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Numerical Analysis Group Progress Report
January 2010 - December 2011

JA Scott (ed)

January 2012

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Numerical Analysis Group Progress Report
January 2010 – December 2011

Jennifer 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 Science and Technology Facilities Council for the period January 2010 to December 2011. This work was principally supported by EPSRC grants EP/E053351/1 and EP/I013067/1.

Keywords: large-scale optimization, sparse matrices, direct methods, iterative methods, ordering techniques, stopping criteria, parallel, multicore, numerical linear algebra, HSL, GALAHAD, CUTEr.

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

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Jennifer Scott.
Group Leader.
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Iain Duff
Sparse matrices and high-performance computing.

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

Jonathan Hogg
HSL, parallel linear algebra, optimization.

Sue Thorne (née Dollar)
Preconditioners, saddle-point problems and sparse linear systems.

Karen McIntyre
Part-time administrative and secretarial support.

Post-doctoral student (until August 2010): Daniel Robinson (Oxford)
Nonlinear optimization.

CASE student: Philip Browne (Bath)
Structural optimization.

Honorary Scientist: John Reid
HSL, sparse matrices, automatic differentiation, and Fortran.

Visiting Scientist: Coralia Cartis (Edinburgh)
Interior-point methods, complexity analysis.

Long term visitor (January - March 2010):

Dominique Orban (Ecole Polytechnique de Montreal and GERAD, Canada)
Large-scale optimization, nonlinear equations and inequalities.

1 Overview

This report covers the period January 2010 to December 2011 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 EP/E053351/1 and, since 1 October 2011, EP/I013067/1.

A significant achievement for the Group during the period of this report was successfully applying to EPSRC for a new research grant *Linear Algebra and Optimization: Structure, Sparsity, Algorithms and Software*. This grant will fund most of the Group's activities until October 2015. In the current tough economic climate, this is clearly a huge success that will guarantee the continued existence of the Group for the next few years. In addition, Nick Gould and Jennifer Scott were involved in the bid to establish a new CCP (Collaborative Computational Project) entitled *Software and Algorithms for Emerging Architectures*. The chair is Anne Trefethen from Oxford; our main involvement initially is a Flagship grant that we secured as part of the CCP application. This will involve developing linear programming and quadratic programming solvers for use on GPU systems. Since at the heart of such solvers lies the need to efficiently solve sparse linear systems of equations, this will involve the development of GPU sparse direct solvers. We are currently advertising for someone to work with us on this project over the next two years.

Another important achievement for the Group was finally securing a new contract with Aspentech. Aspentech was previously responsible for all marketing and distributions of the HSL mathematical software library to non-academic users. Unfortunately, although this arrangement had been mutually beneficial in the past, over the last few years it had not worked well and we were anxious to loosen ties with Aspentech. This proved quite difficult but we are pleased that we now have almost full control of HSL while retaining a good relationship with Aspentech, who remain an important user and customer of HSL.

On the staff front, the big news is that Sue Thorne went on maternity leave in October of this year and Jessica Alice was born in Oxford on 18 December. Congratulations to Sue and James. We will look forward to welcoming Sue back to the Group (on a part time basis) early in the autumn of 2012.

Other personal successes for Group members were the promotion in 2011 of Nick Gould to Senior STFC Fellow and of Jennifer Scott to STFC Fellow, and the election of Iain Duff to SIAM Fellow in 2010. Jonathan Hogg is to be congratulated on successfully defending his PhD thesis *High Performance Cholesky and Symmetric Indefinite Factorizations with Applications* in Edinburgh in September 2010. Furthermore, Jonathan's employment contract has now been moved from fixed-term to permanent.

In April 2011, John Reid's status changed from part-time contractor to Honorary Scientist. This has meant that we no longer see John quite so frequently but, at present, he retains his office at RAL and we are pleased that we generally see him once a week. Jonathan has now taken over from John all responsibilities for the day-to-day running of HSL and is successfully combining his role as HSL manager with research and software development.

We are delighted to have recently been able to recruit a new member to the Group, Tyrone Rees. Tyrone studied for his DPhil *Preconditioning Iterative Methods for PDE Constrained Optimization* in Oxford under the supervision of Andy Wathen and currently holds a post doctoral position at the University of British Columbia in Vancouver. We very much look forward to Tyrone joining us in April 2012. Tyrone's research interests are in numerical linear algebra and PDE-constrained optimization. He works on preconditioning Krylov subspace methods, particularly to solve saddle-point problems and is interested in solving such problems that are derived from the field of optimal control of PDEs. We thus anticipate that he will be able to contribute to the Group's EPSRC grant, as well as pursuing new but related areas of research.

We continue to have a CASE student associated with the Group who is partially funded by sales of HSL software. Phil Browne is a fourth year graduate student at the University of Bath. His supervisors at Bath are Professor Chris Budd from the Department of Mathematics and Dr Alicia Kim from the

Department of Mechanical Engineering. Phil's research work is on structural optimization. He is looking at a formulation of compliance minimisation subject to buckling constraints in order to reach a solution that is not structurally unstable.

During the last two years, we have been pleased to welcome a number of visitors to the Group. In particular, Dominique Orban (Ecole Polytechnique de Montreal and GERAD, Canada) visited the Group during the early part of 2010, financed by an EPSRC visiting researcher grant. Shorter visits were made by Chris Budd and Alicia Kim (Bath), Coralia Cartis (Edinburgh), Yifan Hu (AT&T), Margherita Porcelli (Firenze), Wil Schilders (Technische Universiteit Eindhoven), Philippe Toint (Namur), and Miroslav Tůma (Academy of Sciences of the Czech Republic). In addition, we hosted a number of seminar speakers (Section 8).

The remainder of this report is organised as follows. In Section 2, Group members present brief personal statements. 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 in HSL (formerly the Harwell Subroutine Library) and GALAHAD along with a brief synopsis of their purposes. Briefer lists of conferences and seminars are given in Sections 6 and 7. We finish with a list of seminars held at RAL (in our joint series with Oxford), in Section 8.

Current information on the research and software-related activities of the Group and on individual Group members can be found at `https://www.cse.scitech.ac.uk/nag`

Jennifer Scott (jennifer.scott@stfc.ac.uk)

2 Personal statements

2.1 Mario Arioli

Mario's work revolves around linear algebra and the numerical solution of PDEs. Mario has collaborated with Jennifer on the error analysis of Chebyshev methods used to accelerate iterative refinement processes. In particular, these methods have been shown, both theoretically and numerically, to significantly reduce the number of operations needed to recover full backward stability of the solution when a linear system is solved by Gaussian elimination in single precision.

Mario has investigated the use of Golub-Kahan bi-diagonalization methods in solving augmented systems. In particular, this study focused on augmented systems describing the mixed finite-element approximation of differential systems in variational form. The stopping criteria introduced are linked to the approximation error; they terminate the bi-diagonalization process when the energy norm of the error between the exact solution of the system and the numerical solution at some stage of the bi-diagonalization process has the same order of magnitude as the approximation error. The results stimulated a new collaboration between Mario and Dominique Orban (Montreal). They are studying the use of the Golub-Kahan method in order to solve symmetric quasi-definite systems that emerge in the solution of regularized weighted least-squares problems and differential systems.

The collaboration with Daniel Loghin (Birmingham), investigating the square root approximation of special elliptic operators using the generalised Lanczos method and its use in computing preconditioners for Krylov methods applied to Steklov-Poincare operators, has continued. The theoretical results have been used in domain decomposition applications in collaboration with Drosos Kourounis (Ioannina and Stanford) and the resulting paper has been accepted for publication. During 2010, in relation to this Domain Decomposition project, Mario studied the numerical solution of differential problems on metric graphs (also known as Quantum Graphs). The study was presented at Daresbury and at ENSEEIHT and at CERFACS, Toulouse.

More recently, in collaboration with Jorg Liesen, Agnieszka Miedlar (Berlin), and Zdenek Strakos (Prague), Mario is involved in writing a survey paper at the invitation of the organizers of the GAMM

2012 conference. The study concerns the problem of global convergence of adaptive finite-element methods applied to elliptic equations and to eigenvalue-eigenfunction in variational form, where the solutions on each grid are only approximated by the conjugate gradient method or by a Lanczos process.

Mario contributed the package `HSL_EA20` to the 2011 release of HSL (see Section 5.1).

2.2 Iain Duff

Iain continues in his joint roles of research associated with the Group's EPSRC grant and as an ambassador for STFC in his capacity as an STFC Senior Fellow. Iain is a scientific advisor 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. With his French hat, Iain was a chairman on a French PhD defence jury. 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 and hybrid methods as well as direct methods, and in the exploitation of parallel computers. One of his current interests is in developing combinatorial techniques both in the solution of sparse equations by direct methods and in the preprocessing of matrices prior to the solution of the equations. Recent research in this area has included work on matching algorithms, novel ordering strategies, and preconditioning using a hierarchical decomposition. He is supervising a co-tutelle student from Nottingham who is currently at CERFACS working on block methods for solving systems from high order discretizations applicable to the solution of neutron transport equations. In addition to his CERFACS involvement, Iain spent some time at ENSEEIHT in Toulouse where he co-supervised students working on the efficient generation of explicit entries of the inverse both in an out-of-core and a parallel environment and on the development of the block Cimmino algorithm.

Iain is on the Institute of Mathematics and its Applications Council, is a member of the Research Committee, is chairman of the Journals Board of Management, is an IMA representative on the International Committee that oversees the ICIAM international conferences on applied mathematics, and is an editor of the IMA Journal of Numerical Analysis. He was reelected to be Chairman of the Board of Trustees of SIAM in 2010 and 2011 and is on the SIAM Council, the SIAM Compensation Committee, and the SIAM Cabinet. Iain was elected as a SIAM Fellow in 2010. He was on a review panel for the Czech Academy of Sciences, has been on the Programme and Organizing Committee for several international meetings, and has given invited talks at meetings in Aguas de Lindoia, Amsterdam, Barcelona, Bordeaux, Darmstadt, Lake Tahoe, Reno, Stellenbosch, Vancouver, and Vigo. He continues to serve on the EPSRC College.

