Efficient parallel "black-box" preconditioners for Finite Element Problems
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Personnel supported:
Dr Jonathan Boyle as PDRA (17 months; 11/10/04–01/05/06). Jonathan subsequently took up a three year PDRA position in the School of Mathematics at the University of Manchester.
Dr Alison Durham as PDRA (part-time; 1/10/06–31/12/06).

Introduction. The design of scalable parallel linear solvers for discretized elliptic PDE problems remains an important but very challenging problem. The resources required for accurate three-dimensional finite element approximation test even the most advanced of supercomputer hardware. A major issue that arises using iterative solvers is the need to ensure that convergence is rapid (preferably independent of the mesh size and other problem parameters). The goal of this project was to develop, implement, and test parallel processor software that enables optimal performance across a wide set of engineering application areas. An end product of the research is a library-quality software package that will be made available to the international engineering community.

Key advances and supporting methodology. In the project we built computational tools that provide effective, easy to use, off-the-shelf building blocks for the iterative solution and preconditioning of large, sparse systems of linear algebraic equations that arise from discretization of partial differential equations. Over the period of the project we made important advances commensurate with those envisaged on the original proposal—these are detailed below.

• We developed a prototype code, written in Matlab, that implements algebraic multigrid (AMG) preconditioning based on the "classical" Ruge-Stüben coarsening algorithm. This choice of coarsening was influenced by its observed robustness in the context of the both diffusion and convection-dominated problems. The Matlab implementation was used as a test bed to perform efficiency studies and to enable performance optimization by vectorization of the innermost loops. The functionality of the code is included in the freely available PIFISS toolbox [3], and the source will be made available in the next release of the IFISS toolbox [1]. Both these software packages are widely used for both teaching and research in universities around the world.†

• We developed a library-quality Fortran 95 version of the sequential algebraic multigrid preconditioner [5]. This package of subroutines is now in its final testing phase and will be included in the next release of the HSL Fortran library. For details see `http://www.cse.clrc.ac.uk/nag/hsl/`. This software will then be freely available for all UK academics.

• We installed the Trilinos and Hypre software suites, distributed by Sandia and Livemore National Laboratories respectively, on the CSAR and HPCx architectures. The Trilinos suite is a collection of compatible software packages that support parallel linear algebra and the solution of linear, non-linear and eigen-systems of equations and related capabilities. The majority of this software is written in `C++` using object-oriented techniques and parallel implemention is done using MPI. The algebraic multigrid component of Trilinos is based on a user-specified domain decomposition together with a state-of-the-art smoothed agglomeration coarsening approach. Having installed and optimized this code on HPCx (a non-trivial task, see [6]), we tested its potential as a parallel "black-box" preconditioner for GMRES in the context of solving convection-diffusion problems. A sample set of results (taken from [6]) is given below. These experiments demonstrate excellent scalability and parallel efficiency of the solver when solving problems using sequences of structured grids that are adapted to resolve shear layers.

† A Google search for "ifiss software" typically generates over 200 hits!

number of iterations						
	uniform grid			stretched grid		
grid size	1 proc	4 procs	16 procs	1 proc	4 procs	16 procs
512×512	21	20	19	19	18	18
1024×1024		14	15		15	15
2048×2048			11			8

HPCx solution time in seconds						
	uniform grid			stretched grid		
grid size	1 proc	4 procs	16 procs	1 proc	4 procs	16 procs
512×512	15.8	3.7	1.1	14.6	3.5	1.2
1024×1024		12.2	3.7		12.6	3.7
2048×2048			14.0			10.7

• We assessed the effectiveness of our algebraic multigrid preconditioning code in the context of solving complex coupled PDE problems, such as the C^1 discretisation of the biharmonic equation, mixed approximation of potential flow with highly variable coefficients, incompressible flow modelled by the Navier-Stokes equations and thermal convection problems in two and three dimensions. A new smoothing approach, based on the damped Jacobi method, proved to be surprisingly effective for fine grid resolution of convection dominated problems, see [4]. We have also established that this damped Jacobi smoothing methodology can be combined with the novel Schur complement approximations that are developed in [2] to give a scalable parallel preconditioning methodology for stabilized mixed approximation of the Navier-Stokes equations. In the context of C^1 (Hermitian element) discretisation of the biharmonic equation, using algebraic multigrid with ILU(0) smoothing proved to be an effective approximation of the inverse of a sparse Schur complement matrix [7]. Effective and robust preconditioners were also developed for thermal convection problems arising from both steady and time-dependent bouyancy driven flow [8].

Project plan review. Over the period of the project we made important advances which are commensurate with the aims and objectives envisaged in the original proposal. The exception to this is the anticipated development of a completely new parallel algebraic mutigrid code. We will elaborate on this issue in this section of the report.

