.

A highlight from the past two years was Nick's month-long visit as a Senior Visiting Scientist at Argonne National Laboratory in the autumn of 2004 to work on theoretical aspects of the nonlinear programming solver mentioned above. A major new responsibility has been his appointment as editor-in-chief of the SIAM Journal on Optimization from 2005. He has also added the IMA Journal of Numerical Analysis to his existing associate editorial duties with Mathematical Programming and the ACM Transactions on Mathematical Software. In addition, Sven Leyffer, Philippe Toint and Nick co-edited a special issue of Mathematical Programming to celebrate the 65th birthday of Roger Fletcher from Dundee. He has been busy as usual with his Visiting Professorship in Edinburgh and the associated MSc teaching both in Edinburgh and Oxford. Nick has also organised a number of successful one-day meetings, notably the (now) annual Oxford-Cambridge Optimization Day, the fourth in our series of joint Bath-RAL Numerical Analysis Days, and a Mathematical Interdisciplinary Research Day on Optimization in Warwick.

### 2.4 Jennifer Scott

Major projects that Jennifer has spent much of her time on include collaborating with John Reid on developing a new out-of-core sparse direct solver for the solution of very large symmetric systems and working with Nick Gould and Yifan Hu of Wolfram Research on comparing the performance of sparse direct solvers on large symmetric systems. The results of this study are now available. The out-of-core solver is currently being performance tested, although more work remains for the indefinite case. Jennifer has also continued to work on sparse matrix orderings, including unsymmetric band reduction algorithms and efficient orderings to bordered block diagonal form.

Jennifer has enjoyed a number of short visits to other research groups, notably to the University of British Columbia and the University of Basel. She gave invited talks at CERFACS, Bath, Vancouver, and Basel and invited lectures on HSL at an e-social science workshop at the University of Lancaster and to MSc students at the University of Edinburgh. She has strengthened her contacts with the University of Manchester through being the external examiner for the PhD thesis of Craig Lucas and supervising (with David Silvester) a postdoctoral student Jonathan Boyle. She continues to act as the coordinator for the Group's joint seminar series with Oxford University and has presented, jointly with Iain, MSc lectures on sparse direct methods at Oxford in 2004 and 2005.

She has recently become one of two UK coordinators for European Women in Mathematics and a member of the London Mathematical Society Women in Mathematics Committee. She has also accepted an invitation to represent mathematics on the National Coordinating Committee for WISE (Women into Science, Engineering and Construction). At RAL, she has been acting as a mentor for a more junior female member of staff. She recently became a Fellow of the Institute of Mathematics and Applications. Fitting all this into her part-time working hours is proving a challenge!

## 3 Direct Methods

### 3.1 Pivoting strategies for symmetric indefinite matrices (I.S. Duff and S. Pralet)

This work concerns the direct solution of sparse symmetric indefinite matrices. We consider ways of implementing preordering and scaling for symmetric systems and show the effect of using this technique with a multifrontal code for sparse symmetric indefinite systems. We have developed a new method for scaling, and we propose a way of using an approximation to a symmetric weighted matching to predefine $1 \times 1$ and $2 \times 2$ pivots prior to the ordering and analysis phase. We also present new classes of orderings called "relaxed constrained orderings" that mix structural and numerical criteria.

Furthermore, we propose original approaches that are designed for parallel distributed factorization. We show that our pivoting strategies are numerically robust and that the factorization is significantly faster because of this static/numerical combination. 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.

More recently, further work with Mario Arioli and Serge Gratton has looked at ways to improve the robustness of static pivoting through using more sophisticated iterative methods like GMRES and FGMRES.

[1] I.S. Duff and S. Pralet. Strategies for scaling and pivoting for sparse symmetric indefinite problems. *SIAM J. Matrix Analysis and Applications,* **27**, 313–340, 2005.

[2] 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 RAL-TR-2005-007, 2005.

### 3.2 Multilevel hybrid spectral element ordering algorithms (J. A. Scott)

For frontal solvers to perform well on finite-element problems it is essential that the elements are ordered for a small wavefront. We introduce multilevel element ordering algorithms, which have their origins in the profile reduction algorithm of Sloan but for large problems often give significantly smaller wavefronts. We examine a number of multilevel variants with the aim of finding the best methods to include within our new state-of-the-art frontal solver `HSL_MA42_ELEMENT` (see Section 3.6). Both direct and indirect versions of the reordering algorithm are considered and used in combination with spectral orderings and the Hager exchange algorithm. Numerical experiments are performed using a range of problems arising from real applications and comparisons are made with existing element ordering algorithms. In general, the best orderings are obtained using the indirect hybrid multilevel algorithm but it is faster to compute a Sloan ordering using our HSL ordering code `MC63` and, for the smaller test problems, these orderings are generally of a similar quality.

[1] J.A. Scott. Multilevel hybrid spectral element ordering algorithms. *Commun. Numer. Meth. Engng*, **21**, 233–245, 2005.

### 3.3 Reducing the total bandwidth of a sparse unsymmetric matrix (J.K. Reid and J. A. Scott)

For a sparse symmetric matrix, there has been much attention given to algorithms for reducing the bandwidth. As far as we can see, little has been done for the unsymmetric matrix $A$, which has distinct lower and upper bandwidths $l$ and $u$. When Gaussian elimination with row interchanges is applied, the lower bandwidth is unaltered while the upper bandwidth becomes $l + u$. With column interchanges, the upper bandwidth is unaltered while the lower bandwidth becomes $l+u$. We therefore seek to reduce $\min(l, u) + l + u$, which we call the *total* bandwidth.

We compare applying the reverse Cuthill-McKee algorithm to $A + A^T$, to the row graph of $A$, and to the bipartite graph of $A$. We also propose an unsymmetric variant of the reverse Cuthill-McKee algorithm. In addition, we have adapted the node-centroid and hill climbing ideas of Lim, Rodrigues and Xiao to the unsymmetric case. We have found that using these to refine a Cuthill-McKee based ordering can give significant further bandwidth reductions.