He was chairman of the Working Group on Numerical Libraries, Solvers and Algorithms for the European Exascale Software Initiative which reported to the European Union in October 2011. He has been invited to chair a working group in the follow-up proposal EESI-2. Iain continues to write articles for a general audience, including for encyclopedias and SIAM News.

2.3 Nick Gould

Nick's work continues to revolve around optimization and related linear algebra issues. A new release of GALAHAD occurred in early 2011, and downloads are currently running at around two per day.

Nick, Coralia Cartis (Edinburgh) and Philippe Toint (Namur) have been heavily involved in trying to understand the theoretical limitations of popular and evolving optimization algorithms. The key question they have addressed is how many evaluations of the objective and/or constraint functions might be needed, in the worst case, to find a point that is close to locally optimal. The main finding is that, in this sense, common line-search and trust-region variants of Newton's method may be no better than steepest descent for non-convex problems, while globalizations based on so-called cubic regularization are provably better. Initial analysis focused on unconstrained optimization, but similar results for problems with convex and recently non-convex constraints have been derived. Specialised analyses for convex optimization, non-linear least squares and non-linear equations have been performed, and extensions to derivative-free algorithms are possible. Of course, this does not necessarily mean that typical behaviour of algorithms reflects the worst-case, and it is interesting to see that many of the features that seem to help cubic regularization can actually also be used to enhance, say, trust region methods, as work with Philippe and Margherita Porcelli (Firenze) confirmed.

Nick has also been working with Dominique Orban (Montreal) during his EPSRC-sponsored visit (EP/H026053/1) as described by Sue Thorne (below). As a by-product of this visit, Nick, Dominique and Daniel Robinson (Johns Hopkins) investigated high-order interior-point methods for convex quadratic programming. Of particular note, methods that are capable of finding highly-accurate solutions of degenerate problems have been derived and appear to work well in practice as the new GALAHAD package `CQP` attests.

Having avoided the area for decades, Nick has finally set off into the murky world of global optimization. Nick, Chris Farmer (Oxford), and D.Phil. student Jari Fowkes have looked at Bayesian surrogate-based approaches, as well as specialised methods for problems with Lipschitz continuous Hessians–these include common surrogates—that have some similarities with the cubic regularization ideas mentioned above. Nick, Jari and Coralia are continuing this work as part of Jari's new post doc in Edinburgh and hope to exploit the obvious embarrassing-parallelism to solve realistic problems.

Nick achieved a personal goal of issuing a technical report every month during 2011, and published his 100th refereed paper in November. He has started writing a new book with Coralia and Philippe on the complexity of non-convex optimization. His Oxford D.Phil. student, Jari Fowkes, successfully defended his thesis in July and has now moved to a post doc in Edinburgh. Moreover, his EPSRC-funded post doc (EP/F005369/1) Daniel Robinson has moved into a Faculty position at Johns Hopkins University (via Northwestern) after a successful three years at Oxford and RAL.

Nick's six-year term as Editor-in-Chief of the SIAM Journal of Optimization ended on Christmas Day 2010, and he was presented by SIAM with a handsome clock to celebrate increasing the submission rate by 70% during his tenure. He continues to serve on the editorial board of the Journal as well as on the boards of Mathematical Programming Series A, the ACM Transactions on Numerical Software and the IMA Journal on Numerical Analysis. In addition, Nick has been appointed to the Publications Committee of the Mathematical Optimization Society and to the SIAM Journal Subcommittee. He also served on the organising committees for the SIAM Conference of Optimization (Darmstadt, 2011) and IMA Conferences on Optimisation and Linear Algebra (Birmingham, 2010 & 2012), and was a member of the 15th Leslie Fox prize committee, for the prize presented in Manchester in June 2011.

Nick has been re-appointed to Visiting Professorships at Edinburgh and Oxford and also to the EPSRC College. He is now an STFC Senior Fellow, having been promoted to Individual-Merit Band H during 2011.

2.4 Jonathan Hogg

Jonathan's time is split evenly between research and his role as HSL Manager. As such, his work has two major focuses. The first is his continued collaboration with Jennifer on new and improved sparse direct linear solvers. The second is support of HSL 2011, including substantial technical work for the release of HSL 2011 and the addition of interfaces to C and MATLAB.

The linear solver work has been focused on support for multicore and many-core architectures. This has included the extension of DAG-based techniques to the indefinite case (`HSL_MA86`), in which the challenges of incorporating pivoting had to be addressed. Further work looking at parallelization of the solve phase highlighted the new importance of this phase as it increasingly becomes a bottleneck due to its memory-bound nature.

To prepare for upcoming work on the Group's new EPSRC grants, Jonathan has written a new analysis phase that significantly reduces the memory movement involved. This work included the development of a new technique for problems in element form that is an order of magnitude faster than previous methods. In collaboration with Jennifer, a new multifrontal solver (`HSL_MA97`) was then developed to provide a basis for future work on parallel pivoting techniques. The design is such that bit-compatible results are achieved regardless of the number of threads used.

Much of Jonathan's HSL-related work is described in Section 5.1. In addition to managing the release of HSL 2011, Jonathan is the main point of contact for user support and sales. He is also responsible for providing tools for the Group to use in the development of HSL, which includes maintenance of the Group's computers in conjunction with Nick.

Specific HSL 2011 packages that Jonathan has written (or co-authored) are `HSL_MC56`, `HSL_MC69`, `HSL_MC78`, `HSL_MA86`, `HSL_MA97`, and `HSL_MATLAB`. He has also written C and/or MATLAB interfaces to `HSL_MA77`, `HSL_MA86`, `HSL_MA87`, `HSL_MC68`, `HSL_MC69` and `HSL_MI20`. Jonathan has prepared tools for the development of HSL software and associated interfaces and was involved in writing (revised) guidelines for HSL software development. Finally, Jonathan has developed and tested Ipopt interfaces for both `HSL_MA86` and `HSL_MA97`, enabling more widespread adoption of the new solvers.

To support his work, Jonathan has attended a number of management training courses. This included qualifying as a PRINCE2 practitioner.

2.5 Jennifer Scott

During the last couple of years, Jennifer has been involved in research and software projects with most members of the Group. With Mario, Jennifer collaborated on the error analysis of Chebyshev methods used to accelerate iterative refinement processes. With Sue and Iain, Jennifer has been working on the development of a novel approach to efficiently computing nested dissection orderings for use with our HSL sparse direct solvers. Another interesting sparse matrix ordering problem that is being studied by Jennifer in collaboration with Yifan Hu (AT&T) is that of antibandwidth maximization. This is the dual of the usual bandwidth minimization problem and involves ordering a sparse matrix so that its off-diagonal entries are as far from the diagonal as possible. One application area is that of map colouring. Jennifer and Yifan are looking at the feasibility of adapting techniques from the bandwdith minimization problem to the antibandwidth problem. Initial results for level-based heuristics are encouraging, particularly for problems with an underlying mesh.

Jennifer has continued to work with Jonathan on the development of sparse direct solvers. The main interest has been in solvers designed for multicore machines. As noted by Jonathan, a new sparse indefinite multicore solver `HSL_MA87` has been developed and included in HSL 2011. In addition, a new multifrontal code `HSL_MA97` has just been released. Both packages take advantage of our work on the development of an efficient implementation of the analyse phase.

Jennifer's collaboration with Mirek Tůma (Prague) on the development of incomplete Cholesky factorization preconditioners has continued. The Group was pleased to host week-long visits by Mirek to Rutherford in January 2010 and November 2011. Having completed their study of level-based schemes, Jennifer and Mirek are now starting to look at using robust incomplete Cholesky second order factorizations.

A major success for Jennifer has been completing the long and protracted negotiations between STFC and Aspentech over the future of the Group's software library HSL. After more than two years, a new contract was finally signed in May 2010. This gives STFC almost full control of HSL and secures an annual payment from Aspentech for their continued use of HSL software.

Jennifer is still the editor of the IMA Numerical Analysis Newsletter and produces three editions of the newsletter a year. The newsletter is now mainly distributed in electronic form and is also available via the IMA webpages. Jennifer remains active in promoting women in mathematics in the UK. She is the UK coordinator for European Women in Mathematics and is a member of the Women in Mathematics Committee of the London Mathematical Society.

A significant personal achievement in 2011 was that Jennifer was promoted to Individual-Merit Band G STFC Fellow. Jennifer was also elected to membership of the IFIP Working Group on Numerical on Numerical Software (WG2.5).

2.6 Sue Thorne

Sue's work continues to revolve around linear algebra and optimization. One of her main areas of work has been the linear algebra behind PDE-constrained optimization problems. She has analysed the properties of the linear systems that need solving for Poisson distributed and boundary control problems, and also developed new preconditioners. Sue then extended these preconditioners to Helmholtz control problems, where the linear systems are now complex Hermitian, rather than real and symmetric.

In April 2010, Sue was awarded a first prize in the Bill Morton Prize competition. This is awarded to a paper on computational fluid dynamics by a young researcher within 5 years of obtaining their doctorate. In Sue's case, this was for her paper *Distributed control and constraint preconditioners*, which has since appeared in *Computers and Fluids.*

Between January and May 2010, Dominique Orban (Montreal) visited the Group. During this period, Nick and Sue worked with Dominique on PDE-constrained optimization problems in which the PDE is nonlinear. Dominique has developed a Python package to perform the optimization-side of the solution process and form the associated linear systems: an appropriate linear solver can then be plugged-in. The aim is to form appropriate preconditioners that can be used in conjunction with an iterative solution method to solve these linear systems.

