Abstracts and schedule of talks.

Workshop on the Use of Iterative Methods for Large-Scale Eigenvalue Problems

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Argonne National Laboratory, May 14-16, 1997

Wednesday, May 14

8:45 am, Opening remarks, Rich Lehoucq.

- Eigenvalue algorithms with several factorizations - a unified theory yet?, Axel Ruhe, 9:00 am
- A Projection Framework for a Truncated QZ-like Method for Large Generalized Eigenproblems, Dan Sorensen, 9:45 am

Break, 10:30 am

- A Parallelizable and Fast Algorithm for Very Large Generalized Eigenproblems, Henk van der Vorst (joint with Diederik Fokkema and Gerard Sleijpen), 11:00 am
- Expanding Efficiently Effective Search Subspaces for Jacobi-Davidson Type of Methods, Gerard Sleijpen (joint with Diederik Fokkema and Henk van der Vorst) 11:30 am

Wednesday Lunch, Noon (Cafeteria, private dining room)

Moderator for the afternoon session: Steve Vavasis.

- Some Unusual Eigenvalue Problems, Gene Golub (joint with Z. Bai and his colleagues), 1:30 pm
- Variants of Krylov Projection Methods, Yousef Saad, 2:00 pm

Break 2:30 pm

- On the Calculation of Eigenvalues of Large-Scale Generalized Eigenvalue Problems by the Rational Krylov Method, Karl Meerbergen, 2:45 pm
- A Truncated RQ-Iteration for Large-Scale Eigenvalue Calculations, Chao Yang (joint with Danny Sorensen), 3:15 pm

Break 3:45 pm

- Using Harmonic Ritz Values with Preconditioned Eigenvalue Methods and with GMRES, Ron

Morgan 4 pm
- Trapping Lanczos Eigenvalues and Why Rubies are Red, Christopher Beattie, 4:30 pm

Workshop adjourns for the day, 5:00 pm
Hors D'oeuvres, snacks, and drinks, Freund Lodge at ANL, 6:00-8:00 pm

Thursday, May 15

Moderator for the morning session: Steve Wright.

- Some History of Preconditioned Iterative Methods for Symmetric Eigenvalue Problems, Andrew Knyazev, 8:30 am
- Preconditioning Techniques for Large Eigenvalue Problems, Kesheng Wu (joint with Yousef Saad and Andreas Stathopoulos) 9:00 am

Break 9:30 am

- Restarting Techniques for Preconditioned Symmetric Eigenvalue Methods, Andreas Stathopoulos (joint with Yousef Saad) 10 am.
- Variants of the Inverse Iteration Method for Large-Scale Eigenproblems, Tong Zhang, 10:30 am.
- Eigenvalue Approaches for Large Scale SVD Computations in Linear Geophysical Inverse Problems, Osni Marques (joint with Don Vasco) 11:00 pm.
- A Structural Dynamics Parallel Sparse Eigensolver, David Day 11:30 am.

Thursday Lunch, Noon (Cafeteria, private dining room)

Afternoon session moderator: James Lyness

- An Iterative Block Method for Computing a Few Close Eigenvalues of a Large Sparse Symmetric Matrix, James Baglama (joint D. Calvetti, L. Reichel, and A. Ruttan) 1:30 pm
- Quasi-Leja Shifts in the Implicitly Restarted Lanczos Method, Lothar Reichel, 2:00 pm

Break 2:30 pm

- Computing Guided Waves in Optical Fibers, Lawrence Cowsar (joint with Rich Lehoucq), 2:45 pm
- On Computing Eigenvalues of the Discretized Navier Stokes Equation, 3:15 pm Jennifer Scott (joint with Rich Lehoucq)

Break 3:45 pm

- Resolvent Norm Approximations and Effective Stability Studies of Large Matrices, Valeria Simoncini, 4 pm
- Adaptively Preconditioned GMRES Algoritihms, Daniela Calvetti (joint with J. Baglama, G. Golub, and L. Reichel), 4:30 pm
- Lanczos Process for Pole and Residual Computations in Large Linear Circuits, Qiang Ye (joint with Zhaojun Bai) 5:30 pm

Workshop adjourns for the day, 5:30 pm

Workshop Dinner 7:00 pm at Emilio's Tappas bar and restaurant in Naperville, Illinois.