Numerical results for a range of practical problems are presented and comparisons made with the recent lexicographical method of Baumann, Fleishmann and Mutzbauer.

[1] J.K. Reid and J.A. Scott. Reducing the total bandwidth of a sparse unsymmetric matrix. Technical Report RAL-TR-2005-001, 2005. To appear in *SIAM J. Matrix Analysis and Applications*.

### 3.4 A numerical evaluation of sparse direct solvers for the solution of large sparse, symmetric linear systems of equations (N. I. M. Gould, Y. Hu, and J. A. Scott)

In recent years a number of solvers for the direct solution of large sparse, symmetric linear systems of equations have been developed. These include solvers that are designed for the solution of positive-definite systems as well as those that are principally intended for solving indefinite problems. The available choice can make it difficult for users to know which solver is the most appropriate for their applications. In this study, we use performance profiles as a tool for evaluating and comparing the performance of serial sparse direct solvers on an extensive set of symmetric test problems taken from a range of practical applications.

To be able to compare the different solvers, we had to familiarise ourselves with each of the solvers and to write drivers for them. Our experiences of using the different packages to solve a wide range of problems arising from real applications were mixed. In [1] we present numerical findings and in [3] we highlight some of our experiences of using the solvers with the aim of providing advice to both software developers and users of sparse direct solvers. We conclude that while performance is an essential factor to consider when choosing a code, there are other factors that a user should also consider that vary significantly between packages.

[1] N.I.M. Gould and Y. Hu and J.A. Scott. A numerical evaluation of sparse direct solvers for the solution of large, sparse, symmetric linear systems of equations. In “PARA’04 Workshop on state-of-the-art in scientific computation” (J. Dongarra, K. Madsen and J. Waśniewski, eds.), Springer LNCS proceedings, (2005) 818:827

[2] N.I.M. Gould, Y. Hu, and J.A. Scott. Complete results for a numerical evaluation of sparse direct solvers for the solution of large, sparse, symmetric linear systems of equations. Numerical Analysis Internal Report 2005-1, Rutherford Appleton Laboratory, 2005.

[3] Y. Hu and J.A. Scott. Experiences of sparse direct symmetric solvers. Technical Report RAL-TR-2005-014, 2005.

### 3.5 Stabilized block diagonal forms for parallel sparse solvers (I. S. Duff and J. A. Scott)

One possible approach to the solution of large sparse linear systems $Ax = b$ is to reorder the system matrix to bordered block diagonal form and then to solve the block system in parallel. We consider the duality between singly bordered and doubly bordered block diagonal forms. The idea of a stabilized doubly bordered block diagonal form is introduced. We show how a stable factorization of a singly bordered block diagonal matrix results in a stabilized doubly bordered block diagonal matrix. We propose using matrix stretching to generate a singly bordered form from a doubly bordered form. Matrix stretching is compared with two alternative methods for obtaining a singly bordered form and is shown to be efficient both in computation time and the quality of the resulting block structure.

[1] I.S. Duff and J.A. Scott. Stabilized bordered block diagonal forms for parallel sparse solvers. *Parallel Computing*, **31**, 275–289, 2005.

### 3.6 `MA42_ELEMENT` - a state-of-the-art frontal solver for finite-element applications. (J. A. Scott)

In recent years there have been a number of important developments in frontal algorithms for solving the large sparse linear systems of equations that arise from finite-element problems. We have designed and developed a new fully portable and efficient frontal solver for large-scale real and complex unsymmetric linear systems from finite-element problems that incorporates these developments. The new package offers both a flexible reverse communication interface and a simple to use all-in-one interface, which is designed to make the package more accessible to new users. Other key features include automatic element ordering using our state-of-the-art hybrid multilevel spectral algorithm (see Section 3.2), minimal main memory requirements, the use of high level BLAS, and facilities to allow the solver to be used as part of a parallel multiple front solver. The new solver is written using Fortran 95 and has been tested on a range of problems from practical applications. It is available as package `HSL_MA42_ELEMENT` within the HSL mathematical software library. For element problems, it supersedes the well-known `MA42` package.

[1] J.A. Scott. `MA42_ELEMENT` - a state-of-the-art frontal solver for finite-element applications Technical Report RAL-TR-2004-026, 2004.

[2] J.A. Scott. A frontal solver for the 21st century. *Commun. Numer. Meth. Engng*, to appear.

### 3.7 Automatic ordering for a symmetric sparse direct solver (I.S. Duff and J. A. Scott)

In recent years, nested dissection has grown in popularity as the method of choice for computing a pivot sequence for use with a sparse direct symmetric solver. This is particularly true for very large problems. For smaller problems, minimum degree based algorithms often produce orderings that lead to sparser matrix factors. Furthermore, minimum degree orderings are frequently significantly cheaper to compute than nested dissection. We consider whether we can predict, using only the sparsity pattern of the matrix, which ordering will be better when used with the HSL direct solver `MA57`. Based on a wide range of large problems from different application areas, we find that it can be worthwhile to have an automatic selection strategy, particularly if only few factorizations follow the analysis. The automatic strategy is also a good option for users who wish to treat the software as a black box and who have no interest in understanding the use of orderings or in tuning the code for their problem.

[1] I.S. Duff and J.A. Scott. Towards an automatic ordering for a symmetric sparse direct solver. Technical Report RAL-TR-2006-001, 2006.