Sue was involved in the development of a number of new packages for inclusion within HSL 2011: `HSL_MC69`, `HSL_MC79`, and `HSL_MI27` (see Section 5.1 for details).

Much of Sue's work during 2011 centered on the development of a novel nested dissection routine that computes elimination orderings for large sparse symmetric matrices (in collaboration with Iain and Jennifer). The aim is to produce an HSL package that computes elimination orderings of similar quality to the well-known graph-partitioning package MeTiS but is more efficient in both CPU time and memory. As Sue is currently on maternity leave, this project will be completed on her return.

Since January 2010, Sue has been the secretary for the SIAM Activity Group on Linear Algebra. She is on the scientific committee for the 2012 SIAM Conference on Applied Linear Algebra. Sue gave a 10 lecture MSc course on Advanced Numerical Solution of Differential Equations at the University of Reading in February-March 2010 and again in February-March 2011.

3 Technical Reports that appeared in 2010-2011

Copies of Rutherford Technical Reports are available at `http://www.stfc.ac.uk/CSE/randd/nag/36276.aspx`

RAL-TR-2009-018 *Properties of linear systems in PDE-constrained optimization. Part II: Boundary control.*
H. S. Thorne.

Optimization problems with constraints that contain a partial differential equation arise widely in many areas of science. In this paper, we consider Neumann boundary control problems in which the 2- and 3-dimensional Poisson problem is the PDE. If a discretize-then-optimization approach is used to solve the optimization problem, then a large dimensional, symmetric and indefinite linear system must be solved. In general, boundary control problems include a regularization term, the size of which is determined by a real value known as the regularization parameter. The spectral properties and, hence, the condition number of the linear system are highly dependent on the size of this regularization parameter. We derive intervals that contain the eigenvalues of the linear systems and, using these, we are able to show that if the regularization parameter is larger than a certain value, then backward-stable direct methods will compute solutions to the discretized optimization problem that have relative errors of the order of machine precision: changing the value of the regularization parameter within this interval will have negligible effect on the accuracy but the condition number of the system may have dramatically changed. We also analyse the spectral properties of the Schur complement of the saddle-point system. Throughout the paper, we complement the theoretical results with numerical results.

RAL-TR-2010-001 *Numerical Analysis Group Progress Report: January 2008 - December 2009.*
J. A. Scott (editor).

We discuss the research activities of the Numerical Analysis Group in the Computational Science and Engineering Department at the Rutherford Appleton Laboratory of the Science and Technology Facilities Council for the period January 2008 to December 2009. This work was principally supported by EPSRC grants EP/E053351/1, EP/F006535/1 and EP/F005369/1.

RAL-P-2010-001 *Design, implementation, and analysis of maximum transversal algorithms.*
I. S. Duff, K. Kaya and B. Uçar.

We report on careful implementations of seven algorithms for solving the problem of finding a maximum transversal of a sparse matrix. We analyse the algorithms and discuss the design choices. To the best of our knowledge, this is the most comprehensive comparison of maximum transversal algorithms based on augmenting paths. Previous papers with the same objective either do not have all the algorithms discussed in this paper or they use non-uniform implementations from different researchers. We use a common base to implement all of the algorithms and compare their relative performance on a wide range of graphs and matrices. We systematize, develop and use several ideas for enhancing performance. One of these ideas improves the performance of one of the existing algorithms in most cases, sometimes significantly.

CERFACS-TR/PA/10/14 *Semi-local and global convergence of the Newton-HSS method for systems of nonlinear equations.*
X.-P. Guo and I. S. Duff.

Newton-HSS methods, that are variants of inexact Newton methods different from Newton-Krylov methods, have been shown to be competitive methods for solving large sparse systems of nonlinear equations with positive definite Jacobian matrices [Bai and Guo, 2008]. In that paper, only local convergence was proved. In this paper, we prove a Kantorovich-type semilocal convergence. Then we introduce Newton-HSS methods with a backtracking strategy and analyse their global convergence. Finally, these globally convergent Newton-HSS methods are shown to work well on several typical examples using different forcing terms to stop the inner iterations.

RAL-TR-2010-004 *The importance of structure in algebraic preconditioners.*
J. A. Scott and M. Tůma.

In this paper, we consider level-based preconditioning, which is one of basic approaches to algebraic preconditioning of iterative methods. It is well-known that while structure-based preconditioners can be very useful, excessive memory demands can limit their usefulness. Here we present an improved strategy that considers the individual entries of the system matrix and restricts small entries to contributing to fewer levels of fill than the largest entries. Using symmetric positive definite problems arising from a wide range of practical applications, we show that the use of variable levels of fill can yield incomplete Cholesky factorization preconditioners that are more efficient than those resulting from the standard level-based approach. The concept of level-based preconditioning, which is based on the structural properties of the system matrix, is then transferred to the numerical incomplete decomposition. In particular, the structure of the incomplete factorization determined in the symbolic factorization phase is explicitly used in the numerical factorization phase. Further numerical results demonstrate that our level-based approach can lead to much sparser but efficient incomplete factorization preconditioners.

RAL-TR-2010-007 *A note on the solve phase of a multicore solver.*
J. D. Hogg and J. A. Scott.

When using a direct solver to solve large sparse linear systems of equations, the solve phase that follows the numerical factorization performs a relatively small proportion of the total number of numerical operations. However, it is responsible for a much higher proportion of the memory traffic. This makes it a potential bottleneck on newer multicore architectures that have a higher ratio of computational power to memory bandwidth than exhibited by traditional shared-memory parallel machines.

In this note, we illustrate the problem through experiments and test a number of different approaches that aim to improve the performance of the solve phase on multicore machines. We extend the DAG-based approach that has been successfully used for the factorize phase on multicore machines to the solve phase and explore techniques for reducing memory throughput. Numerical experiments that illustrate the difficulties and the effectiveness of our approaches are performed on large-scale problems from practical applications using the sparse multicore solver `HSL_MA87`.

RAL-TR-2010-008 *Generalized Golub-Kahan bidiagonalization and stopping criteria.*
M. Arioli.

The Golub-Kahan bidiagonalization algorithm has been widely used in solving least-squares problems and in the computation of the SVD of rectangular matrices. Here we propose an algorithm based on the Golub-Kahan process for the solution of augmented systems that minimizes the norm of the error and, in particular, we propose a novel estimator of the error similar to the one proposed by Hestenes-Stiefel for the conjugate gradient. This estimator gives a lower bound for the error, and can be used as a reliable stopping criterion for the whole process. We also propose an upper bound of the error base on Gauss-Radau quadrature. Finally, we show how we can transform and optimally precondition augmented systems rising from the mixed finite-element approximation of differential problems.

RAL-TR-2010-011 *An indefinite sparse direct solver for large problems on multicore machines.*
J. D. Hogg and J. A. Scott.

The sparse direct solver `HSL_MA87` uses a DAG-based algorithm to obtain fine-grain parallel execution of the factorization phase on multicore architectures. The first release of the package performed the Cholesky factorization of symmetric positive-definite systems. In this report, we discuss the changes we have made to `HSL_MA87` to accommodate symmetric indefinite systems. The main changes stem from the inclusion of threshold partial pivoting for numerical stability. In particular, we use a new combined factorize_column task that replaces the separate tasks of the Cholesky factorization. Numerical results for a range of practical problems are given to illustrate the effectiveness of the DAG-based approach for solving indefinite linear systems on multicore machines. We find that speedups in excess of 6 can be achieved for some of the largest problems on our 8-core machine.

RAL-TR-2010-016 *Distributed control and constraint preconditioners.*
H. S. Thorne.

Optimization problems with constraints that involve a partial differential equation arise widely in many areas of the sciences and engineering, in particular in problems of design. The solution of such PDE-constrained optimization problems is usually a major computational task. Here we consider simple problems of this type: distributed control problems in which the 2- and 3-dimensional Poisson problem is the PDE. Large dimensional linear systems result from the discretization and need to be solved: these systems are of saddle-point type. We introduce an optimal preconditioner for these systems that leads to convergence of symmetric Krylov subspace iterative methods in a number of iterations which does not increase with the dimension of the discrete problem. These preconditioners are block structured and involve standard multigrid cycles. The optimality of the preconditioned iterative solver is proved theoretically and verified computationally in several test cases. The theoretical proof indicates that these approaches may have much broader applicability for other partial differential equations.

RAL-TR-2010-019 *A preconditioned block conjugate gradient algorithm for computing extreme eigenpairs of symmetric and Hermitian problems.*
E. E. Ovtchinnkov and J. K. Reid.

This report describes an algorithm for the efficient computation of several extreme eigenvalues and corresponding eigenvectors of a large-scale standard or generalized real symmetric or complex Hermitian eigenvalue problem. The main features are: (i) a new conjugate gradient scheme specifically designed for eigenvalue computation; (ii) the use of the preconditioning as a cheaper alternative to matrix factorization for large discretized differential problems; (iii) simultaneous computation of several eigenpairs by subspace iteration; and (iv) the use of efficient stopping criteria based on error estimation rather than the residual tolerance.

RAL-TR-2010-022 *A robust two-level incomplete factorization for (Navier-)Stokes saddle point matrices.*
F. W. Wubs and J. Thies.

We present a new hybrid direct/iterative approach to the solution of a special class of saddle point matrices arising from the discretization of the steady incompressible Navier-Stokes equations on an Arakawa C-grid. The two-level method introduced here has the following properties: (i) it is very robust, even close to the point where the solution becomes unstable; (ii) a single parameter controls fill and convergence, making the method straightforward to use; (iii) the convergence rate is independent of the number of unknowns; (iv) it can be implemented on distributed memory machines in a natural way; (v) the matrix on the second level has the same structure and numerical properties as the original problem, so the method can be applied recursively; (vi) the iteration takes place in the divergence-free space, so the method qualifies as a constraint preconditioner; (vii) the approach can also be applied to Poisson problems. This work is also relevant for problems in which similar saddle point matrices occur, for instance when simulating electrical networks, where one has to satisfy Kirchhoff's conservation law for currents.

