Parallel Methods for PDE Eigenvalue Problems - GR/M59075/01

1 Background

The numerical solution of large sparse eigenvalue problems arising from discretised PDEs is an important problem in computational mathematics with many and varied applications. It arises, for example, in stability assessment in structural mechanics and in the computation of resonances in electromagnetics. In this project our main target application was in fluid flow problems governed by the incompressible Navier-Stokes equations, where Hopf bifurcations are typically detected by linearised stability analysis. With respect to our target application, the PI had worked for many years with K.A. Cliffe of SERCO Assurance on iterative methods for eigenvalues, based on shift-invert strategies, but only when the systems were small enough to admit a *direct* inner solver (e.g. [5]). These fail to work in the case of practically important model problems such as the stability of 2D flow in an expanding pipe to 3D perturbations.

The main aims of the present project were (i) to produce a numerical analysis of eigenvalue iterations based on *inexact* inner solves and (ii) to build parallel software based on this analysis (using domain decomposition methods for the inexact inner solves) to compute eigenvalues of linear PDEs, in particular the linearised Navier-Stokes equations.

When the project started there was relatively little analysis on eigenvalue iterative methods with inexact inner solves. However during the course of the project there has been a considerable growth of interest in this problem - e.g. [7, 14]. Our work, for example in the large paper [2] (recently submitted), has improved on both of these papers in a way made precise below and we believe that our work is internationally competitive in this area. In order to build parallel iterative methods suitable for solving Navier-Stokes equations, we have benefitted from contacts with active UK groups working in this area – e.g. [13, 11]. These groups have not however been working on parallel algorithms. Our work has built parallel preconditioners, using techniques in [13, 11] combined with our own original ideas to produce Navier-Stokes solvers with good parallel performance and a solution time which scales close to linearly with problem size. This part of the work is at the practical end of the project; but the selection of our paper [9] as a distinguished paper at an international conference shows that we are internationally competitive in this direction too. As far as industrial relevance is concerned, we now have an eigenvalue solver which outperforms the direct-solver-based algorithms previously used at SERCO Assurance and so we consider this outcome to be successful also. In the following we give some more detail of our results (see `http://www.maths.bath.ac.uk/~igg/evalues/`).

2 Shift-invert eigenvalue solvers with inexact inner solves - achievements

This aspect of the project was concerned with the analysis and development of algorithms for generalised eigenvalue problems of the form $A\mathbf{x} = \lambda M\mathbf{x}$ where A and M are large sparse matrices arising from discretised PDEs. Many "shift-invert" based algorithms, ranging from classical inverse iteration to the recent PARPACK Arnoldi software [12], are based on repeated application of the operation $\mathbf{y} \leftarrow (A - \sigma M)^{-1}M\mathbf{x}$ which is implemented as $(A - \sigma M)\mathbf{y} = M\mathbf{x}$, where σ is called the shift. Nowadays there is great interest in the efficient solution of these shifted linear systems using preconditioned iterative methods. However, these iterative methods only solve the linear systems to a prescribed tolerance, and the resulting eigenvalue algorithms should then be thought of as "inexact shift-invert" algorithms. Consequently, there is much interest both in fundemental questions of convergence and in the development of efficient eigenvalue algorithms in this setting. Most of the work described in this part of the project was carried out by Mr J. Berns-Müller, a PhD student supported by this grant, and Professors A. Spence and I.G. Graham.

In general terms the main achievements of this part of the project are:

- A general convergence analysis of inexact inverse iteration applied to symmetric matrices.
- An analysis of the performance of the preconditioned Krylov solver MINRES applied to shifted symmetric linear systems, for general preconditioners.

- A general convergence analysis of inexact inverse iteration applied to nonsymmetric generalised eigenvalue problems.
- An analysis of the performance of preconditioned GMRES applied to (possibly complex) shifted nonsymmetric linear systems, for general preconditioners
- The development of a new eigenvalue strategy based on initial approximation using the (fixed shift) Arnoldi method, and accurate refinement using (variable shift) inexact inverse iteration.
- A convergence theory for a wide class of eigenvalue problems using an Inexact Newton technique.

More details of these achievements are described in the following subsections.