### 3.8 An out-of-core direct solver for large sparse symmetric linear systems (J.K. Reid and J. A. Scott)

The popularity of direct methods for solving large sparse linear systems of equations $Ax = b$ stems from their generality and robustness. Their main weakness is that, in general, the memory required grows more rapidly than the problem size. We are designing and developing a sparse symmetric out-of-core direct solver for inclusion within HSL. Both the system matrix $A$ and its factors are stored externally. The code, which is written in Fortran 95 and called `HSL_MA77`, implements a multifrontal algorithm. By incorporating numerical pivoting using $1 \times 1$ and $2 \times 2$ pivots, the package is intended for the solution of both positive-definite and indefinite problems. To minimise storage for the system data, a reverse communication interface is used. Input of $A$ is either by rows or by elements. An important feature of the package is that all input and output to disk is performed through a set of Fortran subroutines that manage a virtual memory system so that actual i/o occurs only when really necessary (see Section 3.10). For the dense linear algebra computations that lie at the heart of the factorization and solve, `HSL_MA77` uses another new HSL package `HSL_MA54` (see Section 3.11)

### 3.9 A partial condition number for linear least-squares problems (M. Arioli, M. Baboulin, and S. Gratton)

In [1], 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 $b$. 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 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 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 $A$.

[1] M. Arioli, M. Baboulin, and S. Gratton, Partial condition number for least-squares problems. Technical Report RAL-TR-2004-029, 2004.

### 3.10 Efficient i/o handling (J. K. Reid and J. A. Scott)

The package `HSL_OF01` is being developed for use by `HSL_MA77`, but is general-purpose and could be used elsewhere. It provides read/write facilities for one or more direct-access files through a single in-core buffer, so that actual input-output operations are often avoided. The buffer is divided into fixed-length pages and all input-output is performed by transferring a single page to or from a single record of the file(s) (the length of a record is equal to the length of a page).

Each set of data is addressed as a virtual array, that is, as if it were a very large array. It is so large that long (64-bit) integers are used to refer to data within it. Without regard to page boundaries, an array of any length may be sent to a contiguous section of the virtual array by a call to `OF01_write`, or received from it by a call to `OF01_read`. The virtual array is permitted to be too large to be accommodated on a single file, in which case secondary files are used.

### 3.11 Partial Cholesky factorization with efficient use of cache (J. K. Reid)

The package `HSL_MA54` is an adaptation of the block hybrid Cholesky factorization [1] to provide the partial factorizations and solutions that are needed in a frontal or multifrontal code. The block hybrid format is designed to make good use of cache. It stores the matrix as a block matrix with each block held contiguously by rows, which allow Level-3 BLAS to be used.

The modification involves limiting the eliminations to the leading $p$ columns. The factorization takes the form

$$A = \begin{pmatrix} A_{11} & A_{21}^T \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} L_{11} & \\ L_{21} & I \end{pmatrix} \begin{pmatrix} I & \\ & S_{22} \end{pmatrix} \begin{pmatrix} L_{11}^T & L_{21}^T \\ & I \end{pmatrix}$$

where $L_{11}$ is lower triangular and both $A_{11}$ and $L_{11}$ have order $p$. We use the lower blocked hybrid format for the lower triangular parts of both $A_{11}$ and $A_{22}$. Each is held by blocks of order $nb$, except that the final block may be smaller. The rectangular matrix $A_{21}$ is held as a block matrix with matching block sizes. During factorization, these matrices are overwritten by the lower triangular parts of $L_{11}$ and $S_{22}$ and by $L_{21}$. We call this format for $A$ and its factorization the *double blocked hybrid* format.

Subroutines are provided for efficiently rearranging a matrix in lower packed format to double blocked hybrid format and vice-versa, solving sets of equations after a full factorization ($p = n$), and for partial forward and back substitution:

$$\begin{pmatrix} L_{11} & \\ L_{21} & I \end{pmatrix} X = B \quad \text{and} \quad \begin{pmatrix} L_{11}^T & L_{21}^T \\ & I \end{pmatrix} X = B.$$

[1] B. S. Andersen, J. A. Gunnels, F. G. Gustavson, J. K. Reid, and J. Wasniewski. A fully portable high performance minimal storage hybrid format Cholesky algorithm. *ACM Trans. on Math. Software*, **31**, 201-227, 2005.

# 4 Iterative methods

## 4.1 Combining direct and iterative methods (I.S. Duff)

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, usually 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 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.

[1] I.S. Duff, Combining direct and iterative methods for the solution of large systems in different application areas. Technical Report RAL-TR-2004-033, 2004.

## 4.2 Spanning trees and network programming for solving Darcy's equation (M. Arioli and G. Manzini)

In [2], a null space algorithm is considered for solving the augmented system produced by the mixed finite-element approximation of Darcy's Law. The method is based on the combination of a $LU$ factorization technique for sparse matrices with an iterative Krylov solver. The computational efficiency of the method relies on the use of spanning trees to compute the $LU$ factorization without fill-in and on a suitable stopping criterion for the iterative solver. We experimentally investigate its performance on a realistic set of selected applications.

In [3], we use the null-space algorithm approach to solve the augmented systems produced by the mixed finite-element approximation of Darcy's laws. Taking into account the properties of the graph representing the triangulation, we adapt the null space technique proposed in [1], where an iterative-direct hybrid method is described. In particular, we use network programming techniques to identify the renumbering of the triangles and the edges, which enables us to compute the null space without floating-point operations. Moreover, we extensively take advantage of the graph properties to build efficient preconditioners for the iterative algorithm. Finally, we present the results of several numerical tests.

[1] M. Arioli and L. Baldini, A backward error analysis of a null space algorithm in sparse quadratic programming. *SIAM J. Matrix Anal. Appl.*, 23, pp. 425–442, 2001.

[2] M. Arioli and G. Manzini, Null space algorithm and spanning trees in solving Darcy's equation. *BIT Numerical Mathematics*, 43, 839–848, 2003.

[3] M. Arioli and G. Manzini, A network programming approach in solving Darcy's equations by mixed finite-element methods. *Electronic Transactions on Numerical Analysis, Special Volume on Saddle Point Problems: Numerical Solution and Applications.*,22, 40–70, 2006.