RAL-TR-2010-026 *Optimal multilateral well placement.*
C. L. Farmer, J. M. Fowkes and N. I. M. Gould.

One is often faced with the problem of finding the optimal location and trajectory for an oil well. Increasingly this includes the additional complication of optimising the design of a multilateral well. We present a new approach based on the theory of expensive function optimisation.

The key idea is to replace the underlying expensive function (i.e. the simulator response) by a cheap approximation (i.e. an emulator). This enables one to apply existing optimisation techniques to the emulator. Our approach uses a radial basis function interpolant to the simulator response as the emulator. Note that the case of a Gaussian radial basis function is equivalent to the geostatistical method of Kriging and radial basis functions can be interpreted as a single-layer neural network. We use a stochastic model of the simulator response to adaptively refine the emulator and optimise it using a branch and bound global optimisation algorithm.

To illustrate our approach we apply it numerically to finding the optimal location and trajectory of a single multilateral well in a reservoir simulation model using the industry standard ECLIPSE simulator. We compare our results to existing approaches and show that our technique is comparable, if not superior, in performance to these approaches.

RAL-TR-2010-027 *On computing inverse entries of a sparse matrix in an out-of-core environment.*
P. R. Amestoy, I. S. Duff, Y. Robert, F.-H. Rouet, and B. Uçar.

The inverse of an irreducible sparse matrix is structurally full, so that it is impractical to think of computing or storing it. However, there are several applications where a subset of the entries of the inverse is required. Given a factorization of the sparse matrix held in out-of-core storage, we show how to compute such a subset efficiently, by accessing only parts of the factors. When there are many inverse entries to compute, we need to guarantee that the overall computation scheme has reasonable memory requirements, while minimizing the cost of loading the factors. This leads to a partitioning problem that we prove is NP-complete. We also show that we cannot get a close approximation to the optimal solution in polynomial time. We thus need to develop heuristic algorithms, and we propose: (i) a lower bound on the cost of an optimum solution; (ii) an exact algorithm for a particular case; (iii) two other heuristics for a more general case; and (iv) hypergraph partitioning models for the most general setting. We illustrate the performance of our algorithms in practice using the `MUMPS` software package on a set of real-life problems as well as some standard test matrices. We show that our techniques can improve the execution time by a factor of 50.

RAL-TR-2010-029 *On the oracle complexity of first-order and derivative-free algorithms for smooth nonconvex minimization.*
C. Cartis, N. I. M. Gould and Ph. L. Toint.

The (optimal) function/gradient evaluations worst-case complexity analysis available for the Adaptive Regularizations algorithms with Cubics (ARC) for nonconvex smooth unconstrained optimization is extended to finite-difference versions of this algorithm, yielding complexity bounds for first-order and derivative free methods applied on the same problem class. A comparison with the results obtained for derivative-free methods by Vicente (2010) is also discussed, giving some theoretical insight on the relative merits of various methods in this popular class of algorithms.

RAL-TR-2010-030 *Evaluation complexity of adaptive cubic regularization methods for convex unconstrained optimization.*
C. Cartis, N. I. M. Gould and Ph. L. Toint.

The adaptive cubic regularization algorithms described in Cartis, Gould & Toint (2009, 2010) for unconstrained (nonconvex) optimization are shown to have improved worst-case efficiency in terms of the function- and gradient-evaluation count when applied to convex and strongly convex objectives. In particular, our complexity upper bounds match in order (as a function of the accuracy of approximation), and sometimes even improve, those obtained by Nesterov (2004, 2008) and Nesterov & Polyak (2006) for these same problem classes, without employing the Hessian's Lipschitz constant explicitly in the algorithms or requiring exact or global solution of the subproblem. An additional outcome of our approximate approach is that our complexity results can naturally capture the advantages of both first- and second-order methods.

RAL-TR-2010-031 *A modern analyse phase for sparse tree-based direct methods.*
J. D. Hogg and J. A. Scott.

The analyse phase of a sparse direct solver for symmetrically structured linear systems of equations is used to determine the sparsity pattern of the matrix factor. This allows the subsequent numerical factorization and solve phases to be executed efficiently. The analyse phase typically involves identifying supernodes, amalgamating supernodes to form relaxed supernodes and computing their variable lists, and determining the assembly tree.

Two main approaches have been used. The first, based on the initial work of Duff and Reid in the early 1980s, originates from their development of the multifrontal method. This approach emphasises the identification of supervariables of A and, in later versions, handles pre-specified 2×2 block pivots; it has been successfully used in both out-of-core and parallel solvers. The second approach, following the work of Gilbert, Ng and Peyton a decade or so later, adopts a graph theoretic view of assembled matrices, exploiting this to determine column counts for the matrix factor without finding the explicit pattern of the factor. This allows supernodes to be amalgamated before a symbolic factorization is performed, leading to significant savings in the analyse time.

The aims of this paper are two-fold: to incorporate supervariables into the Gilbert, Ng and Peyton approach and to describe an adaptation for matrices in elemental form (such as arise in finite-element applications), without explicitly assembling the system matrix. Various implementation details designed to enhance performance are described. Modifications to support block pivots are introduced. Numerical experiments using problems from practical applications are used throughout and demonstrate that it is advantageous, in terms of both memory and time, to work directly with the elemental form.

RAL-P-2011-001 *Preconditioners based on strong components.*
I. S. Duff and K. Kaya.

This paper proposes an approach for obtaining block triangular preconditioners that can be used for solving a linear system $\mathbf{Ax} = \mathbf{b}$ where $\mathbf{A}$ is a large, nonsingular, real, $n \times n$ sparse matrix. The proposed approach uses Tarjan's algorithm for hierarchically decomposing a digraph into its strong components. To the best of our knowledge, this is the first work that uses Tarjan's algorithm for preconditioning purposes. We describe the method, analyse its performance, and compare it with preconditioners from the literature such as `ILUT` and `XPABLO` and show that it is the best preconditioner for many matrices.

RAL-TR-2011-002 *Complexity bounds for second-order optimality in unconstrained optimization.*
C. Cartis, N. I. M. Gould and Ph. L. Toint.

This paper examines worst-case evaluation bounds for finding weak minimizers in unconstrained optimization. For the cubic regularization algorithm, Nesterov & Polyak (2006) and Conn, Gould & Toint (2010) show that at most $O(\epsilon^{-3})$ iterations may have to be performed for finding an iterate which is within ϵ of satisfying second-order optimality conditions. We first show that this bound can be derived for a version of the algorithm which only uses one-dimensional global optimization of the cubic model and that it is sharp. We next consider the standard trust-region method and show that a bound of the same type may also be derived for this method, and that it is also sharp in some cases. We conclude by showing that a comparison of the worst-case behaviour of the ARC and trust-region algorithms favours the first of these methods.

RAL-TR-2011-005 *On the evaluation complexity of composite function minimization with applications to nonconvex nonlinear programming.*
C. Cartis, N. I. M. Gould and Ph. L. Toint.

We estimate the worst-case complexity of minimizing an unconstrained, nonconvex composite objective with a structured nonsmooth term by means of some first-order methods. We find that it is unaffected by the nonsmoothness of the objective in that a first-order trust-region or quadratic regularization method applied to it takes at most $\mathcal{O}(\epsilon^{-2})$ function-evaluations to reduce the size of a first-order criticality measure below ϵ. Specializing this result to the case when the composite objective is an exact penalty function allows us to consider the objective- and constraint-evaluation worst-case complexity of nonconvex equality-constrained optimization when the solution is computed using a first-order exact penalty method. We obtain that in the reasonable case when the penalty parameters are bounded, the complexity of reaching within ϵ of a KKT point is at most $\mathcal{O}(\epsilon^{-2})$ problem-evaluations, which is the same in order as the function-evaluation complexity of steepest-descent methods applied to unconstrained, nonconvex smooth optimization.

RAL-TR-2011-006 *Corrigendum: nonlinear programming without a penalty function or a filter.*
N. I. M. Gould, D. P. Robinson 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 filter, and yet can be proved to be globally convergent to first-order stationary points. It uses different trust-regions to cope with the nonlinearity of the objective and constraint functions, 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-2011-007 *Updating the regularization parameter in the adaptive cubic regularization algorithm.*
N. I. M. Gould, M. Porcelli and Ph. L. Toint.

The adaptive cubic regularization method (Cartis, Gould & Toint, Math. Programming, DOI: 10.1007/s10107-009-0286-5 & 10.1007/s10107-009-0337-y) has been recently proposed for solving unconstrained minimization problems. At each iteration of this method, the objective function is replaced by a cubic approximation which comprises an adaptive regularization parameter whose role is related to the local Lipschitz constant of the objective's Hessian. We present new updating strategies for this parameter based on interpolation techniques, which improve the overall numerical performance of the algorithm. Numerical experiments on large nonlinear least-squares problems are provided.

RAL-TR-2011-008 *On the complexity of finding first-order critical points in constrained nonlinear optimization.*
C. Cartis, N. I. M. Gould and Ph. L. Toint.

The complexity of finding ϵ-approximate first-order critical points for the general smooth constrained optimization problem is shown to be no worse that $O(\epsilon^{-2})$ in terms of function and constraints evaluations. This result is obtained by analyzing the worst-case behaviour of a first-order shorts-step homotopy algorithm consisting of a feasibility phase followed by an optimization phase, and requires minimal assumptions on the objective function. Since a bound of the same order is known to be valid for the unconstrained case, this leads to the conclusion that the presence of possibly nonlinear/nonconvex inequality/equality constraints is irrelevant for this bound to apply.

