Science & Technology Facilities Council

Numerical Analysis Group Progress Report: January 2006 – December 2007

J.A. Scott (Editor)

2 January 2008

RAL-TR-2008-001

Library and Information Services
SFTC Rutherford Appleton Laboratory
Harwell Science and Innovation Campus
Didcot
OX11 0QX
UK
Tel: +44 (0)1235 445384
Fax: +44(0)1235 446403
Email: library@rl.ac.uk

ISSN 1358-6254

RAL-TR-2008-001

Numerical Analysis Group Progress Report
January 2006 – December 2007

J. A. Scott (Editor)

ABSTRACT

We discuss the research activities of the Numerical Analysis Group in the Computational Science and Engineering Department at the Rutherford Appleton Laboratory of the STFC for the period January 2006 to December 2007. This work was principally supported by EPSRC grants GR/S42170 and EP/E053351/1.

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.

Current reports are available from `http://www.numerical.rl.ac.uk/reports/reports.html`.

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

January 2, 2008

Contents

Personnel in Numerical Analysis Group

Staff

Jennifer Scott.
Group Leader. Sparse linear systems and sparse eigenvalue problems.

Mario Arioli
Numerical linear algebra, numerical solution of PDEs, error analysis.

Coralia Cartis (from 10 July 2006 until 26 July 2007).
Interior-point methods, complexity analysis.

Sue Dollar (from 5 June 2006).
Preconditioners, saddle-point problems and sparse linear systems.

Iain Duff
Sparse matrices and vector and parallel computers and computing.

Nick Gould
Large-scale optimization, nonlinear equations and inequalities.

Angela Vernon (until June 2006).
Administrative and secretarial support.

Sandra Hodgetts (from June 2006 until March 2006).
Administrative and secretarial support.

Sue Hitchcox (from March 2006 until September 2007).
Administrative and secretarial support.

Karen McIntyre (after September 2007).
Administrative and secretarial support.

Consultants

Mike Hopper Support for HSL and for TSSD.

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

Visiting Scientist

Coralia Cartis (Edinburgh) (from August 2007).
Interior-point methods, complexity analysis.

1 Introduction

This report covers the period January 2006 to December 2007 and summarises the activities of the Numerical Analysis Group within the Computational Science and Engineering Department at the STFC Rutherford Appleton Laboratory. This work was principally supported by EPSRC grant GR/S42170 and, from October 2007, EPSRC grant EP/E053351/1.

As will be seen from the personal statements of the Group members, the last two years have been a time of considerable change. In mid 2006, we welcomed to the Group first Sue Dollar (a former student of Andy Wathen at Oxford) and then Coralia Cartis (previously a post doc with Raphael Hauser at Oxford). Sue is now well settled in the Group but Coralia was only with us for 12 months. Coralia left for the very best of reasons: she married in August 2007 and she and her husband, Jared Tanner, have both taken up positions at the University of Edinburgh. Clearly, our loss is Edinburgh's gain and we wish Coralia and Jared well for the future. Coralia retains close contacts with Group; she continues to collaborate with Nick Gould and plans to visit us at RAL on a regular basis.

The other main changes have involved longer-standing Group members. Nick Gould was appointed Professor of Numerical Optimisation at Oxford and Tutorial Fellow in Mathematics at Exeter College. Despite this, he continues to be a very active and valuable part time Group member, spending time outside the Oxford terms at RAL. Iain Duff took the opportunity offered by his sixtieth birthday to move to part time working, thus allowing himself greater freedom to pursue his own research interests and largely freeing himself of managerial responsibilities; Jennifer Scott has taken over as Group Leader.

The support and development of the mathematical software libraries HSL (formerly the Harwell Subroutine Library) and GALAHAD continues to be one of the Group's major activities. There was a release of both libraries in autumn 2007. Currently, marketing and distribution outside the UK academic community is supported by AspenTech Inc. However, Lawrence Daniels, who led the team at AspenTech, very sadly died in the spring of this year after a long and extremely courageous battle with cancer. Lawrence was a highly valued colleague and we miss him very much. In the coming months, it is likely that we will take full responsibility for all aspects of HSL and GALAHAD and for this we rely very much on the help of John Reid, who we continue to employ as a consultant using HSL funds. We have also benefited this year from the consultancy of Mike Hopper who helps us both in typesetting and the ongoing commitment to higher software standards.

During the last two years, we have welcomed a number of visitors to the Group, including Patrick Amestoy (EINSEEIHT), Matthias Bollhöfer (TU Braunschweig), Jack Dongarra (Tenessee), Caroline Edwards (Bath), Martin van Gijzen (Delft), David Gleich (Stanford), Gene Golub (Stanford), Laura Grigori (INRIA), Ekaterina Kostina (Heidelberg), Jan Magnus (Tilburg), Scott McLachlan (TU Delft), Dubravka Mijuca (Belgrade), Daniel Robinson(Oxford), Philippe Toint (Namur), Mirek Tuma (Academy of Sciences of the Czech Republic), and Abigail Wacher (Finavera Renewables Ltd).

The remainder of this report is organised as follows. Group members present brief personal statements in Section 2. We follow this in Section 3 by a list of technical reports written by Group members, each accompanied by its abstract; this serves to summarize our research. Next we list our journal and conference publications in Section 4. Since producing software is our other main preoccupation, we then list new packages from HSL and GALAHAD along with a brief synopsis of their purposes. Briefer lists of conferences attended, seminars presented, and teaching and tutorial activities are given in Sections 6 to 8. We finish with a list of seminars (in the joint series with Oxford), in Section 9.

Current information on the activities of the Group and on Group members can be found at `www.cse.clrc.ac.uk/nag`

Jennifer Scott (j.a.scott@rl.ac.uk)

2 Personal statements

2.1 Mario Arioli

Mario has continued his collaboration with Daniel Loghin (University of Birmingham), investigating approximating the square roots of special elliptic operators using the generalised Lanczos method and its use in computing preconditioners for Krylov methods applied to Steklov-Poincaré operators. The preliminary numerical experiments are very positive and the intention now is to apply the technique to variational problems arising in image modelling and denoising.

Mario has collaborated with Iain Duff, Serge Gratton (CNES, CERFACS), and Stéphane Pralet (SAMTECH, Liège) on the error analysis of Krylov methods. In particular, FGMRES has been shown both theoretically and numerically to be the best method to recover full backward stability of the solution of a linear system when the HSL direct solver `MA57` with static pivoting is used as the preconditioner. Mario and Iain are now studying the use of FGMRES for recovering full double precision backward stability when a linear system is solved by Gaussian elimination in single precision. Recently, Mario and Miro Rozloznik (Academy of Sciences of the Czech Republic) started work on extending the FGMRES theoretical results to other Krylov methods.

For the latest release of HSL (see Section 5.1), Mario contributed `MI15`, which implements FGMRES, and developed Matlab interfaces for the sparse solvers `MA48` and `MA57`. The `MA57` interface has been successfully used by Nick Gould, Sue Dollar, and Andy Wathen (Oxford) in their work on iterative methods and implicit-factorization preconditioners for regularized saddle-point systems, and by other colleagues in Oxford and the Université de Limoges (France).

This autumn, Mario was responsible for organizing the Bath/RAL Numerical Analysis Day, which was held at Rutherford on 25^{th} September.

2.2 Coralia Cartis

Cora's appointment has strengthened the optimization interests and activities of the Group. She holds a PhD from Cambridge (2005) in numerical optimization with Mike Powell, and was completing a postdoctoral position at Oxford working on computational complexity of optimization problems with Raphael Hauser when she was appointed to the Group. Before joining the Group, she collaborated with Nick Gould on feasibility problems with linear constraints (see RAL-TR-2006-016), and this collaboration expanded while Cora was a member of the Group to include trust-region methods and regularizations of Newton's method (see RAL-TR-2007-007). She also continued to work with Raphael Hauser, investigating connections between the stiffness of the vector fields of search directions and the complexity of the optimization algorithms generated using these directions. The latter work involved — in the case when only approximate search directions are computed — perturbation and backward error analysis for linear systems which led to very useful and fruitful interactions with the linear algebra experts in the Group, notably Mario Arioli (technical report forthcoming).

Due to personal circumstances (getting married to an American mathematician), Cora left the Group to take up a lectureship in the School of Mathematics at the University of Edinburgh, where her husband also has an appointment. She would not have left the Group, where she really enjoyed her research time and interactions, were it not for these particular circumstances. However, she holds a Permanent Visitor status at RAL and intends to visit on a regular basis. Her collaborations with Nick Gould continue apace, even from afar.

2.3 Sue Dollar

Sue joined the Group in June 2006 after having spent a year as a lecturer at Reading University. Before that she was a student of Andy Wathen (Oxford) working on the efficient solution of saddle-point problems arising within constrained optimization problems: in collaboration with Nick Gould, Sue has implemented some of this work within the HSL package `HSL_MI13` and GALAHAD's `SBLS` package. Sue has continued to collaborate with Andy Wathen and they, along with Nick and Tyrone Rees (Oxford), are investigating the iterative solution of PDE-constrained optimization problems.