### 4.3 Stopping criteria (M. Arioli, D. Loghin, and A. Wathen)

The conjugate gradient method has been successfully used for many years in the solution of symmetric and positive definite systems obtained by the finite element approximation of self-adjoint elliptic partial differential equations. In [2] we take into account recent results that make it possible to approximate the energy norm of the error during the conjugate gradient iterative process. We adapt the stopping criterion introduced in [1]. Moreover, we show that the use of efficient preconditioners does not require changing the energy norm used by the stopping criterion. Finally, we present the results of several numerical tests that experimentally validate the effectiveness of our stopping criterion.

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

Finally, Daniel and Mario are developing new stopping criteria for saddle point problems. Some preliminary results were presented at the Householder Symposium XVI (2005) and at the $21^{st}$ Numerical Analysis Conference (2005) in Dundee.

[1] M. Arioli, E. Noulard, and A. Russo, Stopping criteria for iterative methods: Applications to PDE's. *CALCOLO*, 38 (2001), pp. 97–112.

[2] M. Arioli. A stopping criterion for the conjugate gradient algorithm in a finite element method framework. *Numer. Math.*, 97(1):1–24, 2005.

[3] M. Arioli, D. Loghin, and A. Wathen, Stopping criteria for iterations in finite-element methods. *Numer. Math.*, 99(1):381–410, 2005.

### 4.4 MI31 (M. Arioli and G. Manzini)

In [1], we present an implementation of the preconditioned conjugate gradient method that is based on reverse communication to allow the user to incorporate his or her own matrix-vector multiplication routine and preconditioning algorithm. Our implementation also includes new stopping criteria that take into account some recent results on the approximation of the energy norm of the error during the conjugate gradient iterative process. We present the results of several numerical tests that experimentally validate the effectiveness of the stopping criteria on finite-element approximations of selected 2D and 3D problems. During the visit of Gianmarco Manzini in the summer of 2005, we added some new techniques to the previous version of the HSL_MI31 package that can improve the convergence rate when a non null starting point is used. Moreover, we have extensively tested HSL_MI31 on elasticity problems in 3D domains and have started a study on the extension of the stopping criteria to nonlinear cases.

[1] M. Arioli and G. Manzini, MI31: a conjugate gradient algorithm implementation with energy-norm stopping criteria. Technical Report RAL-TR-2005-004, 2005.

## 4.5 Dual variable methods for mixed-hybrid finite element approximation of the potential fluid flow problem in porous media (M. Arioli, J. Maryška, M. Rozložník, and M. Tůma)

Mixed-hybrid finite element discretization of Darcy's law and the continuity equation that describe the potential fluid flow problem in porous media leads to symmetric indefinite saddle-point problems. In [1] we consider solution techniques based on the computation of a null-space basis of the whole or part of the left lower off-diagonal block in the system matrix and on the subsequent iterative solution of a projected system. This approach is mainly motivated by the need to solve a sequence of such systems with the same mesh but different material properties. A fundamental cycle null-space basis of the whole off-diagonal block is constructed using the spanning tree of an associated graph. It is shown that such a basis may be theoretically rather ill-conditioned. Alternatively, the orthogonal null-space basis of the sub-block used to enforce continuity over faces can be easily constructed. In the former case, the resulting projected system is symmetric positive definite and so the conjugate gradient method can be applied. The projected system in the latter case remains indefinite and the preconditioned minimal residual method (or the smoothed conjugate gradient method) should be used. The theoretical rate of convergence for both algorithms is discussed

[1] M. Arioli, J. Maryška, M. Rozložník, and M. Tůma, A stopping criterion for the conjugate gradient algorithm in a finite element method framework. *Electronic Transactions on Numerical Analysis, Special Volume on Saddle Point Problems: Numerical Solution and Applications.*,22, 17–40, 2006.

## 4.6 Parallel preconditioners based on partitioning (I.S. Duff, S. Riyavong, and M.B. Van Gijzen)

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.


[1] I.S. Duff, S. Riyavong, and M.B. Van Gijzen, Parallel preconditioners based on partitioning sparse matrices. Technical Report RAL-TR-2004-040, 2004.


# 5 Optimization

## 5.1 A filter-trust-region method for unconstrained optimization (N.I.M. Gould, C. Sainvitu, and Ph. L. Toint)

A new filter-trust-region algorithm for solving unconstrained nonlinear optimization problems is introduced. Based on the filter technique introduced by Fletcher and Leyffer, it extends an existing technique of Gould, Leyffer and Toint (SIAM J. Optimization 15(1):17-38, 2005) for nonlinear equations and nonlinear least-squares to the fully general unconstrained optimization problem. The new algorithm is shown to be globally convergent to at least one second-order critical point, and numerical experiments indicate that it is very competitive with more classical trust-region algorithms.


[1] N. I. M. Gould, C. Sainvitu and Ph. L. Toint, A filter-trust-region method for unconstrained optimization. *SIAM Journal on Optimization,* 16(2) (2006) 341:357


## 5.2 Sensitivity of trust-region algorithms to their parameters (N.I.M. Gould, D. Orban, A. Sartenaer, and Ph. L. Toint)

The sensitivity of trust-region algorithms on parameters related to the step acceptance test and to the update of the trust region radius are examined. In the context of unconstrained programming, it is shown that the numerical efficiency of these algorithms can easily be improved by choosing appropriate parameters. Ranges of values for these parameters are recommended, based on extensive numerical tests.


[1] N. I. M. Gould, D. Orban, A. Sartenaer and Ph. L. Toint, Sensitivity of trust-region algorithms to their parameters. *4OR,* 3(1) (2005) 227:241.