RAL-TR-2011-009 *How good are extrapolated bi-projection methods for linear feasibility problems?*
N. I. M. Gould.

We consider extrapolated projection methods for solving linear feasibility problems. Both successive and sequential methods of a two-set projection scheme are examined. The best algorithm in the class of algorithms that we considered was an extrapolated sequential method. When this was compared to an interior point method using the CUTEr/Netlib linear programming test problems it was found that the bi-projection method was fastest (or equal fastest) for 31% of the cases, while the interior point code was fastest in 71% of the cases. The interior-point method succeeded on all examples, but the best bi-projection method considered here failed to solve 37% of the problems within reasonable CPU time or iteration thresholds.

RAL-TR-2011-010 *Chebyshev acceleration of iterative refinement.*
M. Arioli and J. A. Scott.

We analyse how variants of the Chebyshev algorithm can be used to accelerate the iterative refinement procedure without loss of numerical stability and at a computational cost at each iteration that is only marginally greater than that of iterative refinement. An error analysis of the procedure is presented and numerical tests on selected sparse test problems are used to corroborate the theory and illustrate the potential savings offered by Chebyshev acceleration.

RAL-TR-2011-011 *Optimal Newton-type methods for nonconvex smooth optimization problems.*
C. Cartis, N. I. M. Gould and Ph. L. Toint.

We consider a general class of second-order iterations for unconstrained optimization that includes regularization and trust-region variants of Newton's method. For each method in this class, we exhibit a smooth, bounded-below objective function, whose gradient is globally Lipschitz continuous within an open convex set containing any iterates encountered and whose Hessian is $\alpha-$Hölder continuous (for given $\alpha \in [0,1]$) on the path of the iterates, for which the method in question takes at least $\lfloor \epsilon^{-(2+\alpha)/(1+\alpha)} \rfloor$ function-evaluations to generate a first iterate whose gradient is smaller than ϵ in norm. This provides a lower bound on the evaluation complexity of second-order methods in our class when applied to smooth problems satisfying our assumptions. Furthermore, for $\alpha = 1$, this lower bound is of the same order in ϵ as the upper bound on the evaluation complexity of cubic regularization, thus implying cubic regularization has optimal worst-case evaluation complexity within our class of second-order methods

RAL-TR-2011-015 *Guidelines for the development of HSL software, 2011 version.*
J. D. Hogg, J. K. Reid and J. A. Scott

HSL is a collection of portable, fully documented, and tested packages for large-scale scientific computation. HSL is primarily written in Fortran; MATLAB and C interfaces are available for some packages. 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.

This version supersedes RAL-TR-2008-027.

RAL-TR-2011-016 *A note about the complexity of minimizing Nesterov's smooth Chebyshev-Rosenbrock function.*
C. Cartis, N. I. M. Gould and Ph. L. Toint.

This short note considers and resolves the apparent contradiction between known worst-case complexity results for first and second-order methods for solving unconstrained smooth nonconvex optimization problems and a recent note by Jarre (2011) implying a very large lower bound on the number of iterations required to reach the solution's neighbourhood for a specific problem with variable dimension.

RAL-TR-2011-017 *Trajectory-following methods for large-scale degenerate quadratic programming.*
N. I. M. Gould, D. Orban and D. P. Robinson.

We consider a class of infeasible, path-following methods for convex quadratic programming. Our methods are designed to be effective for solving both nondegenerate and degenerate problems, where degeneracy is understood to mean the failure of strict complementarity at a solution. Global convergence and a polynomial bound on the number of iterations required is given. An implementation, `CQP`, is available as part of GALAHAD. We illustrate the advantages of our approach on the CUTErand Maros-Meszaros test sets.

RAL-TR-2011-020 *A branch and bound algorithm for the global optimization of Hessian Lipschitz continuous functions.*
J. M. Fowkes, N. I. M. Gould and C. L. Farmer.

We present a branch and bound algorithm for the global optimization of a twice differentiable nonconvex objective function with a Lipschitz continuous Hessian over a compact, convex set. The algorithm is based on applying cubic regularisation techniques to the objective function within an overlapping branch and bound algorithm for convex constrained global optimization. Unlike other branch and bound algorithms, lower bounds are obtained via nonconvex underestimators of the function. For a numerical example, we apply the proposed branch and bound algorithm to radial basis function approximations.

RAL-TR-2011-022 *A fast method for binary programming using first order derivatives, with application to topology optimization with buckling constraints.*
P. A. Browne, C. J. Budd, N. I. M. Gould, H. A. Kim and J. A. Scott.

We present a method for finding solutions of large-scale binary programming problems where the calculation of derivatives is very expensive. We then apply this method to a topology optimization problem of weight minimisation subject to compliance and buckling constraints. We derive an analytic expression for the derivative of the stress stiffness matrix with respect to the density of an element in the finite-element setting. Results are presented for a number of two-dimensional test problems.

RAL-TR-2011-023 *European Exascale Software Initiative: numerical libraries, solvers and algorithms.*
I. S. Duff.

Computers with sustained Petascale performance are now available and it is expected that hardware will be developed with a peak capability in the Exascale range by around 2018. However, the complexity, hierarchical nature, and probable heterogeneity of these machines pose great challenges for the development of software to exploit these architectures.

This was recognized some years ago by the IESP (International Exascale Software Project) initiative and the European response to this has been a collaborative project called EESI (European Exascale Software Initiative). This initiative began in 2010 and has submitted its final report to the European Commission with a final conference in Barcelona in October 2011. The main goals of EESI are to build a European vision and roadmap to address the international outstanding challenge of performing scientific computing on the new generation of computers.

The main activity of the EESI is in eight working groups, four on applications and four on supporting technologies. We first briefly review these eight chapters before discussing in more detail the work of Working Group 4.3 on Numerical Libraries, Solvers and Algorithms. Here we will look at the principal areas, the challenges of Exascale and possible ways to address these, and the resources that will be needed.

RAL-TR-2011-024 *`HSL_MA97`: a bit-compatible multifrontal code for sparse symmetric systems.*
J. D. Hogg and J. A. Scott.

The multifrontal method is widely used for the numerical solution of large sparse symmetric linear systems of equations. In this report, we discuss the design and implementation of a new multifrontal code `HSL_MA97`. Our motivation for the new code is discussed along with the key design features. `HSL_MA97` is for real and complex problems and is designed to be efficient for both positive-definite and indefinite systems. `HSL_MA97` can be run in serial or in a shared memory environment using OpenMP. An important feature is that in parallel it offers bit-compatible solutions. Numerical results are presented for a range of problems from practical applications and comparisons are made with existing codes. Future plans for `HSL_MA97` are outlined.

RAL-TR-2011-026 *Guidelines for the development of MATLAB interfaces for HSL packages (revised for MATLAB 2011a).*
M. Arioli, I. S. Duff, J. D. Hogg and H. S. Thorne.

In this report, we describe the modus operandi for providing MATLAB interfaces for HSL and GALAHAD codes. We discuss the file structure for the MATLAB interface and how the file should be constructed. We also provide details of the `HSL_MATLAB` package, the user documentation of which complements this report, and discuss how the user can install the resulting software. This report supersedes the previous guidelines for MATLAB interfaces in report RAL-TR-2010-013.

Internal Report 2011-1 *C interfaces to HSL routines.*
J. D. Hogg.

The C programming language is widely used and can be interfaced to almost every serious numerical computational language in existence. By implementing a C interface to HSL routines the number of people able to use HSL software is signicantly increased. Interfacing C and Fortran 77 code in a portable fashion is a non-trivial problem that has a number of established solutions, such as the use of GNU autotools. Fortran 90 introduced modules and derived types that are not catered for by these approaches. Therefore extra attention is required to allow ready use of such software from C. This guide is aimed at HSL developers and both describes how to use standards-compliant interoperability mechanisms for, and recommendations on the implementation of, consistent C interfaces to HSL routines.

4 Publications

P. Amestoy, A. Buttari, I. S. Duff, A. Guermouche, J.-Y. L'Excellent and B. Uçar "MUMPS". To appear in *Encyclopedia of Parallel Computing*, D. Padua (Editor).

P. Amestoy, A. Buttari, I. S. Duff, A. Guermouche, J.-Y. L'Excellent and B. Uçar "The multifrontal method". To appear in *Encyclopedia of Parallel Computing*, D. Padua (Editor).

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5 HSL and GALAHAD

5.1 HSL

John Reid has now fully retired from maintenance of the HSL library, and his responsibilities have been passed to Jonathan. A new release, HSL 2011, was made in February 2011 and included a new website, a ‘package at once’ distribution method and the first C and MATLAB interfaces. A new back-end tool, `hsladmin`, has been written to automate the preparation of HSL packages before release. This includes a decision to use the same standard format for the input of user data to each new sparse matrix package, with checking and conversion routines provided by a new package `HSL_MC69`. The aim here is to make it very easy for user’s to run a scaling and/or ordering package before running a linear solver and also to try out more than one solver with minimal changes to the interface.

Since the launch of HSL 2011, there have been over 1500 downloads from over 750 users at over 500 different universities and companies in 70 countries.

In this section, the new packages that have been made available since January 2010 are described, together with the major changes to older packages made since the same date.