Friday, May 16

Morning session moderator: Paul Plassmann

- Lanczos Method for Complex Symmetric Eigenvalue Problems and Shift-and-Invert Spectral Transformation, Zhaojun Bai, 9:00 am
- Application of Lanczos and Davidson Methods to Multiple-Well Isomerization, Kristyn Maschhoff 9:30 am

Break 10:00 am

- A Block Inverse Iteration Method Using Multigrid for Electronic Structure Calculations, Jean-Luc Fattebert 10:30 am
- Conjugate-gradient Based Electronic Structure Calculations, Bernd Pfrommer, 11:00 am

Friday Lunch, 11:30 am (Cafeteria, private dining room)

- Eigenvalue Test Problems in The Rutherford-Boeing Sparse Matrix Collection, John G. Lewis (joint with Roger G. Grimes and Iain S. Duff) 1:00 pm
- Workshop Wrap-up, G.W. Stewart, 1:30 pm.

Eigenvalue Algorithms with Several Factorizations - A Unified Theory Yet?

***Axel Ruhe*, Chalmers University of Technology**

(40 minutes + 5 minutes for questions)

The success of shifted and inverted iterations for large eigenvalue problems, has prompted further developmens along (at least) 3 tracks, Rational Krylov, Jacobi Davidson and Truncated RQ. They all use Krylov sequences of shifted and inverted operators, but differ in some interesting details:

1. Length of sequence of basis vectors, continuation or restart?
2. Computation of Ritz approximate eigenvalues.
3. Usefulness with inexact factorizations or preconditioners.

A new reformulation of Rational Krylov gives it a closer relation to Arnoldi, and also insights into the close connection between algorithms developed along the 3 tracks. Go back. Next abstract.

A Projection Framework for a Truncated QZ-like Method for Large Generalized Eigenproblems

***Dan Sorensen*, Rice University**

(40 minutes + 5 minutes for questions)

This talk will present a framework for developing and analyzing methods for large scale generalized eigenvalue problems of the form

$A\,x = s\,B\,x$.

This framework is well suited for the development of methods that do not require accurate solution of shift-invert equations. This framework may be viewed as generalized subspace projection. Along with many of the most recently proposed methods, this setting naturally encompasses a truncated form of the QZ-algorithm for dense problems. This can be combined with an implicit restarting technique that naturally extends the implicitly restarted Arnoldi method to the generalized problem. Go back. Next abstract.

A Parallelizable and Fast Algorithm for Very Large Generalized Eigenproblems

***Henk van der Vorst*, Utrecht University (joint with Diederik Fokkema and Gerard Sleijpen)**

(25 minutes + 5 minutes for questions)

In our presentation we will describe a new iterative technique for the computation of a number of selected solutions for the eigenproblem

$(A - s\,B)\,q = 0$,

with A, B general large sparse matrices of order n . The technique is based on the Jacobi-Davidson method with reduction to Schur form. With this technique we are able to compute a number of eigenvalues and eigenvectors, with subspaces of restricted dimension, and without inversion of any of the matrices involved. The standard methods of Arnoldi and Lanczos are not well-suited for this.

In the Jacobi-Davidson method a subspace is generated onto which the given eigenproblem is projected. The much smaller projected eigenproblem is solved by standard direct methods, and this leads to approximations for the eigensolutions of the given large problem. This is the ‘Davidson’ part of the algorithm. Then, a correction equation for a selected eigenpair is set up. The solution of the correction equation defines an orthogonal correction for the current eigenvector approximation; this is the ‘Jacobi’ part of the algorithm. The correction is used for the expansion of the subspace and the procedure is repeated. This is the part of the algorithm where preconditioning can be used. In the new algorithm the large system is projected on a suitable subspace, in a way that may be viewed as a truncated and inexact form of the QZ factorization. The projected system itself is reduced to Schur form by the QZ algorithm. For this reason we refer to the algorithm as JDQZ (=Jacobi-Davidson-QZ). As we will see, the method

lends itself perfectly well for parallel execution. Go back. Next abstract.

Expanding Efficiently Effective Search Subspaces for Jacobi-Davidson Type of Methods

***Gerard Sleijpen*, Utrecht University**

(25 minutes + 5 minutes for questions)

In the Jacobi-Davidson method for generalized eigenproblems, an approximate eigenvector is selected from a search subspace and is tested with respect to a test subspace. The search subspace and the test subspace have the same dimension, which will typically be low. Both subspaces are expanded in each step. The expansion vector for the search subspace is obtained as the solution of a correction equation. The correction equations are linear and may be solved by any method of choice. For larger problems it is often more convenient to do this only approximately, for instance with an appropriate preconditioned iterative linear solver.