2.1 Symmetric Problems

Although our primary interest is in nonsymmetric generalised eigenvalue problems, several key concepts are best understood in the simpler context of the symmetric eigenvalue problem. Even in this case we had to fill gaps in the theory, and the efficient implementation of a preconditioned Krylov solver throws up an unexpected twist. In [2] we discuss in detail the theory of inexact inverse iteration for the symmetric eigenvalue problem $A\mathbf{x} = \lambda\mathbf{x}$ where the inexact solves are carried out by preconditioned MINRES - a Krylov solver for symmetric indefinite systems. Each outer iteration requires the solution of $(A - \sigma I)\mathbf{y} = \mathbf{x}$, where $(\sigma, \mathbf{x})$ approximates an eigenpair of A. It is proved in [2] that such a combination of shift and right-hand side is advantageous for the application of inner Krylov solvers. However the introduction of a preconditioner destroys this advantage, since it yields a new system with right-hand side which may no longer be close to an eigenvector of the preconditioned matrix. A suitable alteration of the right-hand side yields a faster convergent inner iteration and this turns out to produce an overall benefit, even though the convergence of the outer iteration may be damaged. The paper [14] proposed this strategy for Rayleigh quotient shifts and Cholesky preconditioning. Our paper [2] provides a complete theory for this approach, explains in detail why the altered right hand side is advantageous for Krylov solvers, and gives the extension to general preconditioners, including domain decomposition. Chapters 2 and 3 of [1] contain an extensive account of both theoretical and computational issues for the symmetric problem.

2.2 Nonsymmetric Problems

In [3] we extend the above results to the generalised eigenvalue problem $A\mathbf{x} = \lambda M\mathbf{x}$, where A is a general nonsymmetric matrix and M is symmetric positive definite. In this case we use GMRES (and some of its many variants) as the inexact solver for $(A - \sigma M)\mathbf{y} = M\mathbf{x}$. In [3] we provide the first theoretical account of variable shift methods for nonsymmetric problems. We also give an analysis of GMRES applied to $(A - \sigma M)$ when σ is complex, and this leads us to an extensive understanding of the behaviour of GMRES applied to nearly singular shifted systems. We now understand the subtle interplay between the choices of shift, solver tolerance, and right hand side when preconditioning $(A - \sigma M)\mathbf{y} = M\mathbf{x}$. A more detailed account of this work is described in Chapters 4 and 5 of [1]. This analysis is new, has obvious importance for inexact inverse iteration as a method in its own right, and will influence our understanding of the impact of inexact solves on subspace based methods. As a consequence it was decided to leave multi-dimensional splitting methods as discussed in the original proposal for later consideration.

A short account of some of the theory for nonsymmetric problems is also given in [10] where the extension to the nonsymmetric generalised eigenvalue problems that arise from mixed finite element discretisations of the Navier-Stokes equations is discussed. We describe a new efficient strategy based on initial approximation with Arnoldi's method and improvement using inexact inverse iteration with variable shift. This strategy has been tested on the problems described in the next section.

Finally we have also modified the standard inexact Newton theory [6] to apply to any eigenvalue problem, and have obtained convergence results for inexact inverse iteration that have very general applicability. This work is still in progress.

3 A parallel solver for PDE eigenproblems - achievements

In this part of the project, the main tasks which were carried out were:

- The development of efficient parallel preconditioned iterative algorithms for inverting shifted systems coming from block-format discrete PDE systems.
- The use of this technology as an inner solver inside eigenvalue iterations investigated in § 2.
- The testing of the eigenvalue solver in a variety of applications, particularly those arising from the mixed finite element approximation of the incompressible Navier-Stokes equations.

The parallelisation and preconditioning strategy were developed by the PDRA, Dr E. Vainikko together with Prof I.G. Graham. The coupling of this solver to shift-invert eigenvalue solvers for large PDE systems was also done by Dr Vainikko. Applications to stability problems for the Navier-Stokes equations were developed by Vainikko and Graham, together with Prof A. Spence and Mr K.A. Cliffe of SERCO Assurance (formerly AEA Technology).

The appointment of Dr Vainikko was particularly fortuitous. He had exactly the right experience in code development for large applications and particular experience in domain decomposition (through his PhD studies in Bergen) needed to carry out this very computationally intensive programme. The project also benefitted from his maturity. (He obtained also a PhD in Mathematics from St Petersburg during the Soviet era.) Now that this project has ended he has returned to his native Estonia to head a research group in High Performance Computing at the University of Tartu. All the parallel coding of eigenvalue problems for large-scale discretisations of PDE systems was done by Dr Vainikko. Quite a lot of serial development work was done on the SUN Sparc serial machine bought with the equipment fund in the grant. In the summer of 2001 the Department of Mathematical Sciences installed its first Linux Beowulf cluster, with 9 processors. This was upgraded to a 24 processor machine in the summer of 2002, thanks to financial support from the University of Bath. Much of the parallel computing was done on this cluster but some was also done on the Faculty of Science Sun Grid, bought with a JREI grant in 2002.