5.1.1 New packages

`HSL_EA20` is a suite of Fortran 95 procedures for computing the product of the s-root of a sparse self-adjoint positive-definite matrix by a vector using a scalar product derived by a second symmetric positive-definite matrix. Given two $n \times n$ symmetric positive-definite matrices $\mathbf{A}$ and $\mathbf{M}$, and a vector $\mathbf{u}$, the package uses the Lanczos method, applied to the matrix pencil $(\mathbf{M}, \mathbf{A})$, to approximate

$$\left(\mathbf{M}^{-1}\mathbf{A}\right)^s \mathbf{u}, \quad s \in (-1, 1).$$

Reverse communication is used. Control is returned to the user for the products of $\mathbf{A}$ with a vector $\mathbf{z}$, of $\mathbf{M}$ with a vector $\mathbf{x}$, or of $\mathbf{M}^{-1}$ with a vector $\mathbf{w}$.

`HSL_MA86` uses a direct method to solve large sparse symmetric indefinite linear systems of equations $\mathbf{AX} = \mathbf{B}$. This package uses OpenMP and is designed for multicore architectures. It computes the sparse factorization

$$\mathbf{A} = \mathbf{PLD}(\mathbf{PL})^*$$

where $\mathbf{L}^* = \mathbf{L}^\mathbf{T}$ (real symmetric or complex symmetric) or $\mathbf{L}^* = \mathbf{L}^\mathbf{H}$ (complex Hermitian, where $\mathbf{L}^\mathbf{H}$ denotes the conjugate transpose of $\mathbf{L}$), $\mathbf{P}$ is a permutation matrix, $\mathbf{L}$ is unit lower triangular, and $\mathbf{D}$ is block diagonal with blocks of size 1×1 and 2×2. The efficiency of `HSL_MA86` is dependent on the user-supplied elimination order. The HSL package `HSL_MC68` may be used to obtain a suitable ordering. The lower triangular part of $\mathbf{A}$ must be supplied in compressed sparse column format. The

HSL package `HSL_MC69` may be used to convert data held in other sparse matrix formats and also to check the user's matrix data for errors. If $\mathbf{A}$ is known to be positive definite (so that pivoting for numerical stability is not required), we recommend `HSL_MA87`.

`HSL_MA97` uses a direct method to solve large sparse symmetric linear systems of equations $\mathbf{AX} = \mathbf{B}$. This package optionally uses OpenMP and is designed to achieve bit-compatible results regardless of the number of threads used. It computes the sparse factorization

$$\mathbf{A} = \mathbf{PLD}(\mathbf{PL})^\star \qquad \text{(Indefinite)}$$

or

$$\mathbf{A} = \mathbf{PLL}^\star \qquad \text{(Positive-definite)}$$

where $\mathbf{L}^\star = \mathbf{L}^T$ (real symmetric or complex symmetric) or $\mathbf{L}^\star = \mathbf{L}^H$ (complex Hermitian, where $\mathbf{L}^H$ denotes the conjugate transpose of $\mathbf{L}$), $\mathbf{P}$ is a permutation matrix, $\mathbf{L}$ is lower triangular, and $\mathbf{D}$ is block diagonal with blocks of size 1×1 and 2×2.

If $\mathbf{A}$ is large, bit-compatible answers are not required, we recommend using `HSL_MA86` or `HSL_MA87` instead for better efficiency.

`HSL_MC56` To read a file containing a sparse matrix held in Rutherford-Boeing format and manipulate it to the desired sparse matrix format. The user may specify the storage format the matrix is returned in, and random values can be optionally generated to match the matrix pattern. Rutherford-Boeing format can be used to specify either matrix data or supplementary data, however this package only supports matrix data. To read supplementary data, the HSL routine `MC56` can be used. To write data in Rutherford-Boeing format the HSL routines `MC54` and `MC55` can be used for matrix data and supplementary data, respectively.

`HSL_MC69` offers routines for converting matrices held in a number of sparse matrix formats to the compressed sparse column (CSC) format used by many HSL routines. This format requires the entries within each column of $\mathbf{A}$ to be ordered by increasing row index. For symmetric, skew symmetric or Hermitian matrices, only entries in the lower triangle are held. This format is the one used by many of the recent HSL packages; we shall refer to it as the standard HSL format.

Routines are offered for converting matrices held in lower or upper compressed sparse column format or in lower or upper compressed sparse row format or in coordinate format, and for verification and correction of matrices believed to already be in standard HSL format. The conversion routines check the user-supplied data for errors and handle duplicate entries (they are summed) and out-of-range entries (they are discarded).

`HSL_MC78` Given an elimination order, `HSL_MC78` performs common tasks required in the analyse phase of a symmetric sparse direct solver. Either the entire analyse may be performed or individual tasks. No checking is performed on the validity of user data, and failure to supply valid data will result in undefined behaviour.

Given the sparsity pattern of a sparse symmetric matrix $\mathbf{A}$ and permutation $\mathbf{P}$, `HSL_MC78` finds the pattern of the Cholesky factor $\mathbf{L}$ such that $\mathbf{PAP}^{-1} = \mathbf{LL}^T$. The pattern of $\mathbf{A}$ may be provided in either assembled or elemental format. The permutation $\mathbf{P}$ is referred to as the *elimination (pivot) order.*

To reduce the amount of matrix data read during the analysis, supervariables of $\mathbf{A}$ may be identified. A *supervariable* is a set of columns of $\mathbf{A}$ that have the same sparsity pattern.

An *elimination tree* is built that describes the structure of the Cholesky factor in terms of data dependence between pivotal columns. This allows permutations of the elimination order that do not affect the number of entries in $\mathbf{L}$ to be identified and allows fast algorithms to be used in determining the exact structure of $\mathbf{L}$.

A *supernode* is a set of columns that have the same pattern in the matrix **L**. This pattern is stored as a single row list for each supernode. The condensed version of the elimination tree consisting of supernodes is referred to as the *assembly tree*. To increase efficiency in a subsequent factorization phase, supernodes may be merged through a supernode amalgamation heuristic.

`HSL_MC78` supports the use of 2 × 2 and larger block pivots.

`HSL_MC79` Given the sparsity pattern of a rectangular sparse matrix $\mathbf{A} = \{a_{ij}\}_{m\times n}$, `HSL_MC79` has entries to compute a maximum matching, and a row permutation **P** and column permutation **Q** such that **PAQ** is of block triangular form: a coarse Dulmage-Mendelsohn decomposition and a fine Dulmage-Mendelsohn decomposition are available.

A *matching* is a set of the rows $\mathcal{R}$ and columns $\mathcal{C}$, where each row in $i \in \mathcal{R}$ is paired with a unique $j \in \mathcal{C}$ subject to $a_{ij} \neq 0$. The size of a matching is defined to be equal to the number of columns in $\mathcal{C}$. A *maximum matching* of **A** is a matching of **A** that has size greater than or equal to any other matching of **A**. The size of the maximum matching is equal to the *structural rank* of the matrix.

The *Dulmage-Mendelsohn decomposition* consists of a row permutation **P** and a column permutation Q such that

$$\mathbf{PAQ} = \begin{array}{c} \\ \mathcal{R}_1 \\ \mathcal{R}_2 \\ \mathcal{R}_3 \end{array} \begin{array}{c} \begin{array}{ccc} \mathcal{C}_1 & \mathcal{C}_2 & \mathcal{C}_3 \end{array} \\ \left[\begin{array}{ccc} A_1 & A_4 & A_6 \\ 0 & A_2 & A_5 \\ 0 & 0 & A_3 \end{array}\right] \end{array},$$

where A_1, formed by the rows in the set $\mathcal{R}_1$ and the columns in the set $\mathcal{C}_1$, is an underdetermined matrix with m_1 rows and n_1 columns ($m_1 < n_1$ or $m_1 = n_1 = 0$); A_2, formed by the rows in the set $\mathcal{R}_2$ and the columns in the set $\mathcal{C}_2$, is a square, well-determined matrix with m_2 rows; A_3, formed by the rows in the set $\mathcal{R}_3$ and the columns in the set $\mathcal{C}_3$, is an overdetermined matrix with m_3 rows and n_3 columns ($m_3 > n_3$ or $m_3 = n_3 = 0$). In particular, let the set of rows $\mathcal{R}$ and the set of columns $\mathcal{C}$ form a maximum matching of **A**. The sets $\mathcal{R}_1$ and $\mathcal{R}_2$ are subsets of $\mathcal{R}$, and $\mathcal{R}_3 \cap \mathcal{R}$ has n_3 entries. The sets $\mathcal{C}_2$ and $\mathcal{C}_3$ are subsets of $\mathcal{C}$, and $\mathcal{C}_1 \cap \mathcal{C}$ has m_1 entries.

The *coarse Dulmage-Mendelsohn decomposition* orders the unmatched columns as the first columns in **PAQ** and orders the unmatched rows as the last rows in **PAQ**. The output from the coarse Dulmage-Mendelsohn decomposition can be used to find a node separator from an edge separator of a graph.

The *fine Dulmage-Mendelsohn decomposition* computes a row permutation **P** and a column permutation **Q** such that A_1 and A_3 are block diagonal and each diagonal block is irreducible, and A_2 is block upper triangular with strongly connected (square) diagonal blocks. If **A** is reducible and nonsingular, the fine Dulmage-Mendelsohn decomposition of a matrix **A** can be used to solve the linear systems $\mathbf{Ax} = \mathbf{b}$ with block back-substitution.

`HSL_ME57` To solve a sparse complex symmetric or Hermitian system of linear equations. Given a sparse complex symmetric or Hermitian matrix $\mathbf{A} = \{a_{ij}\}_{n\times n}$ and an n-vector **b** or a matrix $\mathbf{B} = \{b_{ij}\}_{n\times r}$, this subroutine solves the system $\mathbf{Ax} = \mathbf{b}$ or the system $\mathbf{AX} = \mathbf{B}$. The matrix **A** can be either complex symmetric or Hermitian. There is an option for iterative refinement.