The correction equation will be formulated in terms of the given problem and low-dimensional projections. As we will see, this formulation allows easy incorporation of the preconditioner. Jacobi-Davidson for standard eigenproblems is based on similar ideas, but for the generalized problems the projections that are involved need more attention.

For standard eigenproblems, the test subspace can be taken equal to the search subspace. For generalized problems, it is less obvious whether such a choice would be the most effective one. In fact, other choices will appear to be more natural. Go back. Next abstract.

Some unusual eigenvalue problems

***Gene Golub*, Stanford University (joint Z. Bai and his colleagues)**

(25 minutes + 5 minutes for questions)

We consider several non-standard eigenvalue problems. this includes estimating the sum of k eigenvalues and modifying a matrix by a matrix of rank one. Our basic tools are Gaussian quadrature, the Lanczos algorithm and monte carlo techniques. Go back. Next abstract.

Variants of Krylov Projection Methods

***Yousef Saad*, University of Minnesota**

(25 minutes + 5 minutes for questions)

Most of the successful methods for solving large eigenvalue problems consist of combining projection-type techniques with a few other strategies such as deflation and preconditioning. The standard Petrov-Galerkin conditions used to define projection methods give rise to a variety of different methods, some of which have been considered in recent years. These methods involve two subspaces: a subspace K from which the approximate eigenvector is extracted (called the "right" subspace) and a subspace L of the same dimension used to define constraints for computing these eigenvectors (the "left" subspace). One common choice is to take the left and right space to be the same and this leads to a standard orthogonal projection method exemplified by the Lanczos algorithm in the Hermitian case and the Arnoldi algorithm in the non-Hermitian case. A somewhat intriguing variation, derived by comparison with the GMRES algorithm for solving linear systems is to take L=AK. An (incorrect) motivation for this approach is that it acts as a projection operator for the inverse of the matrix. We will consider these options and a few others, which involve inverting the operator. We will compare some of these variants both experimentally and theoretically. Go back. Next abstract.

On the Calculation of Eigenvalues of Large-Scale Generalized Eigenvalue Problems by the Rational Krylov Method

***Karl Meerbergen*, LMS Numerical Technologies**

(25 minutes + 5 minutes for questions)

The rational Krylov method (RKS) is well-suited for the calculation of eigenvalues of large generalized eigenvalue problems. The method is an extension of the shift-and-invert Arnoldi method by the fact that the shift may vary on each iteration step. The computed basis vectors satisfy a recurrence relation with two Hessenberg matrices instead of one for the Arnoldi method. This relation is used for the calculation of eigenvalues, eigenvectors or Schur vectors.

The shift-invert Arnoldi method and the Rational Krylov method require the solution of linear systems. In eigenvalue calculations, one often uses matrix factorization, with the aim of solving the linear systems very accurately. Instead, this talk considers solving the resulting linear system in an inexact manner, for example, by using an iterative method. We show that the use of a Cayley transformation within the RKS method allows for the use of approximate solutions of linear systems. A relationship with the (Jacobi) Davidson method is established. The theory is illustrated by numerical examples.

The computation of the shift-invert transformation is the main concern of this talk. The remainder of the talk is devoted to a short presentation of the main idea of the implicitly filtered rational Krylov method. For both the Arnoldi method and rational Krylov, it may happen that the basis required for the accurate calculation of the wanted eigenvalues becomes too large to be stored by the computer. For the Arnoldi method this problem was solved in an elegant manner by the implicitly restarted Arnoldi method. In this talk a similar implicit restart is presented for rational Krylov. Similarly, the main properties of this restart are the preservation of the Hessenberg structure, a relationship with inverse iteration and purging of unwanted eigenspaces. Go back. Next abstract.