## 5.3 On the convergence of successive linear-quadratic programming algorithms (R.H. Byrd, N.I.M. Gould, J. Nocedal, and R.A. Waltz)

The global convergence properties of a class of penalty methods for nonlinear programming are analysed. These methods include successive linear programming approaches, and more specifically, the successive linear-quadratic programming approach presented by Byrd, Gould, Nocedal and Waltz (Math. Programming 100(1):27-48, 2004). Every iteration requires the solution of two trust-region subproblems involving piecewise linear and quadratic models, respectively. It is shown that, for a fixed penalty parameter, the sequence of iterates approaches stationarity of the penalty function. A procedure for dynamically adjusting the penalty parameter is described, and global convergence results for it are established.

[1] R. H. Byrd, N. I. M. Gould, J. Nocedal and R. A. Waltz On the convergence of successive linear-quadratic programming algorithms. *SIAM Journal on Optimization,* 16(2) (2006) 471:489.

### 5.4 Numerical methods for large-scale nonlinear optimization (N.I.M. Gould, D. Orban, and Ph. L. Toint)

Recent developments in numerical methods for solving large differentiable nonlinear optimization problems are reviewed. State-of-the-art algorithms for solving unconstrained, bound-constrained, linearly-constrained and nonlinearly-constrained problems are discussed. As well as important conceptual advances and theoretical aspects, emphasis is also placed on more practical issues, such as software availability.

[1] N. I. M. Gould, D. Orban and Ph. L. Toint, Numerical methods for large-scale nonlinear optimization. *Acta Numerica,* 14 (2005) 299:361.

### 5.5 On implicit-factorization constraint preconditioners (H.S Dollar, N.I.M. Gould, and A.J. Wathen)

Recently Dollar and Wathen (SIAM J. Matrix Analysis and Applications, to appear 2006) proposed a class of incomplete factorizations for saddle-point problems, based upon earlier work by Schilders (Conference talk, 2002). This class of preconditioners is generalized, and the spectral implications of this approach are examined.. Numerical tests indicate the efficacy of the preconditioners proposed.

[1] H. S. Dollar, N. I. M. Gould and A. J. Wathen, On implicit-factorization constraint preconditioners. In *Large Scale Nonlinear Optimization* (G. Di Pillo and M. Roma, eds.) Springer Series on Nonconvex Optimization and Its Applications, Vol. 83, Springer Verlag (2006).

### 5.6 On iterative methods and implicit-factorization preconditioners for regularized saddle-point systems (H.S Dollar, N.I.M. Gould, W.H.A. Schilders, and A.J. Wathen)

Conjugate-gradient like methods for solving block symmetric indefinite linear systems that arise from saddle point problems or, in particular, regularizations thereof are considered. Such methods require preconditioners that preserve certain sub-blocks from the original systems but allow considerable flexibility for the remaining blocks. Fourteen families of implicit factorizations that are capable of reproducing the required sub-blocks and (some) of the remainder are constructed.

These generalize known implicit factorizations for the unregularized case. Improved eigenvalue clustering is possible if additionally some of the non-crucial blocks are reproduced. Numerical experiments confirm that these implicit-factorization preconditioners can be very effective in practice.

[1] H. S. Dollar, N. I. M. Gould, W. H. A. Schilders and A. J. Wathen, On iterative methods and implicit-factorization preconditioners for regularized saddle-point systems. Technical Report RAL-TR-2005-011, 2005. To appear, SIAM Journal on Matrix Analysis and Applications.

### 5.7 Using constraint preconditioners with regularized saddle-point problems (H.S Dollar, N.I.M. Gould, W.H.A. Schilders, and A.J. Wathen)

The problem of finding good preconditioners for the numerical solution of a certain important class of indefinite linear systems is considered. These systems are of a 2 by 2 block (KKT) structure in which the (2,2) block (denoted by -C) is assumed to be nonzero.

Keller, Gould and Wathen (SIAM J. Matrix Anal. Appl., 21(4):1300-1307, 2000) introduced the idea of using constraint preconditioners that have a specific 2 by 2 block structure for the case of $C$ being zero. Results concerning the spectrum and form of the eigenvectors when a preconditioner of the form considered by Keller, Gould and Wathen is used but for which C may not be 0 is given. In particular, the results presented here indicate clustering of eigenvalues and, hence, faster convergence of Krylov subspace iterative methods when the entries of $C$ are small; such a situation arises naturally in interior point methods for optimization and results for such problems validating theoretical conclusions are given.

[1] H. S. Dollar, N. I. M. Gould, W. H. A. Schilders and A. J. Wathen, Using constraint preconditioners with regularized saddle-point problems. Technical Report RAL-TR-2005-026, 2005.

## 6 HSL and GALAHAD

### 6.1 HSL 2004

HSL 2004 was released in September 2004 and contained the following new packages:

`HSL_DC05` solves ordinary differential equations or differential algebraic equations.

`EP25` uses the Lanczos algorithm to compute in parallel the part of the spectrum of a large symmetric matrix that lies in a specified interval.

`HSL_MA42_ELEMENT` solves one or more sets of sparse linear unsymmetric unassembled finite-element equations by the frontal method, optionally using direct access files for the matrix factors.

`MC67` uses Hager's exchange algorithms to refine a profile-reducing permutation of a symmetric matrix.

**HSL_MC73** computes the Fiedler vector of the Laplacian matrix associated with a given symmetric sparsity pattern or computes a symmetric permutation that reduces the profile and wavefront.

**HSL_MC77** calculates scaling factors for a sparse unsymmetric matrix using any given $p$-norm, with $p \geq 1$.

**HSL_MI31** uses the preconditioned conjugate gradient method to solve a linear system with a symmetric positive-definite matrix $A$, implementing several stopping criteria based on lower and upper bounds of the $A$-norm of the error.

**HSL_MP48** solves sets of unsymmetric linear systems of equations in parallel using Gaussian elimination.

In addition, significant improvements were made to these packages in HSL 2004:

**HSL_MA48** has an option for returning the determinant of a square matrix.

**MA51** has an option for returning the determinant of a square matrix.

**MA57** has options for static pivoting, prescaling by a symmetrization of the MC64 scaling, and alternative orderings.

**HSL_MA57** has options for static pivoting, prescaling by a symmetrization of the MC64 scaling, and alternative orderings.