The multifrontal method is used. `HSL_ME57` is a complex version of the code `HSL_MA57`. It is a direct method based on a sparse variant of Gaussian elimination and is discussed further by Duff and Reid, ACM Trans. Math. Software **9** (1983), 302-325. A detailed discussion on the `MA57` strategy and performance is given by Duff, ACM Trans. Math. Software **30** (2004), 118-144. Relevant work on pivoting and scaling strategies is given by Duff and Pralet, SIAM Journal Matrix Analysis and Applications **27** (2005), 313-340. More recent work on static pivoting is given by Duff and Pralet, SIAM Journal Matrix Analysis and Applications **29** (2007), 1007-1024.

The `HSL_ME57` package has a range of options including several sparsity orderings, multiple right-hand sides, partial solutions, error analysis, scaling, a matrix modification facility, 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.

The package has 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.

`HSL_MI27` This package uses the projected preconditioned conjugate gradient method to solve $(n+m)\times(n+m)$ saddle-point systems of the form

$$\begin{bmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & -\mathbf{C} \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} = \begin{bmatrix} \mathbf{C} \\ \mathbf{d} \end{bmatrix},$$

where $\mathbf{A}$ is an $n \times n$ real and symmetric matrix, $\mathbf{C}$ is an $m \times m$ real, symmetric and positive semi-definite (possibly zero) matrix, and $m \leq n$. A preconditioner of the form

$$\mathbf{P} = \begin{bmatrix} \mathbf{G} & \mathbf{B}^T \\ \mathbf{B} & -\mathbf{C} \end{bmatrix}$$

must be available where $\mathbf{G}$ is a real and symmetric matrix. The following assumptions are assumed to hold:

- if $\mathbf{C}$ is positive definite, both $\mathbf{A}+\mathbf{B}^T\mathbf{C}^{-1}\mathbf{B}$ and $\mathbf{G}+\mathbf{B}^T\mathbf{C}^{-1}\mathbf{B}$ are positive definite;
- if $\mathbf{C}=0$ and the columns of the $n \times (n-m)$ matrix $\mathbf{Z}$ span the nullspace of $\mathbf{B}$, both $\mathbf{Z}^T\mathbf{A}\mathbf{Z}$ and $\mathbf{Z}^T\mathbf{G}\mathbf{Z}$ are positive definite;
- if $\mathbf{C}=\mathbf{E}\mathbf{D}\mathbf{E}^T$, where $\mathbf{d}$ is a $p \times p$ nonsingular matrix with $0 < p < m$, the columns of the $m \times (m-p)$ matrix $\mathbf{F}$ span the nullspace of $\mathbf{C}$ and the columns of the $n \times (n-m+p)$ matrix $\mathbf{Z}$ span the nullspace of $\mathbf{F}^T\mathbf{B}$, then both $\mathbf{Z}^T\left(\mathbf{A}+\mathbf{B}^T\mathbf{E}\mathbf{D}^{-1}\mathbf{E}^T\mathbf{B}\right)\mathbf{Z}$ and $\mathbf{Z}^T\left(\mathbf{G}+\mathbf{B}^T\mathbf{E}\mathbf{D}^{-1}\mathbf{E}^T\mathbf{B}\right)\mathbf{Z}$ are positive definite.

If these assumptions do not hold, then negative curvature may occur and, consequently, the method terminates with an error.

The projected preconditioned conjugate gradient method iteratively finds the vector $\mathbf{x}$ and then, once $\mathbf{x}$ has been computed to a high enough level of accuracy, the vector $\mathbf{y}$ is computed by performing one additional solve with the preconditioner $\mathbf{P}$. Reverse communication is used for preconditioning and matrix-vector products of the form $\mathbf{As}$, $\mathbf{Bs}$, $\mathbf{B}^T\mathbf{s}$ and $\mathbf{Cs}$. `HSL_MI13` may be used to efficiently form suitable preconditioners and carry out the required preconditioning solves; `HSL_MC65` may be used to form the required matrix-vector products. `HSL_MI13` and `HSL_MC65` are both available as part of `HSL 2011`.

5.1.2 Changed packages

`HSL_EA19` uses a subspace iteration method to compute the leftmost eigenvalues and corresponding eigenvectors of a real symmetric (or Hermitian) operator $\mathbf{A}$ acting in the n-dimensional real (or complex) Euclidean space R^n, or, more generally, of the problem

$$\mathbf{Ax} = \lambda\mathbf{Bx},$$

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

The convergence may be accelerated by the provision of a symmetric positive-definite operator $\mathbf{T}$ that approximates the inverse of $(\mathbf{A} - \sigma\mathbf{B})$ for a value of σ that does not exceed the leftmost eigenvalue. Computation time may also be reduced by supplying vectors that are good approximations to some of the eigenvectors.

`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.

5.2 MATLAB Interfaces to HSL

New mex interfaces for the HSL packages `MA57`, `HSL_MA86`, `HSL_MA87`, `HSL_MA97`, `HSL_MC64`, `HSL_MC73`, `ME57` and `HSL_MI20` have been written. Some of these are new, while others are based on old beta-release interfaces that have undergone significant upgrades to support the forced migration of mex dependency from the g95 to the gfortran compiler and the issues that then arose for 64-bit platforms.

These interfaces are supported by the new `HSL_MATLAB` that was developed to provide a type-safe and forwards compatible wrapper to the MATLAB API. Guidelines for the development of HSL interfaces are given in the report RAL-TR-2011-026.

5.3 C Interfaces to HSL

For the first time, C interfaces to some HSL packages are now being offered. In particular, C interfaces for `HSL_MA77`, `HSL_MA86`, `HSL_MA87`, `HSL_MA97`, `HSL_MC68`, `HSL_MC69` and `HSL_MI20` have been written.

Guidelines for the development of C interfaces to HSL packages are given in the Numerical Analysis Group internal report 2011-1.

5.4 GALAHAD

Version 2.4 of GALAHAD was released in January 2011. This included support for shared-memory parallelism using OpenMP and hooks for further external software were added. In addition, a major overhaul of makefiles and numerous improvements to existing packages was performed. New packages include:

`CQP:` This package uses an primal-dual interior-point method to solve the *convex quadratic programming problem*

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

subject to the general linear constraints

$$c_i^l \leq \mathbf{a}_i^T\mathbf{x} \leq c_i^u, \quad i = 1, \ldots, m,$$

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, positive-semi-definite matrix $\mathbf{H}$, the vectors $\mathbf{g}$, $\mathbf{a}_i$, $\mathbf{c}^l$, $\mathbf{c}^u$, $\mathbf{x}^l$, $\mathbf{x}^u$ and the scalar f are given. Any of the constraint bounds c_i^l, c_i^u, x_j^l and x_j^u may be infinite. Full advantage is taken of any zero coefficients in the matrix $\mathbf{H}$ or the matrix $\mathbf{A}$ of vectors $\mathbf{a}_i$.

`QP:` This package provides a common interface to other GALAHAD packages for solving the *quadratic programming problem*

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

subject to the general linear constraints

$$c_i^l \leq \mathbf{a}_i^T\mathbf{x} \leq c_i^u, \quad i = 1, \ldots, m,$$

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 $\mathbf{H}$, the vectors $\mathbf{g}$, $\mathbf{a}_i$, $\mathbf{c}^l$, $\mathbf{c}^u$, $\mathbf{x}^l$, $\mathbf{x}^u$ and the scalar f are given. Any of the constraint bounds c_i^l, c_i^u, x_j^l and x_j^u may be infinite. Full advantage is taken of any zero coefficients in the matrix $\mathbf{H}$ or the matrix $\mathbf{A}$ of vectors $\mathbf{a}_i$.

`SCALE:` This package calculates and applies shift and scale factors for the variables and constraints to try to equilibrate the *quadratic programming problem*

$$\text{minimize } \; \tfrac{1}{2}\mathbf{x}^T\mathbf{H}\mathbf{x} + \mathbf{g}^T\mathbf{x} + f \tag{1}$$

subject to the general linear constraints

$$c_i^l \leq \mathbf{a}_i^T\mathbf{x} \leq c_i^u, \quad i = 1, \ldots, m, \tag{2}$$

and the simple bound constraints

$$x_j^l \leq x_j \leq x_j^u, \quad j = 1, \ldots, n, \tag{3}$$

where the n by n symmetric matrix $\mathbf{H}$, the vectors $\mathbf{g}$, $\mathbf{a}_i$, $\mathbf{c}^l$, $\mathbf{c}^u$, $\mathbf{x}^l$, $\mathbf{x}^u$ and the scalar f are given. Full advantage is taken of any zero coefficients in the matrix $\mathbf{H}$, as well as the matrix $\mathbf{A}$, whose rows are the vectors $\mathbf{a}_i^T$, $i = 1, \ldots, m$. Any of the constraint bounds c_i^l, c_i^u, x_j^l and x_j^u may be infinite.

The derived type is also capable of supporting parametric quadratic programming problems, in which an additional objective term $\theta\delta\mathbf{g}^T\mathbf{x} + \theta\delta f$ is included, and the trajectory of solution are required for all $0 \leq \theta \leq \theta_{\max}$ for which

$$c_i^l + \theta\delta c_i^l \leq \mathbf{a}_i^T\mathbf{x} \leq c_i^u + \theta\delta c_i^u, \quad i = 1, \ldots, m,$$

and

$$x_j^l + \theta x_j^l \leq x_j \leq x_j^u + \delta x_j^u, \quad j = 1, \ldots, n.$$

New variables $\mathbf{X}_s^{-1}(\mathbf{x} - \mathbf{x}_s)$ are calculated, involving the matrix of diagonal variable scaling factors $\mathbf{X}_s$ and a corresponding vector of shifts $\mathbf{x}_s$. Likewise the constraint values are transformed to be $\mathbf{C}_s^{-1}(\mathbf{A}\mathbf{x} - \mathbf{c}_s)$, involving the matrix of diagonal constraint scaling factors $\mathbf{C}_s$ and vector of corrsponding shifts $\mathbf{c}_s$. The value of the objective function is transformed to be $F_s^{-1}(q(x) - f_s)$ using an objective scaling factor F_s and shift f_s.