Sue and Nick have recently formed a collaboration with Ricardo Pong-Wong and John Woolliams (Roslin Institute, Edinburgh) to work on the efficient and robust solution of optimization problems arising within animal breeding programmes. Additionally, Sue has collaborated with Patrick Amestoy (EINSEEIHT), John Reid and Jennifer Scott on improving the performance of the approximate minimum degree algorithm for matrices that have some dense rows: this has resulted in the release of a new version of `MC47` within HSL. Sue and Jennifer also collaborated together to produce `HSL_MC68`, an HSL package for computing a variety of elimination orderings for use with sparse direct solvers.

Sue, along with Nick Trefethen (Oxford), jointly organises the Computational Mathematics and Applications Seminars. During Spring Term 2007, Sue gave a series of ten MSc lectures on advanced boundary value problems at Reading University.

2.4 Iain Duff

Although Iain relinquished Group Leader duties in January 2007, he is continuing in a part time role as an STFC Senior Fellow and is the Principal Investigator for our main research grant. In fact, one highlight of 2007 was the successful renewal of this main grant to ensure funding for the Group until October 2011. Iain still leads a project at the European Centre for Research and Advanced Training in Scientific Computation (CERFACS) at Toulouse in France, where he supervises PhD students and organizes a regular conference "Sparse Days at CERFACS" each year that is usually attended by other members of the Group. Iain also continues to visit Glasgow regularly in his capacity as a Visiting Professor at Strathclyde. His research interests continue to be in all aspects of sparse matrices, including 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. He is collaborating with the Geotechnical Engineering Department at Newcastle in New South Wales on the determination of the rank and nonsingular submatrix of a highly deficient matrix and is studying the solution of very badly scaled indefinite systems in mixed finite element methods with a researcher from Serbia. He is also looking at ways of implementing scaling and matching algorithms in parallel in conjunction with his colleagues in France. A major project at CERFACS involves using hybrid methods to solve Helmholtz equations arising in geophysics.

Although he stood down as Chief Editor of the IMA Journal of Numerical Analysis in January, he remains as an Associate Editor. He is on the Institute of Mathematics and its Applications Council, is a member of the Research Group, is chairman of the Journals Board of Management, and IMA representative on the International Committee that oversees the ICIAM international conferences on applied mathematics. He was reelected for a third year as Chairman of the Board of Trustees of SIAM in December 2007 and is the first non-US resident to hold that position. Iain is on several Advisory Boards and Prize Committees, has been on the Programme and Organizing Committee for more than ten international meetings and has given invited talks at meetings in Armenia, Beijing, California, Colorado, Lijiang, Marseille, Shanghai, and Utrecht, and has presented seminars in Argonne, Lyngby, Manchester, Newcastle (Australia), and Xi'an.

Iain was elected as Fellow of the Royal Society of Edinburgh in 2006 and is a member of the Applied Mathematics Panel for the REsearch Assessment Exercise (RAE 2008), the only non-University person on either Maths Panel.

2.5 Nick Gould

Nick's life changed dramatically over the two years as in October 2006 he was appointed as Professor of Numerical Optimisation at the University of Oxford and as a Tutorial Fellow in Mathematics at Exeter College. While for most people this might seem like a full-time job, Nick is still employed 20% of the time by STFC, and spends much of the University vacation at RAL. Indeed, given the teaching and administrative duties that dominate life during term time, this is more or less the only chance he finds to do research and development!

As always, Nick's work continues to revolve around optimization and its attendant linear-algebraic requirements. GALAHAD continues to evolve and much preparatory work for the upcoming nonlinear optimization solvers continues apace. He has worked (with Coralia Cartis) on methods for finding good initial points when the optimization involves linear constraints. More fundamentally, Coralia, Philippe Toint (Namur) and Nick have developed a complete theory for a new class of unconstrained minimization methods which provide an alternative to the traditional line-search and trust-region paradigms. Most significantly, it has been shown that these adaptive cubic over-regularisation (ACO) methods exhibit better theoretical worst-case behaviour than their older rivals, and just as importantly they also behave better in general in practice. Needless to say, this may have a large impact on future development throughout optimisation, and Nick, Coralia and Philippe are currently exploring a number of extensions to the constrained case. Nick and Philippe are also investigating new methods for constrained optimization whose aim is to limit the interference from globalisation strategies as far as possible. No reliance on penalty functions or filters is made, and the tests for the acceptance of a trial point depends on whether its primary aim is to improve the objective function or constraint violation, not on both together. In tandem, Nick Sven Leyffer and Todd Munson (Argonne National Lab.) and Michael Friedlander (University of British Columbia) have continued to develop their FASTr sequential linear-quadratic programming method, and this has been prototyped as part of GALAHAD. Finally, Nick has started to port sections of GALAHAD into Matlab, but has been somewhat frustrated by the poor support for modern Fortran within this ubiquitous system.

With his Oxford hat on, Nick was recently awarded an EPSRC Responsive Mode grant to support a three-year postdoc to study SQP methods for constrained optimization. The recipient Daniel Robinson (ex University of California at San Diego) has made a promising start, and will spend some of his time at RAL in the future.

2.6 Jennifer Scott

Jennifer's life has also changed quite significantly in the last couple of years. When Sue and Coralia joined the Group in 2006, she became their line manager. Then, in January 2007, she took over as Group leader. The subsequent increase in managerial responsibilities and duties led her to move to full time working in the spring of this year (which really just formalised what was already her working pattern).

On the research side, Jennifer has continued to work with John Reid on their out-of-core multifrontal solvers. The positive definite and unsymmetric solvers, together with separate packages that are designed to efficiently handle the input/output operations and to perform the partial dense factorizations and solves that lie at the heart of the multifrontal method, are included in the recent release of HSL (see Section 5.1). Jennifer has also worked with Jonathan Boyle of the University of Manchester on the development of the

Fortran 95 algebraic multigrid code and with Eugene Ovtchinnikov of the University of Westminster and John Reid on a new eigensolver for very large-scale symmetric problems. Both these collaborations have led to new HSL packages, as has a collaboration with Sue Dollar and John Reid on improving the performance of the approximate minimum degree algorithm for sparse matrices that have some rows with many more entries than the matrix average. In addition, following an invited visit to the Academy of Sciences of the Czech Republic in Prague, Jennifer has started a collaboration with Mirek Tuma on designing and developing preconditioners based on sparse incomplete factorizations. The intention is to produce new packages that will strengthen the preconditioning section of HSL.

With new Group members and new collaborators working with us on software projects, Jennifer and John have written a document (that is available as a RAL Technical Report) that provides guidelines for the design, development and maintenance of HSL codes. The aim is to ensure a common framework is used and that all HSL packages conform to the same high standards.

In April, Jennifer was awarded an 18-month EPSRC grant under the HPC Software Development programme. The grant is to investigate the potential benefits for HSL solvers of using mixed precision computations and of enhancing performance for multicore architectures. We are looking forward to Jonathan Hogg (who is currently a third year PhD student at the University of Edinburgh) joining us in January 2008 for 12 months to work on this project.

In December 2006, Jennifer took over as editor of the IMA Numerical Analysis Newsletter, a role that Iain had undertaken since the first issue in October 1976. So far, she has edited three issues, with the next on its way. In addition, Jennifer has continued to take an active role in promoting women in mathematics in the UK. She is currently the UK coordinator for European Women in Mathematics, and is a member of both the Women's Committee of the LMS and the national coordinating committee for WISE (Women in Science, Engineering and Construction).

3 Technical Reports

RAL-TR-2006-001 *Towards an 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. In this report, we look at whether we can predict which ordering will be better, using only the sparsity pattern of the matrix. Our aim is to choose efficiently a good ordering for a wide range of large problems from different application areas.

RAL-TR-2006-006 *Numerical Analysis Group Progress Report. January 2004–December 2005.*
I. S. Duff (Editor).

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.

RAL-TR-2006-007 *A note on GMRES preconditioned by a perturbed LDL^T decomposition with static pivoting.*
M. Arioli, I. S. Duff, S. Gratton, and S. Pralet,

A strict adherence to threshold pivoting in the direct solution of symmetric indefinite problems can result in substantially more work and storage than forecast by an sparse analysis of the symmetric problem. One way of avoiding this is to use static pivoting where the data structures and pivoting sequence generated by the analysis are respected and pivots that would otherwise be very small are replaced by a user defined quantity. This can give a stable factorization but of a perturbed matrix.

The conventional way of solving the sparse linear system is then to use iterative refinement (IR) but there are cases where this fails to converge. In this paper, we discuss the use of more robust iterative methods, namely GMRES and FGMRES.

We show both theoretically and experimentally that both these approaches are more robust than IR and furthermore that FGMRES is far more robust than GMRES and that, under reasonable hypotheses, FGMRES is backward stable. We also show how restarted variants can be beneficial although again the GMRES variant is not as robust as FGMRES.

RAL-TR-2006-010 *Stopping criteria for mixed finite element problems.*
M. Arioli and D. Loghin.

We study stopping criteria that are suitable in the solution by Krylov space based methods of linear and non linear systems of equations arising from the mixed and the mixed-hybrid finite-element approximation of saddle point problems. Particular emphasis is given to Navier-Stokes equation and to several of its linearization.