The `DOUG` package [8] is a parallel solver, based on domain decomposition, for discretised steady state PDEs on unstructured grids in 2D or 3D domains. When the present project started, the code was able to solve general scalar elliptic PDEs discretised by standard families of finite elements (given in elemental form) on general unstructured meshes. The code had mainly been used for symmetric problems [4] and only a rudimentary Bi-CGSTAB nonsymmetric solver was implemented.

In the code, the set of freedoms of the problem is decomposed into overlapping subdomains and these are used to build the parallel matrix-vector multiplications required for iterative methods. Also preconditioners are constructed from partial solves of the PDE in the subspaces defined by the decomposition. In order to ensure parallel efficiency, the required communication between overlapping freedoms on boundaries of subdomains has to be performed at the same time as the iterative updating of freedoms in the interiors of subdomains. This is done with carefully scheduled message passing. In order to maintain robustness as the number of freedoms increases, this type of "one level" preconditioner needs to be supplemented by the solution of a global coarse problem – a "two-level" method. The "mesh coarsening" procedure in `DOUG` uses some additional (rudimentary) geometric information about the domain of the underlying PDE and is based on the introduction of an adaptively controlled coarse space of low order finite elements (e.g. linear or bilinear elements) on the domain.

Our main computational task in the present project was to enable `DOUG` for the efficient solution of block linear systems, focussing on those highly nonsymmetric systems arising from (linearisation of) discretisations of Navier Stokes equations, especially in the case of fine meshes and high Reynolds numbers.

Our main achievements have been:

(i) The extension of the one-level `DOUG` technology to handle the case of discrete systems of PDEs, rather than a single equation. This is essentially an algebraic process which requires very little knowledge of the underlying PDEs, but the message passing of interface freedoms is more complicated and care must be taken to ensure scalability. Our strategy is described in some detail in [15].

(ii) The addition of cutting edge iterative methods for solving nonsymmetric systems, including GMRES and Flexible GMRES, with efficient parallel versions obtained using the iterated classical Gram-Schmidt algorithm. In particular the results for large Navier-Stokes systems in [15] would have been impossible without Flexible GMRES, which offers comparable performance to standard GMRES, but with a substantially reduced memory requirement.

(iii) In this project a lot of time was invested in the development of efficient (one and two level) parallel preconditioners for mixed finite element approximations of Navier-Stokes equations, since this was the principal target problem for our industrial collaborators. In 2D these have the block form

$$A = \begin{bmatrix} F_{11} & F_{12} & B_1^T \\ F_{21} & F_{22} & B_2^T \\ B_1 & B_2 & 0 \end{bmatrix}, \tag{1}$$

corresponding to the blocking of the unknowns as $(\mathbf{U}_1, \mathbf{U}_2, \mathbf{P})$, with $\mathbf{U}_i$ denoting velocity freedoms and $\mathbf{P}$ corresponding to pressure. We investigated various parallel implementations of the preconditioners of [11, 13] (which are all based on a block LU factorisation of (1)), together with several new versions of these. For continuous pressure elements we devised [9, 10] a new parallel counterpart of the "Green's function based" preconditioner in [11] which has the property of robustness to mesh refinement. We found this preconditioner not to work well for the discontinuous pressure elements which are most popular with our industrial collaborator. The paper [15] studies the discontinuous case in detail. The interesting result there is that the preconditioner (which we call WHOLE in [15]), which is based on the direct application of the `DOUG` technology to the block matrix (1) (without block LU decomposition) works much better than our best block-LU method. In particular the problem of stability of flow in an expanding pipe could not be solved without this preconditioner.

As an example of the capability of our solver, here are wall clock times for a single solve for 2D flow around a cylinder with biquadratic velocities and discontinuous linear pressures at $Re = 25$, solved by Flexible GMRES with the WHOLE preconditioner on a cluster with 12 slave nodes.

#DOF	18622	52158	102590
Sec	42.8	73.0	128.0

These clearly show better than linear complexity with number of degrees of freedom. (The low complexity growth is aided by the well-known phenomenon that parallel speed-ups usually increase as the volume of data increases.) This preconditioner suffers some degradation as Re increases but remains usable at $Re = 300$.