`SLS:` This package *solves dense or sparse symmetric systems of linear equations* using variants of Gaussian elimination. Given a sparse symmetric matrix $\mathbf{A} = \{a_{ij}\}_{n\times n}$, and an n-vector $\mathbf{b}$ or a matrix $\mathbf{B} = \{b_{ij}\}_{n\times r}$, this subroutine solves the system $\mathbf{A}\mathbf{x} = \mathbf{b}$ or the system $\mathbf{A}\mathbf{X} = \mathbf{B}$. The matrix $\mathbf{A}$ need not be definite.

The method provides a common interface to a variety of well-known solvers from HSL and elsewhere. Currently supported solvers include `MA27/SILS`, `HSL_MA57`, `HSL_MA77` , `HSL_MA86`, `HSL_MA87` and `HSL_MA97` from HSL, `PARDISO` from the Pardiso Project and `WSMP` from the IBM alpha Works, as well as `POTR`, `SYTR` and `SBTR` from LAPACK. Note that the solvers themselves do not form part of this package and must be obtained separately. Dummy instances are provided for solvers that are unavailable. Also note that additional flexibility may be obtained by calling the solvers directly rather that via this package.

5.5 MATLAB Interfaces to GALAHAD

New mex interfaces for the GALAHAD packages `BQP`, `CQP`, `EQP`, `QP`, `QPA`, `QPB` and `SBLS` have been written, and significant upgrades have been made to other interfaces to support the forced migration of Mex dependency from the g95 to the gfortran compiler and the issues that then arose for 64-bit platforms.

6 Conference and workshop presentations

15 March 2010, SANUM 2010. The 34th Annual South African Symposium on Numerical and Applied Mathematics, Stellenbosch, South Africa.
I. S. Duff, *The solution of really large linear systems arising from discretizations of three-dimensional problems.*

14 April 2010, ICFD Conference on Numerical Methods for Fluid Dynamics, Reading.
H. S. Thorne, *Challenges from PDE-constrained optimization and some methods to circumvent these issues.*

21 May 2010, III Workshop G-HPC 2010: High Performance Computing Applications, Vigo, Spain.
I. S. Duff, *The solution of really large linear systems arising from discretizations of three-dimensional problems.*

15 June 2010, Sparse Days 2010, Toulouse.
M. Arioli, *Generalized Golub-Kahan bidiagonalization and stopping criteria.*

15 June 2010, Sparse Days 2010, Toulouse.
J. A. Scott, *The multicore challenge: the sparse indefinite case.*

1 July 2010, Parallel Matrix Algorithms and Applications 2010, Basel, Switzerland.
J. A. Scott, *Designing sparse direct solvers for multicore architectures.*

2 July 2010, Parallel Matrix Algorithms and Applications 2010, Basel, Switzerland.
J. D. Hogg, *The challenge fo the solve phase of a multicore solver.*

13 September 2010, 2nd IMA Conference on Numerical Linear Algebra and Optimisation, Birmingham.
J. A. Scott, *Designing sparse direct solvers for multicore architectures.*

13 September 2010, 2nd IMA Conference on Numerical Linear Algebra and Optimisation, Birmingham.
J. D. Hogg, *The challenge fo the solve phase of a multicore solver.*

15 September 2010, 2nd IMA Conference on Numerical Linear Algebra and Optimisation, Birmingham.
H. S. Thorne, *PDE-constrained optimisation: why is it so challenging and some methods to overcome these challenges.*

16 September 2010, Optimization, Design and Control Workshop, Oxford.
H. S. Thorne, *PDE-constrained optimisation: from linear to nonlinear constraints.*

22 September 2010, CNMAC 2010. XXXIII Congresso Nacional de Matematica Aplicada e Computacional, Aguas de Lindoia, SP, Brazil.

I. S. Duff, *Solving really large sparse linear problems from a range of applications.*

25 November 2010, OPTEC Workshop on Large Scale QP, Leuven, Belgium.
N. I. M. Gould, *CQP: a Fortran 90 module for large-scale convex quadratic programming.*

4 January 2011, The Second International Conference on Numerical Analysis and Optimization. Sultan Qaboos University, Muscat, Oman.
I. S. Duff, *The use of direct methods in the solution of sparse linear equations from optimization and other applications.*

11 April 2011, BAMC, Birmingham.
M. Arioli, *Linear regression models and stopping criteria for Krylov methods.*

15 May 2011, Preconditioning Techniques, Bordeaux, France.
J. A. Scott, *A novel approach to level-based preconditioners.*

20 May 2011, SIAM Conference on Optimization, Darmstadt, Germany.
N. I. M. Gould, *CQP: a Fortran 90 module for large-scale convex quadratic programming.*

11 June 2011, Symposium on Eigenvalues, Model Order Reduction and Trust Regions in celebration of Danny Sorensen's 65th birthday, Reno, Nevada, USA.
I. S. Duff, *Partitioning Strategies for the Block Cimmino algorithm.*

13 June 2011, Householder Symposium XVII, Tahoe City, California.
M. Arioli, *Generalized Golub-Kahan bidiagonalization and stopping criteria.*

13 June 2011, Householder Symposium XVII, Tahoe City, California.
I. S. Duff, *Preconditioners based on strong components.*

13 June 2011, Householder Symposium XVII, Tahoe City, California.
H. S. Thorne, *Preconditioners for PDE-constrained optimisation problem.*

15 June 2011, Householder Symposium XVII, Tahoe City, California.
J. A. Scott, *The robust and efficient partial factorization of dense symmetric indefinite matrices.*

19 July 2011, ICIAM 2011, Vancouver, Canada.
I. S. Duff, *The use of direct methods in the solution of sparse linear equations for constrained optimization.*

29 June 2011, 24th Biennial Conference on Numerical Analysis, Strathclyde University.
N. I. M. Gould, *Puiseux-based extrapolation for large-scale degenerate quadratic programming.*

29 June 2011, 24th Biennial Conference on Numerical Analysis, Strathclyde University.
J. D. Hogg, *Experience of Linear Solvers in a Nonlinear Interior Point Method.*

5 August 2011, IFIP WG 2.5 Business Meeting, Boulder, Colorado.
J. A. Scott, *The multicore challenge for linear systems.*

29 August 2011, HPSS 2011, EuroPar 2011, Bordeaux.
I. S. Duff, *European Exascale Software Initiative: Numerical Libraries, Solvers and Algorithms.*

6 September 2011, Sparse Days 2011, Toulouse.
J. A. Scott, *An introductory look at the antibandwidth problem.*

11 October 2011, EESI Final Conference, Barcelona, Spain.
I. S. Duff, *Numerical libraries, solvers and algorithms.*

7 Seminars and other talks

18 March 2010, Birmingham University.
J. A. Scott, *The multicore challenge for sparse linear systems.*

12 May 2010, Uppsala University, Sweden.
H. S. Thorne, *Challenges from PDE-constrained optimization and some methods to circumvent these issues.*

20 July 2010, STFC Daresbury Laboratory.
M. Arioli, *An introduction to Quantum Graphs theory.*

12 November 2010, University of Basel, Switzerland.
H. S. Thorne, *PDE-constrained optimisation: from linear to nonlinear constraints.*

9 December 2010, ENSEEIHT Toulouse.
M. Arioli, *An introduction to Quantum Graphs theory.*

7 October 2011, NAG Ltd, Oxford.
J. D. Hogg, *The HSL Mathematical Software Library: Past, present and future.*

6 December 2011, AT&T New Jersey.
J. A. Scott, *An introduction to the world of sparse direct solvers.*

7 December 2011, Temple University, Philadelphia.
I. S. Duff, *Preconditioners based on strong subgraphs.*

7 December 2011, IBM Research Centre, Yorktown Heights, New York.
J. A. Scott, *Antibandwidth maximization: a map coloring problem.*

9 December 2011, Courant Institute, New York University.
J. A. Scott, *Antibandwidth maximization: a map coloring problem.*

8 Seminars at RAL

21 January 2010	Prof Ernesto Estrada (University of Strathclyde) An excursion through the world of complex networks guided by matrix theory.
11 February 2010	Dr Melina Freitag (University of Bath) Resolution of sharp fronts in the presence of model error in variational data assimilation.
29 April 2010	Prof Dominique Orban (Ecole Polytechnique de Montreal and GERAD, Canada) A Primal-Dual Regularized Interior-Point Method for Convex Quadratic Programs.
20 May 2010	Dr Jan Van lent (UWE Bristol) Numerical Methods for Monge-Kantorovich Transportation Problems.
25 November 2010	Dr Vanessa Styles (University of Sussex) Primal-dual active set methods for solving Non-local Allen-Cahn Systems.
2 December 2010	Dr Julian Hall (University of Edinburgh) A high performance dual revised simplex solver.
27 January 2011	Dr David Titley-Peloquin (University of Oxford) Backward Perturbation Analysis of Linear Least Squares Problems.
10 March 2011	Prof David Silvester (University of Manchester) Optimal Iterative Solvers for Saddle Point Problems.

12 May 2011	Prof Andrew Cliffe (University of Nottingham) Uncertainty Analysis for Flow of an Incompressible Fluid in a Sudden Expansion in Two-Dimensional Channel.
3 November 2011	Dr Bora Uçar (ENS Lyon, France) On hypergraph partitioning based ordering methods for sparse matrix factorization.
17 November 2011	Prof Nancy Nichols (University of Reading) Data assimilation using reduced order modelling for unstable systems.
12 December 2011	Prof Michele Benzi (Emory University) Decay properties of spectral projectors with applications to electronic structure computations.