We reduce the original problem in a finite dimensional space and we take advantage of the Lagrangian formulation in order to use some of the results presented by Arioli, Loghin, and Wathen (*Stopping criteria for iterations in finite-element methods*, Numer. Math., 99, 2005, pp. 381–410.).

RAL-TR-2006-013 *An out-of-core sparse Cholesky solver.*
J. K. Reid and J. A. Scott.

Direct methods for solving large sparse linear systems of equations are popular because of their generality and robustness. Their main weakness is that the memory they require usually increases rapidly with problem size. We discuss the design and development of the first release of a new symmetric direct solver that aims to circumvent this limitation by allowing the system matrix, intermediate data, and the matrix factors to be stored externally. The code, which is written in Fortran and called `HSL_MA77`, implements a multifrontal algorithm. The first release is for positive-definite systems and performs a Cholesky factorization. Special attention is paid to the use of efficient dense linear algebra kernel codes that handle the full-matrix operations on the frontal matrix and to the input/output operations. These are performed using a separate package that provides a virtual-memory system and allows the data to be spread over many files; for very large problems these may be held on more than one device.

Numerical results are presented for a collection of 30 large real-world problems, all of which were solved successfully.

RAL-TR-2006-014 *Sparse system solution and the HSL Library.*
I. S. Duff.

We consider the solution of large sparse systems, sketch their ubiquity, and briefly describe some of the algorithms used to solve these systems.

The HSL mathematical software library started life in 1963 as the Harwell Subroutine Library making it one of the oldest such libraries. The main strengths of the Library lie in packages for large scale system solution. It is particularly strong in direct methods for sparse matrices and optimization. The Library has been used worldwide by a wide range of industries.

We briefly discuss the history of the library and its organization and contents. We discuss the evolution of some of our current packages and the efforts to ensure reliability, robustness, and efficiency.

We describe in some detail the functionality of one of our most popular sparse direct codes.

RAL-TR-2006-015 *How good are projection methods for convex feasibility problems?*
N. I. M. Gould.

We consider simple projection methods for solving convex feasibility problems. Both successive and sequential methods are considered, and heuristics to improve these are suggested. Unfortunately, particularly given the large literature which might make one think otherwise, numerical tests indicate that in general none of the variants considered are especially effective or competitive with more sophisticated alternatives.

RAL-TR-2006-016 *Finding a point in the relative interior of a polyhedron.*
C. Cartis and N. I. M. Gould.

A new initialization or 'Phase I' strategy for feasible interior point methods for linear programming is proposed that computes a point on the primal-dual central path associated with the linear program. Provided there exist primal-dual strictly feasible points — an all-pervasive assumption in interior point method theory that implies the existence of the central path — our initial method (Algorithm 1) is globally Q-linearly and asymptotically Q-quadratically convergent, with a provable worst-case iteration complexity bound. When this assumption is not met, the numerical behaviour of Algorithm 1 is highly disappointing, even when the problem is primal-dual feasible. This is due to the presence of implicit equalities, inequality constraints that hold as equalities at all the feasible points. Controlled perturbations of the inequality constraints of the primal-dual problems are introduced — geometrically equivalent to enlarging the primal-dual feasible region and then systematically contracting it back to its initial shape — in order for the perturbed problems to satisfy the assumption. Thus Algorithm 1 can successfully be employed to solve each of the perturbed problems. We show that, when there exist primal-dual strictly feasible points of the original problems, the resulting method, Algorithm 2, finds such a point in a finite number of changes to the perturbation parameters. When implicit equalities are present, but the original problem and its dual are feasible, Algorithm 2 asymptotically detects *all* the primal-dual implicit equalities and generates a point in the relative interior of the primal-dual feasible set. Algorithm 2 can also asymptotically detect primal-dual infeasibility. Successful numerical experience with Algorithm 2 on linear programs from NETLIB and CUTEr, both with and without any significant preprocessing of the problems, indicates that Algorithm 2 may be used as an *algorithmic preprocessor* for removing implicit equalities, with theoretical guarantees of convergence.

RAL-TR-2006-026 `HSL_OF01`*, a virtual memory system in Fortran.*
J. K. Reid and J. A. Scott.

`HSL_OF01` is a Fortran 95 package that provides facilities for reading from and writing to direct-access files. A buffer is used to avoid actual input/output operations whenever possible. The data may be spread over many files and for very large problems these may be held on more than one device. We describe the design of `HSL_OF01` and comment on its use within an out-of-core sparse direct solver.

RAL-TR-2006-027 *The design and use of a sparse direct solver for skew symmetric matrices.*

I. S. Duff.

We consider the LDL^T factorization of sparse skew symmetric matrices. We see that the pivoting strategies are similar, but simpler, to those used in the factorization of sparse symmetric indefinite matrices, and we briefly describe the algorithms used in a forthcoming direct code based on multifrontal techniques for the factorization of real skew symmetric matrices. We show how this factorization can be very efficient for preconditioning matrices that have a large skew component.

RAL-TR-2006-031 *Guidelines for the development of HSL software.*

J. K. Reid and J. A. Scott.

HSL is a collection of portable, fully documented, and tested Fortran packages for large-scale scientific computation. It has been developed by the Numerical Analysis Group at the Rutherford Appleton Laboratory, with additional input from other experts and collaborators.

The aim of this report is to provide clear and comprehensive guidelines for those involved in the design, development and maintenance of software for HSL. It explains the organisation of HSL, including the use of version numbers and naming conventions, the aims and format of the user documentation, the programming language standards and style, and the verification and testing procedures.

RAL-TR-2007-001 *Co-arrays in the next Fortran Standard.*

J. K. Reid and R. W. Numrich.

The WG5 committee, at its meeting in Delft, May 2005, decided to include co-arrays in the next Fortran Standard. A Fortran program containing co-arrays is interpreted as if it were replicated a fixed number of times and all copies were executed asynchronously. Each copy has its own set of data objects and is called an image. The array syntax of Fortran is extended with additional trailing subscripts in square brackets to give a clear and straightforward representation of access to data on other images.

References without square brackets are to local data, so code that can run independently is uncluttered. Any occurrence of square brackets is a warning about communication between images.

The additional syntax requires support in the compiler, but it has been designed to be easy to implement and to give the compiler scope both to apply its optimizations within each image and to optimize the communication between images.

The extension includes execution control statements for synchronizing images and intrinsic procedures to return the number of images, to return the index of the current image, and to perform collective operations.

The paper does not attempt to describe the full details of the feature as it now appears in the draft of the new standard. Instead, we describe a subset and demonstrate the use of this subset with examples.

RAL-TR-2007-002 *Multigrid based preconditioners for the numerical solution of two-dimensional heterogeneous problems in geophysics.*

I. S. Duff, S. Gratton, X. Pinel, and X. Vasseur.

We study methods for the numerical solution of the Helmholtz equation for two-dimensional applications in geophysics. The common framework of the iterative methods in our study is a combination of an inner iteration with a geometric multigrid method used as a preconditioner and an outer iteration with a Krylov subspace method. The preconditioning system is based on either a pure or shifted Helmholtz operator. A multigrid iteration is used to approximate the inverse of this operator. The proposed solution methods are evaluated on a complex benchmark in geophysics involving highly variable coefficients and high wavenumbers. We compare this preconditioned iterative method with a direct method and a hybrid method that combines our iterative approach with a direct method on a reduced problem. We see that the hybrid method outperforms both the iterative and the direct approach.

RAL-TR-2007-006 *Analysis of the out-of-core solution phase of a parallel multifrontal approach.*
P. Amestoy, I. S. Duff, A. Guermouche, and T. Slavova.

We consider the parallel solution of sparse linear systems of equations in a limited memory environment. A preliminary out-of core version of a sparse multifrontal code called MUMPS (MUltifrontal Massively Parallel Solver) has been developed as part of a collaboration with members of the INRIA project GRAAL.

In this context, we assume that the factors have been written on the hard disk during the factorization phase, and we discuss the design of an efficient solution phase. Two different approaches are presented to read data from the disk, with a discussion on the advantages and the drawbacks of each one.

Our work differs and extends the work of Rothberg and Schreiber (1999) and Rotkin and Toledo (2004) because firstly we consider a parallel out-of-core context, and secondly we focus on the performance of the solve phase.

RAL-TR-2007-007 *Adaptive cubic overestimation methods for unconstrained optimization.*
C. Cartis, N. I. M. Gould and Ph. L. Toint.

An Adaptive Cubic Overestimation (ACO) algorithm for unconstrained optimization, generalizing a method due to Nesterov & Polyak (*Math. Programming* **108**, 2006, pp 177-205), is proposed. At each iteration of Nesterov & Polyak's approach, the global minimizer of a local cubic overestimator of the objective function is determined, and this ensures a significant improvement in the objective so long as the Hessian of the objective is Lipschitz continuous and its Lipschitz constant is available. The twin requirements of global model optimality and the availability of Lipschitz constants somewhat limit the applicability of such an approach, particularly for large-scale problems. However the promised powerful worst-case theoretical guarantees prompt us to investigate variants in which estimates of the required Lipschitz constant are refined and in which computationally-viable approximations to the global model-minimizer are sought. We show that the excellent global and local convergence properties and worst-case iteration complexity bounds obtained by Nesterov & Polyak are retained, and sometimes extended to a wider class of problems, by our ACO approach. Numerical experiments with small-scale test problems from the CUTEr set show superior performance of the ACO algorithm when compared to a trust-region implementation.