(iv) The algorithms described above were applied to fluid flow problems, with the aim of computing the "critical" Reynolds number, corresponding to the onset of instability. After a period of testing our algorithm on the problem of flow around cylinder (where the critical Re is known), we then put most of our effort into computing the instability of 2D flows in an expanding pipe to 3D perturbations. This is a very challenging problem, since (a) the onset of instability is thought to be in the $Re = 200 - 300$ range; (b) The flow is complex, a large number of degrees of freedom $10^5 - 10^6$ are needed, and the matrices (3D variants of (1)) are highly nonsymmetric; (c) the base flow features a recirculation region of length $O(Re)$, the computational domain must be lengthened as Re increases and to avoid further blowup of dimension, highly anisotropic meshes are employed.

The eigenvalue codes at SERCO Assurance fail for this application. Our work on this problem has produced an eigenvalue solver which has comparable performance to that of the much easier flow around the cylinder problem. We are currently running intensive experiments to identify the point of instability for the expanding pipe problem. We expect that when we have isolated this instability it will be of sufficient interest to merit publication in the fluid dynamics literature.

4 Project Plan Review

There was an approved four month break from 1/3/2002 till 30/6/2002 in the Postdoctoral part of the project. There were no significant changes to the project plan.

5 Dissemination

Many seminars, invited and contributed conference talks and posters, and research visits directly related to this project have been given both in the UK and abroad by all four people directly involved in this project. Briefly, Berns-Müller has talked at Durham(twice), Dundee, Copper Mountain (Colorado), Lexington (Kentucky) and presented posters at two EPSRC Days. Graham has talked at Dundee, Greenwich (LMS Workshop), Institut Francais du Petrole (Paris), Max-Plank-Institut (Leipzig), Strathclyde, RAL, BAMC Warwick, CERFACS (Toulouse) and the EPSRC Spectral Theory Network Sussex meeting. Spence has talked at Oxford(twice) Dundee, Strathclyde, Imperial College, Sandia Labs (Albuquerque) and at the EPSRC Spectral Theory Network meeting at Cardiff. Vainikko has talked at Durham, Greenwich (LMS Workshop), Paderborn (Euro-Par2002) and Neuchatel (Parallel Matrix Algorithms and Applications, 2002). Spence is an invited participant at the Pacific Institute for the Mathematical Sciences (PIMS) conference in November 2003 on "Theory and Numerics of Matrix Eigenvalue Problems", at Banff (Canada).

6 Future plans

On the eigenvalue theory side, we plan to use our understanding of inexact solves in inverse iteration to attack the analysis of inexact subspace-based eigenvalue solvers, such as Arnoldi's method. This is of particular relevance when preconditioned solves are used in conjunction with software packages such as ARPACK/PARPACK [12] and at present there is no analysis available on this topic.

On the practical side, we plan to publish our results on the onset of instability in the expanding pipe, once the critical Re has been conclusively isolated. As far as we are aware, we are the only group worldwide with the capability to do this. Further instability calculations for other flow problems should also be possible. We are continuing to work collaboratively with Dr E. Vainikko (Tartu) and have applied for a Royal Society European Science Exchange Project with Estonia for two year's support for bilateral visits between Bath and Tartu. This collaboration has already been active during the lifetime of the grant, since a postgraduate student from Tartu has written a web interface to `DOUG` which allows easy remote running of jobs on the Bath machines. The problem of preconditioning in the presence of anisotropic mesh refinement (mentioned in §2 (iv)) is of particular current interest to I.G. Graham, and he has just obtained an EPSRC VF Grant (GR/S43399/01) for Dr W. McLean (Sydney) to visit Bath in 2003-04 to work on this problem.

7 Research Impact

- As described in §2, our results should be of significant interest to academic researchers working on large sparse eigenvalue problems, particularly those arising from systems of discretised PDEs.
- As described in §3 (iv), our techniques extend the capability of the eigenvalue solver currently available in ENTWIFE (the general purpose Finite Element software marketed by SERCO), which applies subspace iteration to a Cayley Transform of $A\mathbf{x} = \lambda M\mathbf{x}$ and uses direct inner solves. As a spin-off, SERCO have also expressed strong interest in using our linear solvers as stand-alone techniques for

finding the base flow for difficult flow problems. (At present their solvers are based on the multifrontal method. Iterative solvers are of particular interest in 3D.)

- The interest generated by the present project has contributed to the setting up of a new PhD EPSRC CASE Award (Quota: 02304195) jointly with SERCO Assurance on the numerical analysis of methods for computing turbulent flows.

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