A major update to HSL 2004 was made by Mike Hopper in March 2005 to improve its portability. FD15 now uses Fortran 95 intrinsic functions to provide those machine constants that are needed within the library. Previously, FD05 and ID05 required these and other constants to be supplied explicitly for each machine.

## 6.2 GALAHAD

Version 1.5 of GALAHAD was released in May 2004. This added a Python-based GUI as a front-end to the two major packages. New and forthcoming GALAHAD packages include:

| | |
|---|---|
| EQP | solves an equality-constrained quadratic program using a preconditioned, projected conjugate-gradient iteration |
| QPC | solves a general quadratic program using an interior-point active-set crossover scheme |
| QPS | scales the data for a a general quadratic program to try to make subsequent solution easier |
| RPD | assembles quadratic programming data from a user-supplied problem data file |
| SPPS | provide preconditioners for saddle-point problems |

WCP finds a well-centered point within a polytope

FASTR solves nonlinear programming problems via a filter active-set trust-region method based on sequential regularized linear programming with EQP acceleration

## 7 Conferences

SVG Meeting, Stanford, California, USA. 9-10 January 2004. I. Duff, *Jim Varah, Alan George, and Mike Saunders 60th Birthday Meeting,* After-dinner talk.

SIAM Conference on Parallel Processing for Scientific Computing. San Francisco, California, USA. 24-27 February 2004. Invited minisymposia. J.A. Scott† and I.S. Duff, *SBBD orderings and parallel direct solvers,* I.S. Duff, G. Golub, F. Kwok†, and J.A. Scott, *Combining direct and iterative methods to solve partitioned linear systems,* T.A. Drummond†, I.S. Duff, and D. Ruiz, *Partitioning strategies for the block Cimmino algorithm,* P.A. 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.* I.S. Duff, Organizing Committee and Minisymposia organizer.

CSC Workshop, San Francisco, California, USA. 27-28 February 2004. I.S. Duff and S. Pralet†, *Symmetric weighted matching and applications to indefinite multifrontal solvers.*

GAMM 75th Annual Meeting, Dresden, Germany. 26 March 2004. N.I.M. Gould, *A filter-trust-region method for unconstrained optimization.*

European Conference on Computational Optimization, Dresden, Germany. 29 March 2004. N.I.M. Gould, *An interior-point l1-penalty method for nonlinear optimization.*

Copper Mountain Meeting on Iterative Methods, Colorado, USA. March/April 2004. I.S. Duff, Organizing committee, Workshop chair.

Workshop on Large Scale Nonlinear and Semidefinite Programming, University of Waterloo, Ontario, Canada. 13 May 2004. N.I.M. Gould, *An interior-point l1-penalty method for nonlinear optimization.*

IMAT 2004 in honour of Owe Axelsson, Prague. 25-28 May 2004. M. Arioli, *A Chebyshev-based two-stage iterative method as an alternative to the direct solution of linear systems.*

CERFACS Sparse Days Meeting, 3 June 2004. J.A. Scott, *A numerical evaluation of sparse solvers for the direct solution of large sparse symmetric linear systems.* I.S. Duff, Organizer.

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

PARA04 Conference, Copenhagen, Denmark. 20-23 June 2004. I.S. Duff, *Partitioning and parallelism in the solution of large sparse systems,* Y. Hu† and J.A. Scott, *Efficient ordering techniques for bordered block diagonal forms for unsymmetric parallel sparse direct solvers,* J.K.

Reid, *Fortran is getting more and more powerful,* B. Andersen, J. Gunnels, F. Gustavson, J.K. Reid†, and J. Wasniewski, *A fully portable high performance minimal storage hybrid format Cholesky algorithm,* J.A. Scott†, N.I.M. Gould, and Y. Hu, *A numerical evaluation of sparse direct solvers for the solution of large, sparse, symmetric linear systems of equations.*

Large-scale Nonlinear Optimization Workshop, Erice, Sicily, Italy. 28 June 2004. N.I.M. Gould, *Constraint preconditioners for large-scale nonlinear optimization.*

SIAM Annual Meeting, Portland, Oregon, USA. 14-19 July 2004. I.S. Duff, Organizer of Invited (by SIAGLA) Minisymposium on "Sparse direct methods and their applications", Member of Board of Trustees.

Optbridge 2004, Oxford University, England. 13 August 2004. N.I.M. Gould, *Nonlinear scaling for bound-constrained optimization.*

International Conference of Numerical Analysis and Applied Mathematics 2004 (ICNAAM 2004), Chalkis, Greece. 11-14 September 2004. I.S. Duff, *Partitioning and parallelism in the solution of large sparse systems.*

Workshop on Structured Numerical Linear Algebra Problems: Algorithms and Applications, Cortona, Italy. 20-24 September 2004. M. Arioli, *A Chebyshev-based two-stage iterative method as an alternative to the direct solution of linear systems.*

3rd Bath-RAL Numerical Analysis Day, University of Bath, England. 1 October 2004. J.A. Scott, *Which sparse direct symmetric solver?* M. Arioli, *A Chebyshev-based two-stage iterative method as an alternative to the direct solution of linear systems.*

Conference in Honour of Alfonso Laratta, Modena, 13 October 2004. M. Arioli, *Problemi di accuratezza relativi alla soluzione di sistemi sottodeterminati.*

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.*

E-social Science Workshop, University of Lancaster. 6 April 2005. J.A. Scott, *HSL and an introduction to sparse linear systems.*

SIAM Conference on Optimization, Stockholm, Sweden. 17 May 2005. N.I.M. Gould, *Useful linear algebra for large-scale nonlinear optimization.*

Householder Symposium XVI, Seven Springs Mountain Resort, Pennsylvania, USA. 24 May 2005. M. Arioli, *Block partitioned matrices, inf-sup conditions, and stopping criteria,* I.S. Duff† and S. Pralet, *Further advances in the solution of sparse indefinite systems,* J.K. Reid and J.A. Scott†, *On solving large sparse linear systems out-of-core,* J.K. Reid† and J.A. Scott, *Reducing the bandwidths and profiles of a sparse unsymmetric matrix.*

Second International Workshop on Combinatorial Scientific Computing, CERFACS, Toulouse, France. 21 June 2005. J.A. Scott, *Reducing the total bandwidth of a sparse unsymmetric* *matrix,* I.S. DUFF, Co-chairman (with Alex Pothen and John Gilbert) of Programme Committee.