RAL-TR-2007-014 *An efficient out-of-core multifrontal solver for large-scale unsymmetric element problems.*
J. K. Reid and J. A. Scott.

In many applications where the efficient solution of large sparse linear systems of equations is required, a direct method is frequently the method of choice. Unfortunately, direct methods have a potentially severe limitation: as the problem size grows, the memory needed generally increases rapidly. However, the in-core memory requirements can be limited by storing the matrix and its factors externally, allowing the solver to be used for very large problems. We have designed a new out-of-core package for the large sparse unsymmetric systems that arise from finite-element problems. The code, which is called HSL_MA78, implements a multifrontal algorithm and achieves efficiency through the use of efficient dense linear algebra kernels and specially designed code for handling the input/output operations. We describe the design of HSL_MA78, explain its user interface and the options it offers, and illustrate its performance using problems from a range of practical applications.

RAL-TR-2007-016 *Nonlinear programming without a penalty function or a filter.*
N. I. M. Gould and Ph. L. Toint.

A new method is introduced for solving equality constrained nonlinear optimization problems. This method does not use a penalty function, nor a barrier or a filter, and yet can be proved to be globally convergent to first-order stationary points. It uses different trust-regions to cope with the nonlinearities of the objective function and the constraints, and allows inexact SQP steps that do not lie exactly in the nullspace of the local Jacobian. Preliminary numerical experiments on CUTEr problems indicate that the method performs well.

RAL-TR-2007-020 *An approximate minimum degree algorithm for matrices with dense rows.*
P. Amestoy, H. S. Dollar, J. K. Reid and J. A. Scott.

We present a modified version of the approximate minimum degree algorithm for preordering a matrix with a symmetric sparsity pattern prior to the numerical factorization. The modification is designed to improve the efficiency of the AMD algorithm when some of the rows and columns have significantly more entries than the average for the matrix. Numerical results are presented for problems arising from practical applications and comparisons are made with other implementations of variants of the minimum degree algorithm.

RAL-TR-2007-021 HSL_MI20*: an efficient AMG preconditioner.*
J. Boyle, M. D. Mihajlovic and J. A. Scott.

Algebraic multigrid (AMG) is an efficient multi-level method designed for effective solution of sparse linear systems obtained from the discretisation of scalar elliptic partial differential equations. AMG can be used to compute powerful preconditioners for use with Krylov subspace methods. We report on the design and development of an efficient, robust and portable implementation of AMG that is available as package HSL_MI20 within the HSL mathematical software library. HSL_MI20 implements the classical AMG method and, although it can be used as a "black-box" preconditioner, it offers the user a large number of options and parameters that may be tuned to enhance its performance for specific applications. The performance of HSL_MI20 is illustrated using finite element discretisations of diffusion and convection-diffusion problems in three dimensions.

RAL-TR-2007-022 *A note on fast approximate minimum degree orderings for matrices with some dense rows.*
H. S. Dollar and J. A. Scott.

Recently two different approximate minimum degree algorithms have been proposed that aim to efficiently deal with matrices containing some dense rows. We compare the performance of these algorithms and, as a result, present a new variant that combines the speed of Carmen's method with the robustness of the Amestoy, Dollar, Reid and Scott method for detecting dense rows. Numerical results are presented for problems arising from practical applications.

4 Publications

M. Arioli, M. Baboulin, and S. Gratton, “Partial condition number for least-squares problems” *SIAM J. Matrix Anal. and Applics.*, **29 (2)** (2007) 413–433.

M. Arioli, I. S. Duff, S. Gratton, and S. Pralet S., “A note on GMRES preconditioned by a perturbed LDL^T decomposition with static pivoting”, *SIAM J. Sci. Comput.* **29 (5)** (2007) 2024–2044.

M. Arioli and D. Loghin, “Stopping criteria for mixed finite element problems”, to appear on *ETNA*.

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.

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.

N. I. M. Gould and Ph. L. Toint, “Global Convergence of a Non-monotone Trust-Region SQP-Filter Algorithm for Nonlinear Programming”. in “Multiscale Optimization Methods and Applications” (W. W. Hager, S.-J. Huang, P. M. Pardalos and O. A. Prokopyev, eds.) Springer Series on Nonconvex Optimization and Its Applications, Vol. 82, Springer Verlag (2006) 125–150.

H. S. Dollar, “Constraint-style preconditioners for regularized saddle-point problems”. *SIAM Journal on Matrix Analysis and Applications* **29** (2007) 672–684.

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) 61–82.

H. S. Dollar, N. I. M. Gould, W. H. A. Schilders and A. J. Wathen, “Implicit-factorization preconditioning and iterative solvers for regularized saddle-point systems”. *SIAM Journal on Matrix Analysis and Applications* **28** (2006) 170–189.

H. S. Dollar, N. I. M. Gould, W. H. A. Schilders and A. J. Wathen, “Using constraint preconditioners with regularized saddle-point problems”. *Computational Optimization and Applications* **36 (2-3) (2007)** 249–270.

H. S. Dollar and A. J. Wathen, “Approximate factorization constraint preconditioners for saddle-point matrices”. *SIAM Journal on Scientific Computing* **27** (2006) 1555–1572.

I. S. Duff, “Combining direct and iterative methods for the solution of large systems in different application areas”.

A. H. Siddiqi, I. S. Duff, and O. Christensen (Editors), “Modern Mathematical Models, Methods and Algorithms for Real World Systems”. *In* Modern Mathematical Models, Methods and Algorithms for Real World Systems. Anamaya Publishers, New Delhi, India. Edited by A.H. Siddiqi, I. S. Duff, and O. Christensen (2007) 402–419.

I. S. Duff, “Sparse system solution and the HSL Library”. In *Some Topics in Industrial and Applied Mathematics. Series in Contemporary Applied Mathematics CAM 8, World Scientific, Singapore. Edited by R. Jeltsch, T-T Li, and I.H. Sloan* (2007) 78–94.

I. S. Duff, S. Gratton, X. Pinel, and X. Vasseur, “Multigrid based preconditioners for the numerical solution of two-dimensional heterogeneous problems in geophysics”. *International Journal of Computer Mathematics* **84-88** (2007) 1167–1181.

I. S. Duff and S. Pralet, “Towards stable mixed pivoting strategies for the sequential and parallel solution of sparse symmetric indefinite systems”. *SIAM Journal on Matrix Analysis and Applications* **29 (3)** (2007) 1007–1024.

N. I. M. Gould and Ph. L. Toint, “FILTRANE, a fortran 95 filter-trust-region package for solving nonlinear feasibility problems”. *ACM Transactions on Mathematical Software* **33 (1)** (2007).

N. I. M. Gould, Y. Hu and J. A. Scott, “A numerical evaluation of sparse direct solvers for the solution of large, sparse, symmetric linear systems of equations”. *ACM Transactions on Mathematical Software* **33,** Article 10 (2007) 32 pages.

N. I. M. Gould, “How good are projection methods for convex feasibility problems?” *Computational Optimization and Applications* DOI 10.1007/s10589-007-9073-5 (2007).

J. K. Reid and J. A. Scott, “Reducing the total bandwidth of a sparse unsymmetric matrix”. *SIAM J. Matrix Analysis and Applications* **28 (3)** (2006) 805–821.

J. K. Reid and J. A. Scott, “The design of a new out-of-core multifrontal solver”. *PARA 2006 Conference Proceedings* (2007) 598–607.

J. A. Scott, “A frontal solver for the 21st century”. *Communications in Numerical Methods in Engineering* **22** (2006) 1015–1029.

J. A. Scott and Y. Hu, “Experiences of sparse direct symmetric solvers”. *ACM Transactions on Mathematical Software* **33,** Article 18 (2007) 28 pages.

A. H. Siddiqi, I. S. Duff, and O. Christensen (Editors), “Modern Mathematical Models, Methods and Algorithms for Real World Systems”. *Anamaya Publishers, New Delhi, India.*

5 HSL and GALAHAD

5.1 HSL 2007

HSL 2007 was released in October 2007 and contained the following new packages:

`HSL_EA19` This package is designed to compute the n_e leftmost eigenvalues $\lambda_1 \leq \lambda_2 \leq ... \leq \lambda_{n_e}$ and corresponding eigenvectors $x_1, \ldots, x_{n_e}$ of a real symmetric (or Hermitian) operator A acting in the n-dimensional real (or complex) Euclidean space $\mathcal{R}^n$, or, more generally, of the problem

$$Ax = \lambda Bx, \tag{1}$$

where B a real symmetric (or Hermitian) positive definite operator. By applying `HSL_EA19` to $-A$, the user can compute the n_e rightmost eigenvalues of A and the corresponding eigenvectors. `HSL_EA19` does not perform factorizations of A or B and thus is suitable for solving large-scale problems for which a sparse direct solver for factorizing A or B is either not available or is too expensive.