At the beginning of the project, when evaluating what was “out there” regarding parallel algebraic mutigrid software it was evident that the availability of the Trilinos and Hypre packages meant that our original objective to write such a code was inappropriate. Both of these software packages have had teams of expert programmers and algebraic mutigrid theoreticians working on them for over a decade—we could only afford to employ one experienced researcher (Dr Boyle, an expert in parallel programming but having no prior experience of algebraic mutigrid) for 17 months.‡ Given this situation the emphasis of this aspect of the project was changed to that of testing the effectiveness of the freely available parallel algebraic multigrid solvers on the CSAR and HPCx architectures.

Most of the parallel computing effort was concentrated in the final three months of Dr Boyle’s appointment. Unfortunately, most this work was wasted effort. Having tested and debugged the

‡ In retrospect it is clear that we needed a three year grant if we were to contemplate writing a complete parallel mutigrid code from scratch. This was not permitted within the call for proposals in the “New users to HPC computing” initiative that funded this work.

Trilinos and Hypre packages on the Origin architecture in the Computer Science department in the University of Manchester prior to a rigorous performance analysis on CSAR (the architecture was identical but interactive usage was not "charged") we found out that CSAR was to be switched off, prematurely, at the crucial stage of our project!

Our research effort then shifted to assessing the performance of Trilinos and Hypre on HPCx. For this task we extended the grant by three months and employed a part-time researcher (Dr Durham, an expert in parallel computing using Fortran 95, but having no `C++` experience) to install and evaluate the performance of the two packages on the HPCx architecture. Whilst installation of these packages on the shared memory architecture of CSAR was relatively straightforward, implementation and optimization on HPCx was something of a challenge. In particular, getting the Trilinos software to run efficiently ultimately required a detailed knowledge of HPCx specific features. A report that summarizes the many problems that arose in implementing this software on HPCx is available online [6]. Testing the algebraic multigrid component of the software required us to correct a number of bugs in the TRILINOS code. This severely hampered our progress in the final stages of the project—especially given that we had very few HPCx allocation units to work with.

Research impact and benefits to society. The immediate research impact of our project is summarised in four categories below.

• The most prominent outcome of our work is the forthcoming appearance of a highly optimized AMG solver in the scientific computing software library HSL. This library is freely available to the academic users in the UK, and is a licensed software library for commercial users. As a consequence, we envisage that our software will be accessible to a number of research communities who are involved in numerical simulation of various processes and phenomena in science and engineering. In particular, the AMG preconditioning package will provide an effective "black-box" tool, which, when used in conjuction with standard Krylov subspace iterative solvers (also available in HSL) will create powerful methods for block preconditioning of the complicated linear systems that arise when solving coupled systems of PDEs associated with application areas like solid mechanics, fluid mechanics and heat transfer.

• Our prototype code implementing algebraic multigrid was developed in Matlab, and this is a "built in" component of two educational software packages developed by the Numerical Analysis group in the University of Manchester: IFISS (which is a finite element modelling tool for incompressible fluid dynamics problems, including state-of-the-art iterative solvers and preconditioning techniques); and PIFISS (which is a finite element modelling tool for ground water flow modelling). Both of these packages are extensively used in Manchester and in a number of universities around the world to support the teaching of advanced courses on finite element approximation and fast iterative solvers. The commercial computational fluid dynamics community is becoming increasingly interested in our methodology. For example, a minisymposium in the recent SIAM conference on Computational Science and Engineering† was devoted to evaluating the effectiveness of the preconditioning ideas that are built into the IFISS package.

• The development of our AMG solver is likely to lead to much more effective and robust methods for preconditioning of convection-dominated problems (especially our use of point Jacobi smoothers for problems with recirculating convection fields), as well as for problems in structural mechanics, fluid mechanics and stochastic finite element modelling.

• The outcomes of this project will have long-term benefits to the research in the fields of

† This meeting was held at Orange County in California in February 2007, and attracted over six hundred participants from academia and industry, see `http://www.siam.org/meetings/cse07/`

linear stability of non-linear PDE systems, problems of shape optimization, system control and model order reduction. Projects in these areas are currently underway or else are planned activities for the The Manchester Centre for Interdisciplinary Computational and Dynamical Analysis (CICADA) as part of the recently announced EPSRC project EP/E050441/1.

Explanation of expenditure. The grant funds were used in accordance with the originally proposed schedule. The grant provided funding for the PDRA Dr J. Boyle for the total duration of seventeen months (between 11 October 2004 and 1 May 2006). During this time Dr Boyle developed and tested both Matlab and Fortran 95 (HSL) versions of the sequential AMG solver. Our travel budget was spent in part (as indicated in the original project plan) to provide for his subsistence for several visits to RAL in Oxfordshire. During these visits Dr Boyle worked with Dr J. Scott on the details of testing and writing documentation in preparation for the inclusion of the Fortran 95 code into HSL. The PI and Dr Boyle also made a three day visit to the Sandia Laboratories in Livermore USA. There they had a very productive collaborative exchange with Ray Tuminaro and other members of the research team who put together the AMG component of the Trilinos package.