21st Biennial Conference on Numerical Analysis, Dundee, Scotland. 29 June 2005. M. ARIOLI, *Stopping criteria for Krylov methods applied to the solution of mixed finite-element problems,* N.I.M. GOULD, *Finding a well-centred point for a set of convex polyhedral constraints.* J.K. REID† AND J.A. SCOTT, *Reducing the bandwidths and profiles of a sparse unsymmetric matrix,* J.A. SCOTT, *On solving large sparse linear systems out-of-core,* I.S. DUFF, *Dundee and Dundonians,* After dinner talk.

Optbridge 2005, Cambridge University, England. 16 August 2005. N.I.M. GOULD, *Finding a well-centred point within a polyhedron.*

4th Bath-RAL Numerical Analysis Day Rutherford Appleton Laboratory, England. 27 September 2005. N.I.M. GOULD, *SRLP-EQP filter methods for constrained optimization,* J.K. REID, *Reducing the total bandwidth of a sparse unsymmetric matrix.*

Mathematical Interdisciplinary Research Day on Optimization, University of Warwick, England. 3 October 2005. N.I.M. GOULD, *Optimization - a brief overview.*

2nd European Workshop on Automatic Differentiation, Cranfield University at Shrivenham, England. 18 November 2005. N.I.M. GOULD, *Requirements for automatic differentiation in numerical optimization.*

†Indicates the speaker in multiply authored presentations.

## 8 Seminars

Judge Institute of Management, University of Cambridge, England. 25 February 2004. N.I.M. GOULD, *An interior-point l1-penalty method for nonlinear optimization.*

University of Edinburgh, Scotland. 14 April 2004. N.I.M. GOULD, *An interior-point l1-penalty method for nonlinear optimization.*

Mathematics and Computational Science Division, Argonne National Laboratory, Illinois, USA. 7 September 2004. N.I.M. GOULD, *Constraint preconditioners for large-scale nonlinear optimization.*

Department of Mathematics, The University of British Columbia, Vancouver, Canada. 7 December 2004. J.A. SCOTT, *Which sparse direct solver?*

EPCC, The University of Edinburgh, Scotland. 21 January 2005. J.A. SCOTT, *HSL and the solution of sparse linear systems.*

The University of Edinburgh, Scotland. 21 January 2005. J.A. SCOTT, *Which sparse direct solver?*

University of Basel, Switzerland. 3 February 2005. J.A. SCOTT, *HSL and parallel sparse direct solvers.*

Oxford University Computing Laboratory, England. 17 February 2005. N.I.M. GOULD, *To SQP or not to SQP - modern alternatives in large-scale nonlinear optimization.*

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.*

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.*

University of Manchester, England. 12 October 2005. N.I.M. GOULD, *The (ir)resistible rise of sequential quadratic programming methods for nonlinear optimization.*

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

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

## 9 Lecture Courses, Teaching, Supervision

Oxford MSc Course on Sparse Direct Methods. Hilary Term 2004. I.S. DUFF AND J.A. SCOTT

INPT (Institute National Polytechnique de Toulouse, France). February, 2004. Two-month visiting professorship. Several lectures on *The role of backward stability and dual spaces in the design of iterative methods* were presented. M. ARIOLI.

University of Edinburgh. 12 lecture Operations Research MSc course on Numerical Optimization, April 2004. N.I.M. GOULD

The University of Udine (Dipartimento di Matematica e Informatica). Spring, 2004. Short course on numerical stability in high performance computing (12 lectures). M. ARIOLI.

Thesis defence of Abdou Guermouche, Lyon, France. 28 July 2004. I.S. DUFF.

Thesis defence of Stéphane Pralet, CERFACS, Toulouse, France. 21 September 2004. I.S. DUFF.

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.

University of Edinburgh. 10 lecture Operations Research MSc course on Numerical Optimization, January 2005. N.I.M. GOULD

Oxford University. 12 lecture Computational Mathematics MSc course on Numerical Optimization, January-February 2005. N.I.M. GOULD

Examiner of PhD thesis of Craig Lucas, University of Manchester. 26 January 2005. J.A. SCOTT

Oxford MSc course on Sparse Direct Methods. Hilary Term 2005. I.S. DUFF AND J.A. SCOTT

Two visits by Jonathan Boyle (postdoc. Manchester). 2005. J.A. SCOTT

Thesis defence of Emeric Martin, CERFACS, Toulouse, France. 26 July 2005. I.S. Duff.

Thesis defence of Ahmed Touhami, ENSEEIHT, Toulouse, France. 25 November 2005. M. Arioli, I.S. Duff.

HDR defence of Serge Gratton, CERFACS, Toulouse, France. 13 December 2005. I.S. Duff.