The convergence may be accelerated by the provision of a symmetric positive-definite operator T that approximates the inverse of $(A - \sigma B)$ for a value of σ that initially does not exceed λ_1. The operator T is called *the preconditioner*.

We stress that neither A nor B nor T needs to be available explicitly: `HSL_EA19` only requires the multiplication of sets of vectors by A, B, and T.

HSL_EA19 implements a subspace iteration method, i.e. it generates a sequence of subspaces V^i, $i = 1, 2, ...,$ that contain approximations to the eigenvectors of the problem. All subspaces V^i are of the same dimension $m \geq n_e$. The simplest choice for m is $m = n_e$ but it is desirable that there is a significant gap $\lambda_{m+1} - \lambda_{n_e}$ both for a satisfactory rate of convergence to the right-most eigenvalues of interest and for the error estimation scheme. The subspace iteration method implemented by HSL_EA19 is based on the Jacobi-conjugate preconditioned gradients (JCPG) scheme of Ovtchinnikov. This method requires at least $4m$ vectors of length n (which include m approximate eigenvectors) and two $2m$-by-$2m$ matrices to be stored in main memory. $2m$ additional vectors of length n are needed if the user opts for reducing the number of multiplications by A; in the case of the generalized problem, the same applies to B.

The user may supply any number $n_i \leq m$ of vectors to be used by the package for the construction of a basis in the initial subspace: this option may be used to reduce the computation time in cases where good approximations to some eigenvectors are available. One way of providing such approximations is by restarting from previously calculated eigenvectors.

HSL_KB22 This package is a suite of Fortran 95 procedures for successively arranging a set of real numbers, $\{a_1, a_2, ..., a_n\}$, in increasing order using the Heapsort method of J. W. J. Williams. At the k-th stage of the method, the k-th smallest member of the set is found (where 'smallest' means 'most negative' if negative numbers are present). The method is particularly appropriate if it is not known in advance how many smallest members of the set will be required as the Heapsort method is able to calculate the $k+1$-st smallest member of the set efficiently once it has determined the first k smallest members. The method is guaranteed to sort all n numbers in $O(n \log n)$ operations. If a complete sort is required, the Quicksort algorithm, KB05, may be preferred.

HSL_MA54 For a matrix that is full, symmetric and positive definite, this module performs partial factorizations and solutions of corresponding sets of equations, paying special attention to the efficient use of cache memory. It uses a modification of the code of Andersen, Gunnels, Gustavson, Reid, and Wasniewski (ACM Trans. on Math. Software, **31**, 2005, 201-227). It is suitable for use in a frontal or multifrontal solver, but may also be used for the direct solution of a full set of equations.

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

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} L_{11} & 0 \\ L_{21} & I \end{pmatrix} \begin{pmatrix} I & 0 \\ 0 & S_{22} \end{pmatrix} \begin{pmatrix} L_{11}^T & L_{21}^T \\ 0 & I \end{pmatrix},$$

where L_{11} is lower triangular and both A_{11} and L_{11} have order p. We use the lower blocked hybrid format of Andersen *et al.* (2005) for the lower triangular part of A_{11} and optionally also for the lower triangular part of 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 will call this format for A and its factorization the **double blocked hybrid** format.

The module has facilities for rearranging a lower triangular matrix in lower packed format (that is, packed by columns) to double blocked hybrid format and vice-versa.

Subroutines are provided for partial forward and back substitution, that is, solving equations of the form

$$\begin{pmatrix} L_{11} & 0 \\ L_{21} & I \end{pmatrix} X = B, \quad \begin{pmatrix} L_{11}^T & L_{21}^T \\ 0 & I \end{pmatrix} X = B$$

and the corresponding equations for a single right-hand side b and solution x.

There are also subroutines for solving one or more sets of equations after a full factorization ($p = n$) and for extracting the diagonal of L_{11}.

`HSL_MA74` Given a dense unsymmetric $n \times n$ matrix A, `HSL_MA74` performs partial factorizations and solutions of corresponding sets of equations. High level BLAS are used. It is suitable for use in, for example, a frontal or multifrontal solver or may be used to factorize and solve a full system of equations.

Eliminations are limited to the leading $p \le n$ rows and columns. Stability considerations may lead to $q \le p$ eliminations being performed. The factorization takes the form

$$PAQ = \begin{pmatrix} L_1 & 0 \\ L_2 & I \end{pmatrix} \begin{pmatrix} D_1 & 0 \\ 0 & A_2 \end{pmatrix} \begin{pmatrix} U_1 & U_2 \\ 0 & I \end{pmatrix},$$

where P and Q are permutation matrices, L_1 and U_1 are unit lower and unit upper triangular matrices of order q, and D_1 is diagonal of order q. The permutation matrices P and Q are of the form

$$P = \begin{pmatrix} P_1 & 0 \\ 0 & I \end{pmatrix}, \quad Q = \begin{pmatrix} Q_1 & 0 \\ 0 & I \end{pmatrix},$$

where P_1 and Q_1 are of order p.

Subroutines are provided for partial solutions, that is, solving systems of the form

$$\begin{pmatrix} L_1 & 0 \\ L_2 & I \end{pmatrix} X = B, \quad \begin{pmatrix} D_1 & 0 \\ 0 & I \end{pmatrix} X = B, \quad \begin{pmatrix} D_1 & 0 \\ 0 & I \end{pmatrix} \begin{pmatrix} U_1 & U_2 \\ 0 & I \end{pmatrix} X = B, \quad \begin{pmatrix} U_1 & U_2 \\ 0 & I \end{pmatrix} X = B,$$

and the corresponding equations for a single right-hand side b and solution x.

Subroutines are also provided for partial solutions to transpose systems, that is, solving systems of the form

$$\begin{pmatrix} U_1^T & 0 \\ U_2^T & I \end{pmatrix} X = B, \quad \begin{pmatrix} D_1 & 0 \\ 0 & I \end{pmatrix} \begin{pmatrix} L_1^T & L_2^T \\ 0 & I \end{pmatrix} X = B, \quad \begin{pmatrix} L_1^T & L_2^T \\ 0 & I \end{pmatrix} X = B,$$

and the corresponding equations for a single right-hand side b and solution x.

Options are included for threshold partial pivoting, threshold diagonal pivoting, threshold rook pivoting, and static pivoting.

`HSL_MA77` This package solves one or more sets of sparse symmetric equations $AX = B$ using an out-of-core multifrontal method. The square symmetric matrix A may be either positive definite or indefinite and may be input by the user by square symmetric elements, (such as in a finite-element calculation) or by rows.

The multifrontal method is a variant of sparse Gaussian elimination. In the positive-definite case, it involves the Cholesky factorization

$$A = (PL)(PL)^T$$

where P is a permutation matrix and L is lower triangular. In the indefinite case, it involves the factorization

$$A = (PL)D(PL)^T$$

where P is a permutation matrix, L is unit lower triangular, and D is block diagonal with blocks of size 1×1 and 2×2. The factorization is performed by the subroutine `MA77_factor` and is controlled by an elimination tree that is constructed by the subroutine MA77_analyse. Once a matrix has been factorized, any number of calls to the subroutine MA77_solve may be made for different right-hand sides B. An option exists for computing the residuals. For large problems, the matrix data and the computed factors are held in direct-access files.

For a very large problem, several direct-access files are used. The actual input/output is performed through the package HSL_OF01. If a file become full, HSL_OF01 opens secondary files and treats the primary file and all its secondaries as a single superfile. The primary and secondary files may reside on different devices. If the problem is not very large, the superfiles may be replaced by arrays in memory.

At the heart of the subroutines MA77_factor and MA77_solve there are calls to the packages HSL_MA54 and HSL_MA64 for the efficient partial factorization and partial solution of full sets of symmetric positive definite and symmetric indefinite equations, respectively. These block the matrix to reduce caching overheads.

HSL_MA78 This package solves one or more sets of sparse unsymmetric equations $AX = B$ or $A^T X = B$ using an out-of-core multifrontal method. The matrix A must be in unassembled element form.

The multifrontal method involves the factorization

$$A = PLDUQ$$

where P and Q are a permutation matrices, L and U are unit lower and upper triangular matrices, respectively, and D is a diagonal matrix. The factorization is performed by the subroutine MA78_factor and is controlled by an elimination tree that is constructed by the subroutine MA78_analyse. Once a matrix has been factorized, any number of calls to the subroutine MA78_solve may be made for different right-hand sides B. An option exists for computing the residuals. For large problems, the matrix data and the computed factors are held in direct-access files.

For a very large problem, several direct-access files are used. The actual input/output is performed through the package HSL_OF01. If a file become full, HSL_OF01 opens secondary files and treats the primary file and all its secondaries as a single superfile. The primary and secondary files may reside on different devices. If the problem is not very large, the superfiles may be replaced by arrays in memory.

At the heart of the subroutines MA78_factor and MA78_solve there are calls to the package HSL_MA74 for the efficient partial factorization and partial solution of full sets of unsymmetric equations.