The remainder of the travel budget was spent on the attendance of a number of academic conferences (including those listed below) by both investigators and the PDRA. These conference trips were used as an opportunity for the dissemination of the results of this research to the international academic community. Travel funds were also used to attend the EPSRC–organised meeting for HPC users in London in December 2005.

The grant funds were also used to provide part-time funding for Dr A. Durham, who performed the evaluation of the parallel AMG solver from the Trilinos library on the HPCx architecture.

The grant funds aimed at the purchase of equipment were spent to provide two personal computers, some computer accessories, and the purchase of the software licenses.

Further research and dissemination activities. The research undertaken and the software produced during the course of this project provides a starting point for our ongoing PhD project (EPSRC grant EP/C534875/1) that is funded under the HEC initiative. The aim of this research programme is to develop effective parallel smoothing techniques in the context of both geometric and algebraic multigrid preconditioning of convection-dominated flow problems.

The software produced will also be crucially important for a project currently being put together by the investigators together with Professor Steve Furber, FRS who leads the Advanced Processor Group in the School of Computer Science in Manchester. This project will involve a linear stability analysis of a thermal convection problem arising in the design of a forced cooling system of a novel architecture parallel computer.

Having completed his work on our project Dr Boyle took up a position as a research assistant with Prof. M. Heil on EPSRC project EP/D070422/1. This project is concerned with solving three-dimensional fluid flow problems arising in biomedical engineering. This in turn requires an effective preconditioning strategy for the Navier-Stokes equations that is scalable on a parallel computer architecture. Our understanding is that the experience and the expertise that Dr Boyle gained in writing the AMG software in our project is allowing him to make rapid advances.

Both investigators in the project gave, in addition to conference presentations, a number of invited seminars at academic departments in the UK, Germany and USA (the full list is given below), thus further enhancing the dissemination of the results of this project.

Invited Conference Talks given by David Silvester: Black-Box Multigrid Preconditioning for Steady Incompressible Flows, *Minisymposium on New Algorithmic and Theoretical Developments in Krylov Methods and Preconditioners*, SIAM Conference on Computational Science and Engineering, Orlando, February 2005; Least Squares Preconditioners for Stabilized Mixed Approximation of the Navier-Stokes Equations, Ninth Copper Mountain Conference on Iterative Methods, Colorado, April 2006; Least Squares preconditioners for stabilized mixed approximation of the Navier-Stokes equations, *Minisymposium on Fast Iterative Solvers*, MAFELAP 2006, Brunel University, June 2006; Algebraic Multigrid Preconditioning for Incompressible Flow Problems, *BICS Workshop on Computation of Flow and Transport in Heterogeneous Media,* University of Bath, June 2006.

Research Seminars given by David Silvester: *Efficient Preconditioning Methods for Steady Incompressible Flow Problems*, University of Strathclyde, February 2006; *Adaptive timestepping for incompressible flow problems*, TU Bergakademie Freiberg, Germany, December 2005; University of Strathclyde, February 2006; University of Birmingham, November 2006.

Research Seminars given by Milan Mihajlović: *Efficient AMG preconditioning of problems from structural mechanics*, University of Strathclyde, March 2005; *Efficient multigrid preconditioning of the Navier-Stokes equations with the free surface condition*, University of Leeds, May 2006; University of Bath, June 2006; University of Maryland, USA, September 2006.

Research Seminars and Conference Contributions given by Jonathan Boyle: *Numerical models of stochastic excitable media*, research seminar, University of Manchester, April 2005; *Algebraic multigrid and convection diffusion problems*, Dundee Biennial Conference on Numerical Analysis, June 2005; research seminar, University of Manchester, October 2005; Ninth Copper Mountain Conference on Iterative Methods, April 2006.

Publications: EP/C000528/1

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2. Elman. H., Howle V., Shadid, J., Silvester, D. and Tuminaro, R. Least squares preconditioners for stabilized discretizations of the Navier-Stokes equations, MIMS Eprint 2006.55, April 2006.
3. Silvester, D. and Powell, C. PIFISS: Potential (Incompressible) Flow & Iterative Solution Software Guide, MIMS Eprint 2007.14, February 2007. See also, `http://www.maths.manchester.ac.uk/~djs/ifiss/pifiss.html`.
4. Boyle, J. and Silvester, D. Properties of multigrid smoothers for convection diffusion problems, in preparation. See also, `http://www.maths.manchester.ac.uk/~djs/amg06.pdf`.
5. `http://www.maths.manchester.ac.uk/~djs/hsl_mi20.pdf`.
6. `http://www.maths.manchester.ac.uk/~djs/AD_report.pdf`.
7. Mihajlović, M., Heil, M. and Muddle, R. Algebraic multigrid preconditioning for C^1 approximation of the biharmonic problem, in preparation.
8. Mihajlović, M., Elman, H. and Silvester, D. Algebraic multigrid preconditioning for buoyancy driven flow problems, in preparation.