## 10 Seminars at RAL

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|---|---|
| 22 January 2004 | Professor Simon Chandler-Wilde (Reading)<br>Inverse scattering by rough surfaces. |
| 11 March 2004 | Dr Francoise Tisseur (Manchester)<br>Structured matrix computations. |
| 29 April 2004 | Dr Damien Jenkinson (Huddersfield)<br>Parameterised approximation estimators for mixed noise distributions. |
| 10 June 2004 | Dr Serge Gratton (CERFACS)<br>Practical implementation of an inexact GMRES method. |
| 15 June 2004 | Dr Yifan Hu (Wolfram Research)<br>Fast and high quality display of large relational information with an introduction to recent advances in Mathematica. |
| 18 November 2004 | Dr Angel-Victor de Miguel (London Business School)<br>An interior point method for MPECs based on strictly feasible relaxations. |
| 2 December 2004 | Michael Hagemann (Basel)<br>Weighted matchings for the preconditioning of symmetric indefinite matrices. |
| 27 January 2005 | Dr Ian Jones (ANSYS Europe)<br>The use of coupled solvers for complex multiphase and reacting flows. |
| 10 February 2005 | Dr Eugene Ovtchinnikov (Westminster)<br>Preconditioning for eigenvalue problems: ideas, algorithms, error analysis. |
| 5 May 2005 | Professor Roger Fletcher (Dundee)<br>A new look at Newton's method. |
| 16 June 2005 | Professor Peter Jimack (Leeds)<br>Scale-invariant moving finite-elements for time-dependent nonlinear partial differential equations. |
| 10 November 2005 | Dr Serge Gratton (CERFACS)<br>Sensitivity issues for least-squares problems. |

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|---|---|
| 1 December 2005 | Dr Jean-Yves L'Excellent (Lyons)<br>Dynamic load balancing issues and preliminary out-of-core experiments in a parallel solver. |

## 11 Technical Reports

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|---|---|
| RAL-TR-2004-006 | Stabilized bordered block diagonal forms for parallel sparse solvers. I. S. Duff and J. A. Scott. |
| RAL-TR-2004-009 | A filter-trust-region method for unconstrained optimization. N. I. M. Gould, C. Sainvitu and Ph. L. Toint. |
| RAL-TR-2004-016 | Numerical Analysis Group Progress Report. January 2002 - December 2003. I. S. Duff (Editor). |
| RAL-TR-2004-017 | A fully portable high performance minimal storage hybrid format Cholesky algorithm. B. S. Andersen, J. A. Gunnels, F. G. Gustavson, J. K. Reid, and J. Wasniewski. |
| RAL-TR-2004-018 | Multilevel hybrid spectral element ordering algorithms. J. A. Scott. |
| RAL-TR-2004-020 | Strategies for scaling and pivoting for sparse symmetric indefinite problems. I. S. Duff and S. Pralet. |
| RAL-TR-2004-026 | MA42_ELEMENT - a state-of-the-art solver for finite-element applications. J. A. Scott. |
| RAL-TR-2004-029 | Partial condition number for linear least-squares problems. M. Arioli, M. Baboulin, and S. Gratton. |
| RAL-TR-2004-030 | Sensitivity of trust-region algorithms to their parameters. N. I. M. Gould, D. Orban, A. Sartenaer, and Ph. L. Toint. |
| RAL-TR-2004-031 | On the convergence of successive linear quadratic programming algorithms. R. H. Byrd, N. I. M. Gould, J. Nocedal and R. A. Waltz. |
| RAL-TR-2004-032 | Numerical methods for large-scale nonlinear optimization. N. I. M. Gould, D. Orban, and Ph. L. Toint. |
| RAL-TR-2004-033 | Combining direct and iterative methods for the solution of large systems in different application areas. I. S. Duff. |
| RAL-TR-2004-036 | On implicit-factorization constraint preconditioners. H.S. Dollar, N.I.M. Gould, and A.J. Wathen. |
| RAL-TR-2004-040 | Parallel preconditioners based on partitioning sparse matrices. I.S. Duff, S. Riyavong, and M.B. Van Gijzen. |

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| RAL-TR-2005-001 | Reducing the total bandwidth of a sparse unsymmetric matrix. J.K. Reid and J.A. Scott. |
| RAL-TR-2005-004 | MI31: a conjugate gradient algorithm implementation with energy-norm stopping criteria. M. Arioli and G. Manzini. |
| RAL-TR-2005-001 | A numerical evaluation of sparse direct solvers for the solution of large sparse, symmetric linear systems of equations. N.I.M. Gould, Y. Hu, and J.A. Scott. |
| RAL-TR-2005-007 | Towards a stable static pivoting strategy for the sequential and parallel solution of sparse symmetric indefinite systems. I.S. Duff and S. Pralet. |
| RAL-TR-2005-011 | On iterative methods and implicit-factorization preconditioners for regularized saddle-point systems. H.S. Dollar, N.I.M. Gould, W.H.A. Schilders, and A.J. Wathen. |
| RAL-TR-2005-014 | Experiences of sparse direct symmetric solvers. J. A. Scott and Y. Hu. |
| RAL-TR-2005-026 | Using constraint preconditioners with regularized saddle-point problems. H.S. Dollar, N.I.M. Gould, W.H.A. Schilders, and A.J. Wathen. |

## 12 Publications


P. R. Amestoy, T. A. Davis and I. S. Duff, "Algorithm 837: AMD, an approximate minimum degree ordering algorithm," *ACM Transactions on Mathematical Software*, **30**, 381-388, 2004.

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.

M. Arioli, "A stopping criterion for the conjugate gradient algorithm in a finite element method framework," *Numer. Math.*, 97(1):1–24, 2005.

M. Arioli and D. Loghin and A. Wathen, "Stopping criteria for iterations in finite-element methods," *Numer. Math.*, **99**, 381–410, 2005.

R. H. Byrd, N. I. M. Gould, J. Nocedal and R. A. Waltz "An active set algorithm for nonlinear programming using linear programming and equality constrained subproblems". *Mathematical Programming B* **100:1** 27-48, 2004.

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**, 753-771, 2004.

B. Carpentieri, I. S. Duff, L. Giraud and G. Sylvand. "Combining fast multipole techniques and an approximate inverse preconditioner for large electromagnetism calculations," *SIAM J. Scientific Computing*, **27**, 774-792, 2005.

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