MC58 This package estimates the rank and finds a nonsingular submatrix of a sparse matrix A with m rows and n columns using Gaussian elimination. The main entry performs a sparse LU factorization of the matrix optionally using rook pivoting. The factors are not returned but the routine is much faster than the main MA48 matrix factorization routine, sometimes by two orders of magnitude.

HSL_MC64 Given a sparse matrix $A = \{a_{ij}\}_{m\times n}$, $m \geq n$, this subroutine finds a column permutation vector that makes the permuted matrix have n entries on its diagonal. If the matrix is structurally nonsingular, the subroutine optionally returns a column permutation that maximizes the smallest element on the diagonal, maximizes the sum of the diagonal entries, or maximizes the product of the diagonal entries of the permuted matrix. For the latter option, the subroutine also finds scaling factors that may be used to scale the original matrix so that the nonzero diagonal entries of the permuted and scaled matrix are one in absolute value and all the off-diagonal entries are less than or equal to one in absolute value. The natural logarithms of the scaling factors $u_i, i = 1, ..., m$, for the rows and v_j, $j = 1, ..., n$, for the columns are returned so that the scaled matrix $B = \{b_{ij}\}_{m\times n}$ has entries

$$b_{ij} = a_{ij}\ exp(u_i + v_j).$$

In this Fortran 90 version, there are added facilities from the original `MC64` code for working on rectangular and symmetric matrices. For the rectangular case, a row permutation is returned so that the user can permute the matching to the diagonal and identify the rows in the structurally nonsingular block. For the symmetric case, the user must only supply the lower triangle and, if a scaling is computed, it will be a symmetric scaling with the same property as in the unsymmetric case.

`HSL_MC68` Given a symmetric sparse matrix $A = \{a_{ij}\}_{n\times n}$, `HSL_MC68` computes elimination orderings that are suitable for use with a sparse direct solver. Currently the following choices are available

- Approximate minimum degree ordering (with provision for some dense rows and columns) using `MC47`
- Minimum degree ordering using the methodology of `MA27`
- Nested bisection ordering using MeTiS
- `MA47` ordering for indefinite matrices which may generate a combination of both 1×1 and 2×2 pivots

`MF64` Given a sparse complex matrix $A = \{a_{ij}\}_{n\times n}$, this subroutine finds a column permutation vector that makes the permuted matrix have n entries on its diagonal. If the matrix is structurally nonsingular, the subroutine optionally returns a column permutation that maximizes the smallest modulus of an entry on the diagonal, maximizes the sum of the moduli of the diagonal entries, or maximizes the product of the moduli of the diagonal entries of the permuted matrix. For the latter option, the subroutine also finds scaling factors that may be used to scale the original matrix so that the diagonal entries of the permuted and scaled matrix are one in absolute value and all the off-diagonal entries are less than or equal to one in absolute value. The natural logarithms of the scaling factors u_i, $i = 1, ..., n$, for the rows and v_j, $j = 1, ..., n$, for the columns are returned so that the scaled matrix $B = \{b_{ij}\}_{n\times n}$ has entries

$$b_{ij} = a_{ij}\ exp(u_i + v_j).$$

`HSL_MI13` Given a block symmetric matrix

$$K_H = \begin{pmatrix} H & A^T \\ A & -C \end{pmatrix},$$

where H has n rows and columns and A has m rows and n columns, `HSL_MI13` constructs preconditioners of the form

$$K_G = \begin{pmatrix} G & A^T \\ A & -C \end{pmatrix}. \tag{2}$$

Here, the leading block matrix G is a suitably chosen approximation to H; it may either be prescribed explicitly, in which case a symmetric indefinite factorization of K_G will be formed using `HSL_MA57`, or implicitly. In the latter case, K_G will be ordered to the form

$$K_G = P \begin{pmatrix} G_{11} & G_{21}^T & A_1^T \\ G_{21} & G_{22} & A_2^T \\ A_1 & A_2 & -C \end{pmatrix} P^T \tag{3}$$

where P is a permutation and A_1 is an invertible sub-block ("basis") of the columns of A; the selection and factorization of A_1 uses `HSL_MA48` - any dependent rows in A are removed at this stage. Once the preconditioner has been constructed, solutions to the preconditioning system

$$\begin{pmatrix} G & A^T \\ A & -C \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} a \\ b \end{pmatrix} \tag{4}$$

may be computed.

Full advantage is taken of any zero coefficients in the matrices H, A and C.

`MI15` This package implements the Flexible Generalized Minimal Residual method with restarts every m iterations, **FGMRES**(m), to solve the $n \times n$ unsymmetric linear system $Ax = b$, optionally using preconditioning. **FGMRES**(m) generalises the preconditioned **GMRES**(m) allowing the possibility of using a different right preconditioner $P_R^{(i)}$ at each step in solving the preconditioned system

$$\bar{A}x = \bar{b}$$

where $\bar{A} = P_L A$ and $\bar{b} = P_L b$ and P_L is a left preconditioner.

Reverse communication is used for preconditioning operations and matrix-vector products of the form Az. **FGMRES**(m) needs more memory than **GMRES**(m) and, in particular, stores an additional $n \times m$ real matrix. However, in floating point arithmetic, **FGMRES**(m) is numerically more stable than **GMRES**(m) method.

If Gaussian elimination with static pivoting option has been used to compute an approximate LU factorization of A, **FGMRES**(m) can be used to recover full backward error stability. In this case the left preconditioner should be chosen to be the identity and the right preconditioner should be chosen to be $P_R^{(i)} = P_R = (LU)^{-1}$

`HSL_MI20` Given an $n \times n$ sparse matrix A and an $n-$vector z, `HSL_MI20` computes the vector $x = Mz$, where M is an algebraic multigrid (AMG) v-cycle preconditioner for A. A classical AMG method is used. The matrix A must have positive diagonal entries and (most of) the off-diagonal entries must be negative (the diagonal should be large compared to the sum of the off-diagonals). During the multigrid coarsening process, positive off-diagonal entries are ignored and, when calculating the interpolation weights, positive off-diagonal entries are added to the diagonal.

`HSL_ZB01` Given a rank-one or rank-two allocatable array, `HSL_ZB01` reallocates the array to have a different size, and can copy all or part of the original array into the new array. This will use a temporary array or, if there is insufficient memory, one or more temporary files will be used. The user may optionally force `HSL_ZB01` to only use temporary files and not to attempt to use a temporary array. The user may also optionally supply the name of the temporary file and the filesize; if no name is supplied, then a scratch file will be used. If more than one file is required and a filename has been supplied, then `HSL_ZB01` opens files with names that it constructs from the filename by appending '1', '2',... to the end. All temporary files are deleted upon successful exit. If the array given as input was not already allocated, then `HSL_ZB01` allocates the array to have the desired size.

`HSL_ZD11` This package defines a derived type capable of supporting a variety of sparse matrix storage schemes. Its principal use is to allow exchange of data between HSL subprograms and other codes.

The following packages had major updates in the HSL 2007 release:

`MA57 and HSL_MA57` The `MA57` package solves large sparse symmetric indefinite systems and has undergone several significant enhancements.

The `MA57` package now has a wide range of options including several sparsity orderings (with an automatic selection option), multiple right-hand sides, partial solutions, error analysis, a scaling option that is performed internally to the package, a matrix modification facility, an option for static pivoting, the efficient factorization of highly rank deficient systems, and a stop and restart facility. Although the default settings should work well in general, there are several parameters available to enable the user to tune the code for his or her problem class or computer architecture.

In the Fortran 90 version, there are added facilities for automatic restarts when storage limits are exceeded, the return of information on pivots, permutations, scaling, modifications, and the possibility to alter the pivots a posteriori.

`ME57` The `ME57` package was given a major overhaul in the `HSL 2007` release. The package now offers the solution of sets of linear equations $Ax = b$ where the matrix A can be either Hermitian or complex symmetric. It now includes all the options that are offered in the `MA57` package.

5.2 GALAHAD

Version 2.1 of GALAHAD was released in September 2007. New GALAHAD packages include:

`FDC` Given an under-determined set of linear equations/constraints $a_i^T x = c_i$, $i = 1, \ldots, m$ involving $n \geq m$ unknowns x, this package **determines whether the constraints are consistent, and if so how many of the constraints are dependent**; a list of dependent constraints, that is, those which may be removed without changing the solution set, will be found and the remaining a_i will be linearly independent. Full advantage is taken of any zero coefficients in the vectors a_i.

`GLRM` Given real n by n symmetric matrices H and M (with M positive definite), a real n vector c and scalars $\sigma > 0$ and f_0, this package finds an **approximate minimizer of the regularised objective function** $\mathbf{1/p}\sigma\|x\|_M^p + \frac{1}{2}x^T Hx + c^T x + f_0$**,** where $\|x\|_M = \sqrt{x^T Mx}$ is the M-norm of x. This problem commonly occurs as a subproblem in nonlinear optimization calculations involving cubic regularisation. The method may be suitable for large n as no factorization of H is required. Reverse communication is used to obtain matrix-vector products of the form Hz and $M^{-1}z$.

`LANCELOT_simple` This package provides a convenient interface to the GALAHAD package `LANCELOT B`, and is thus designed to minimize an objective function where the minimization variables are required to satisfy a set of auxiliary, possibly nonlinear, constraints. Bounds on the variables and known values may be specified. Unlike `LANCELOT`, the package completely ignores problem partial separability/sparsity structure, limits the forms under which the problem can be presented to the solver and provides a restricted choice of algorithmic options. It is thus of interest mostly for small-dimensional problems for which ease of interface matters more than numerical performance.

`LSTR` Given a real m by n matrix A, a real m vector b and a scalar $\Delta > 0$, this package finds an **approximate minimizer of** $\|Ax - b\|_2$**, where the vector** x **is required to satisfy the "trust-region" constraint** $\|x\|_2 \leq \Delta$**.** This problem commonly occurs as a trust-region subproblem in nonlinear optimization calculations, and may be used to regularize the solution of under-determined or ill-conditioned linear least-squares problems. The method may be suitable for large m and/or n as no factorization involving A is required. Reverse communication is used to obtain matrix-vector products of the form $u + Av$ and $v + A^T u$.

LSRM Given a real m by n matrix A, a real m vector b and a scalar $\sigma > 0$, this package finds an **approximate minimizer of the regularised linear-least-squares objective function** $\frac{1}{2}\|Ax - b\|_2^2 + {}^{\mathbf{1}}\!/\!_{\mathbf{p}}\sigma\|x\|_2^p$**.** This problem commonly occurs as a subproblem in nonlinear optimization calculations involving cubic regularisation, and may be used to regularise the solution of under-determined or ill-conditioned linear least-squares problems. The method may be suitable for large m and/or n as no factorization involving A is required. Reverse communication is used to obtain matrix-vector products of the form $u + Av$ and $v + A^T u$.

QPC This package uses a crossover method, switching between interior-point and working-set approaches, to solve the **quadratic programming problem**

$$\text{minimize} \;\; q(x) = \tfrac{1}{2}x^T Hx + g^T x + f$$

subject to the general linear constraints

$$c_i^l \leq a_i^T x \leq c_i^u, \quad i = 1, \ldots, m,$$

and the simple bound constraints

$$x_j^l \leq x_j \leq x_j^u, \quad j = 1, \ldots, n,$$

where the n by n symmetric matrix H, the vectors g, a_i, c^l, c^u, x^l, x^u and the scalar f are given. Full advantage is taken of any zero coefficients in the matrix H or the vectors a_i. Any of the constraint bounds c_i^l, c_i^u, x_j^l and x_j^u may be infinite.

If the matrix H is positive semi-definite, a global solution is found. However, if H is indefinite, the procedure may find a (weak second-order) critical point that is not the global solution to the given problem.

SBLS Given a **block, symmetric matrix**

$$K_H = \begin{pmatrix} H & A^T \\ A & -C \end{pmatrix},$$

this package constructs a variety of **preconditioners** of the form

$$K_G = \begin{pmatrix} G & A^T \\ A & -C \end{pmatrix}.$$

Here, the leading-block matrix G is a suitably-chosen approximation to H; it may either be prescribed **explicitly**, in which case a symmetric indefinite factorization of K_G will be formed using the GALAHAD package SILS, or **implicitly**, by requiring certain sub-blocks of G be zero. In the latter case, a factorization of K_G will be obtained implicitly (and more efficiently) without recourse to SILS. In particular, for implicit preconditioners, a reordering

$$K_G = P \begin{pmatrix} G_{11} & G_{21}^T & A_1^T \\ G_{21} & G_{22} & A_2^T \\ A_1 & A_2 & -C \end{pmatrix} P^T$$

involving a suitable permutation P will be found, for some invertible sub-block ("basis") A_1 of the columns of A; the selection and factorization of A_1 uses the GALAHAD package ULS. Once the preconditioner has been constructed, solutions to the preconditioning system

$$\begin{pmatrix} G & A^T \\ A & -C \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} a \\ b \end{pmatrix}$$

may be obtained by the package. Full advantage is taken of any zero coefficients in the matrices H, A and C.

`ROOTS` This package uses classical formulae together with Newton's method to find all the real roots of real polynomials of degree up to four.

`WCP` This package uses a primal-dual interior-point method to **find a well-centered interior point** x for a set of general linear constraints

$$c_i^l \leq a_i^T x \leq c_i^u, \quad i = 1, \ldots, m, \tag{5}$$

and simple bounds

$$x_j^l \leq x_j \leq x_j^u, \quad j = 1, \ldots, n, \tag{6}$$

where the vectors a_i, c^l, c^u, x^l and x^u are given. More specifically, if possible, the package finds a solution to the system of primal optimality equations

$$Ax = c, \tag{7}$$

dual optimality equations

$$g = A^T y + z, \;\; y = y^l + y^u \;\text{ and }\; z = z^l + z^u, \tag{8}$$

and perturbed complementary slackness equations

$$(c_i - c_i^l) y_i^l = (\mu_c^l)_i \;\text{ and }\; (c_i - c_i^u) y_i^u = (\mu_c^u)_i, \quad i = 1, \ldots, m, \tag{9}$$

and

$$((x_j - x_j^l) z_j^l = (\mu_x^l)_j \;\text{ and }\; (x_j - x_j^u) z_j^u = (\mu_x^u)_j, \quad j = 1, \ldots, n, \tag{10}$$

for which

$$c^l \leq c \leq c^u, \;\; x^l \leq x \leq x^u, \;\; y^l \geq 0, \;\; y^u \leq 0, \;\; z^l \geq 0 \;\text{ and }\; z^u \leq 0. \tag{11}$$

Here A is the matrix whose rows are the a_i^T, $i = 1, \ldots, m$, mu_c^l, mu_c^u, mu_x^l and mu_x^u are vectors of strictly positive *targets*, g is another given vector, and (y^l, y^u) and (z^l, z^u) are dual variables for the linear constraints and simple bounds respectively; c gives the constraint value Ax. Since (9)–(11) normally imply that

$$c^l < c < c^u, \;\; x^l < x < x^u, \;\; y^l > 0, \;\; y^u < 0, \;\; z^l > 0 \;\text{ and }\; z^u < 0, \tag{12}$$

such a primal-dual point $(x, c, y^l, y^u, z^l, z^l)$ may be used, for example, as a feasible starting point for primal-dual interior-point methods for solving the linear programming problem of minimizing $g^T x$ subject to (5) and (6).

Full advantage is taken of any zero coefficients in the vectors a_i. Any of the constraint bounds c_i^l, c_i^u, x_j^l and x_j^u may be infinite. The package identifies infeasible problems, and problems for which there is no strict interior, that is one or more of (11) only holds as an equality for all feasible points.

6 Conference and workshop presentations

2-7 April 2006, Copper Mountain Conference on Iterative Methods, Copper, Colorado, USA. I.S. Duff, *A note on GMRES preconditioned by a perturbed LDL^T decomposition with static pivoting.*

25-26 May 2006, Shanghai Forum on Industrial and Applied Mathematics, Shanghai, China. I.S. Duff, *Sparse system solution and the HSL Library.*

15-16 June 2006, Sparse Days, CERFACS, Toulouse, France. M. Arioli, *A note on GMRES preconditioned by a perturbed LDL^T decomposition with static pivoting.* H.S. Dollar, *Implicit-factorization constraint preconditioners and permutations.* N.I.M. Gould, *Finding a well-centred point for a set of polyhedral constraints.*

19-23 June 2006, PARA'06, Umea, Sweden. J.A. Scott, *The design of an out-of-core multifrontal solver for the 21st century.*

22 July 2006, ICCG, BICGSTAB, and Jacobi-Davidson, Utrecht, Netherlands. I.S. Duff, *The perfect preconditioner.*

24-27 July 2006, GAMM-SIAM Conference on Applied Linear Algebra, Dusseldorf, Germany. M. Arioli *Stopping criteria in the context of finite-element discretization.* H.S. Dollar *Constraint style preconditioners for regularized saddle point problems.* J.A. Scott, *Refinement algorithms for bandwidth reduction.*

30 July - 3 August 2006, ISMP 2006, Rio de Janeiro, Brazil. C. Cartis, *A new perspective on the complexity of interior point methods for linear programming.*

23 August 2006, Optbridge, Said Business School, Oxford. N.I.M. Gould, *Successive and simultaneous projection methods for convex feasibility problems.*

5-8 September 2006, ECCOMAS CFD, Egmond aan Zee, The Netherlands. M. Arioli *Stopping criteria for Krylov methods and finite-element approximation of variational problems.*

18 September 2006, Bath-RAL Numerical Analysis Day, University of Bath, England. C. Cartis, *Finding a well-centred point within a polyhedron.* I.S. Duff, *Direct solution of sparse skew symmetric linear systems.*

27 September 2006, International Conference on Numerical Analysis and Optimization, Beijing, China. C. Cartis, *Finding a well-centred point within a polyhedron.* N.I.M. Gould, *SRLP-EQP filter methods for constrained optimization.*

22-26 October 2006, First International Conference on Numerical Algebra and Scientific Computing (NASC06). I.S. Duff, *Design and use of a sparse direct solver for skew-symmetric systems.*

28 October, 2006, International Workshop at Fudan University, Shanghai, China. I.S. Duff, *Design and use of a sparse direct solver for skew-symmetric systems.*

5-6 December 2006, 2nd Internal Numerical Analysis Conference, University of Oxford. H.S. Dollar, *Solving saddle-point problems at a gallop.*

5 February 2007, Scientific and Celebratory Conference, Daresbury Laboratory, UK. I.S. Duff, *Combining direct and iterative methods for the solution of large systems in different application areas.*

17-19 February, 2007, SIAM Workshop on Combinatorial Scientific Computing (CSC07), Cost Mesa, California, USA. I.S. Duff, *Recent developments in multifrontal codes.*

28 March 2007, Berkeley Lab Scientific Computing Workshop, LBNL, Berkeley, California, USA. I.S. Duff, *Recent developments in multifrontal codes.* J.A. Scott, *A virtual memory system for use with an out-of-core solver.*

29-31 March 2007, Stanford 50: State of the Art & Future Directions of Computational Mathematics &

Numerical Computing, Stanford, California, USA. I.S. DUFF, *Combining direct and iterative methods for the solution of large systems in different application areas.*

23 May 2007, Gene Golub Day, University of Leicester. I.S. DUFF, *Direct codes for rank detection and the solution of skew symmetric systems.*

26-29 June 2007, 22nd Biennial Conference on Numerical Analysis, Dundee, Scotland. M. ARIOLI *GMRES preconditioned by a perturbed* LDL^T *decomposition with static pivoting.* C. CARTIS, *A new perspective on the complexity of interior point methods for linear programming.* H.S. DOLLAR *Iterative solution of saddle-point systems with examples from PDE-constrained optimization.* N.I.M. GOULD, *Adaptive cubic over-estimation methods for unconstrained optimization.* J.A. SCOTT, *The performance of a new HSL out-of-core solver.*

9-12 July 2007, International Conference on Preconditioning Techniques, Toulouse, France. H.S. DOLLAR, *Iterative solution of saddle-point systems with examples from PDE-constrained optimization.*

15-20 July 2007, ICIAM 2007, Zurich, Switzerland. C. CARTIS, *Adaptive cubic overestimation methods for unconstrained optimization.* H.S. DOLLAR, *Iterative linear algebra for constrained optimization.* H.S. DOLLAR, *Iterative solution of saddle-point systems with examples from PDE-constrained optimization.* I.S. DUFF, *Developments in matching and scaling algorithms.* I.S. DUFF, *The use of hybrid techniques at CERFACS for the solution of large problems on parallel machines.*

13-18 August 2007, International Conference on Applied Mathematics and Interdisciplinary Research, Lijiang, Yunnan Province, China. I.S. DUFF, *Hybrid techniques for the solution of large scale problems.*

20-24 August 2007, Computational Methods with Applications, Harrachov, Czech Republic. M. ARIOLI *GMRES preconditioned by a perturbed* LDL^T *decomposition with static pivoting.* J.A. SCOTT, *On the direct solution of very large sparse linear systems using out-of-core techniques.*

13-15 September 2007, First IMA Conference on Numerical Linear Algebra and Optimization, Birmingham. M. ARIOLI *GMRES preconditioned by a perturbed* LDL^T *decomposition with static pivoting.* H.S. DOLLAR, *Iterative solution of saddle-point systems with examples from PDE-constrained optimization.* J.A. SCOTT, *Solving large sparse linear systems out of core.*

24-28 September 2007, Sixth International Conference on Computer Science and Information Technologies (CSIT'2007), Yerevan, Armenia. I.S. DUFF, *The use of hybrid techniques for the solution of large scale problems.*

25 September 2007, Bath-RAL Numerical Analysis Day, RAL. H.S. DOLLAR, *Iterative solution of PDE-constrained optimization problems.* J.A. SCOTT, *Solving large sparse linear systems out of core.*

10 October 2007, Sparse Days at CERFACS, Toulouse, France. J.A. SCOTT, *The out-of-core challenge for large-scale problems.*

15-19 October 2007, Matrix Analysis and Applications. CIRM Luminy, Marseille, France. I.S. DUFF, *The use of hybrid techniques at CERFACS for the solution of large scale problems on parallel machines.*

7 Seminars

Institute of Computer Science, Academy of Sciences of the Czech Republic, Prague. 2 November 2006. J.A. Scott, *HSL and its out-of-core solver.*

Department of Mathematics, University of Leicester. 9 November 2006. M. Arioli, *The role of finite dimensional Hilbert spaces and their duals in the design of Krylov subspaces methods.*

Department of Mathematics, University of Utah, USA. 13 November 2006. C. Cartis *Some challenges in interior point methods for linear programming.*

Department of Geotechnical Engineering, University of Newcastle, NSW, Australia. 16 November 2006. I.S. Duff, *Determining the rank of sparse matrices.*

Mathematics and Computer Science Division, Argonne National Laboratory, USA. 17 November, 2006. C. Cartis *Finding a well-centred point within a polyhedron.*

Department of Mathematics, University of Edinburgh. 15 November 2006. H.S. Dollar, *Iterative linear algebra for constrained optimization.*

Mathematics and Computer Science Division, Argonne National Laboratory, USA. 17 November 2006. C. Cartis *Finding a well-centred point within a polyhedron.*

Oxford University Computing Laboratory. 25 January 2007. M. Arioli, *A note on GMRES preconditioned by a perturbed LDL^T decomposition with static pivoting.*

Centre for Operations Research and Management Science, University of Southampton. 1 March 2007. C. Cartis *Some challenges in interior point methods for linear programming.*

IMM Seminar Series, DTU, Lyngby, Denmark. 21 March 2007. I.S. Duff, *Combining direct and iterative methods for the solution of large systems in different application areas.*

Numerical Analysis Group, DTU, Lyngby, Denmark. 23 March 2007. I.S. Duff, *Recent developments in multifrontal codes.*

Department of Mathematics, University of Bath. 11 May 2007. J.A. Scott, *An introduction to HSL and the solution of sparse linear systems.*

Mathematics and Computer Science Division, Argonne National Laboratory, USA. 14 June 2007. I.S. Duff, *Recent developments in rank detection and skew solvers.*

Department of Mathematics, Jiaotong University, Xi'an, China. 23 August 2007. I.S. Duff, *Recent developments in multifrontal codes.*

Department of Mathematics, University of Manchester. 3 October 2007. I.S. Duff, *The use of hybrid techniques for the solution of large scale problems.*

Department of Mathematics, University of Manchester. 26 October 2007. H.S. Dollar, *Iterative solution of PDE-constrained optimization problems.*

8 Lecture Courses, Teaching, Supervision

University of Edinburgh. 10 lecture Operations Research MSc course on Numerical Optimization, 9-13 January 2006. N.I.M. Gould

Oxford University. 16 lecture Part C course on Numerical Optimization, January-March 2006. N.I.M. Gould

Oxford University. 12 lecture MSc course on Sparse Direct Methods, January-March 2006. I.S. Duff and J.A. Scott

Reading University. 10 lecture MSc course on Advanced Boundary Value Problems, February-March 2007. H.S. Dollar

DTU Lyngby, Denmark. Lectures on Advanced Topics in Optimization, March-April 2007. I.S. Duff

9 Seminars at RAL

2 March 2006	Dr Matthias Bollhöfer (TU Braunschweig, Germany) Algebraic multigrid using inverse-based coarsening
9 March 2006	Dr Daniel Loghin (University of Birmingham) Adaptive preconditioners for Newton-Krylov methods
4 May 2006	Dr Dulceneia Becker (Cranfield University) A novel, parallel PDE solver for unstructured grids
25 May 2006	Dr Mirek Tuma (Academy of Sciences of the Czech Republic) Algebraic updates of preconditioners for solving similar linear algebraic systems
9 November 2006	Dr Hou-Duo Qi (University of Southampton) Convex quadratic semi-definite programming problem: algorithms and applications
30 November 2006	Dr Martin van Gijzen (Delft University of Technology, The Netherlands) Spectral analysis of the discrete Helmholtz operator preconditioned with a shifted Laplacian.
1 February 2007	Professor Patrick Amestoy (EINSEEIHT, Toulouse, France) Parallel sparse multifrontal solver in a limited memory environment
15 March 2007	Dr Sven Hammarling (NAG Ltd and the University of Manchester) New developments in LAPACK and ScaLAPACK
27 April 2007	Dr Scott McLachlan (TU Delft, The Netherlands) Multigrid solvers for quantum dynamics - a first look
31 May 2007	Dr Ekaterina Kostina (University of Heidelberg, Germany) Model based design of optimal experiments for dynamic processes
1 November 2007	Dr Laura Grigori (INRIA, Paris, France) Communication avoiding algorithms for dense LU and QR factorizations
15 November 2007	Prof Jan Magnus (Tilburg University, The Netherlands) On the estimation of a large sparse Bayesian system: the Snaer program