A Truncated RQ-iteration for Large Scale Eigenvalue Calculations

***Chao Yang*, Rice University**

(25 minutes + 5 minutes for questions)

We introduce a Krylov subspace iteration for large scale eigenvalue problems that is able to accelerate the convergence through an inexact (iterative) solution to a shift-invert equation. The method also takes full advantage of an exact solution when it is possible to apply a sparse direct method to solve the shift-invert equations. We call this new iteration the Truncated RQ iteration (TRQ). It is based upon a recursion that develops in the leading k columns of the implicitly shifted RQ iteration for dense matrices. Inverse-iteration-like convergence to a partial Schur decomposition occurs in the leading d columns of the updated basis vectors and Hessenberg matrices. The TRQ iteration is competitive with the Rational Krylov Method of Ruhe when the shift-invert equations can be solved directly and with the Jacobi-Davidson Method of Sleijpen and Van der Vorst when these equations are solved inexactly with a preconditioned iterative method. The TRQ iteration is related to both of these but is derived directly from the RQ iteration and thus inherits the convergence properties of that method. Existing RQ deflation strategies may be employed directly in the TRQ iteration. Go back. Next abstract.

Using Harmonic Ritz Values with Preconditioned Eigenvalue Methods and with GMRES

***Ron Morgan*, Baylor University**

(25 minutes + 5 minutes for questions)

Two uses of harmonic Ritz values are discussed. First we look at finding interior eigenvalues with the generalized Davidson method, which uses preconditioning. It is demonstrated that the preconditioning can make a big difference and that using harmonic Ritz values is important. Second, harmonic Ritz values are used in an implicitly restarted GMRES method. The small eigenvalues are deflated in order to improve convergence. Remarkably, a Krylov subspace can be generated that contains selected harmonic Ritz vectors from the previous cycle of GMRES. Comparisons to standard restarted GMRES and transpose-free QMR are given. Go back. Next abstract.

Trapping Lanczos Eigenvalues and Why Rubies are Red

***Christopher Beattie*, Virginia Tech**

(25 minutes + 5 minutes for questions)

A variety of spectral problems in solid-state physics and chemistry involve the difficult task of isolating discrete eigenvalues of differential operators from essential spectra lying nearby. This leads to difficulties both with regard to the appearance of ‘‘ghost’’eigenvalues (approximations that don’t

correspond to real eigenvalues) and with regard to sluggish convergence behavior of the estimates.

Some approaches that have been considered to resolve these problems may give some insight into approaches for accurate and rapidly convergent estimates to matrix eigenvalues that are situated deep in the interior of the spectrum. Go back. Next abstract.

Some History of Preconditioned Iterative Methods for Symmetric Eigenvalue Problems

***Andrew Knyazev*, University of Colorado at Denver**

(25 minutes + 5 minutes for questions)

Iterative methods for symmetric eigenvalue problems are finally becoming a numerical standard for extremely large problems. In this talk we present a survey of some theoretical convergence rate estimates for such methods, derived by soviet scientists. We consider preconditioned analogs of the power method, the steepest descent/ascent method, Chebyshev's methods, and Lanczos-type methods, as well as their block variants. Go back. Next abstract.

Preconditioning Techniques for Large Eigenvalue Problems

***Kesheng Wu*, University of Minnesota (joint with Yousef Saad and Andreas Stathopoulos)**

(25 minutes + 5 minutes for questions)

This research focuses on finding a few eigenvalues and eigenvectors of a large sparse matrix. The approach taken is to find new preconditioning schemes to improve the effectiveness of preconditioned techniques for eigenvalue problems. The basic framework of the preconditioned eigenvalue method we chose to study is that of the Arnoldi method and the Davidson method. Within this framework, we compared five different schemes that are mathematically equivalent without preconditioning. However, the Davidson method is much more successful with many different preconditioners. Despite its success, the preconditioning scheme in the Davidson method is seen as flawed. The Davidson preconditioning scheme is an inexact Newton step. This motivates us to explore other Newton methods to develop new preconditioning schemes without the same flaws. Our research reveals that some of the well known preconditioning schemes can be understood as inexact Newton methods for eigenvalue problems. At the same time we have also developed new versions of Newton methods for eigenvalue problems. This talk will present theoretical properties of these Newton methods and discuss their advantages and disadvantages when used as preconditioners. Go back. Next abstract.

Restarting Techniques for Preconditioned Symmetric Eigennvalue Methods

***Andreas Stathopoulos*, University of Minnesota (joint with Yousef Saad)**

(25 minutes + 5 minutes for questions)

The Jacobi-Davidson method is a popular preconditioned variant of the Arnoldi method for solving large eigenvalue problems. Because of theoretical and practical reasons, the two methods are often used with restarting. This has significant performance shortcomings, since important components of the invariant subspace may be discarded. One way of saving more information at restart, is the idea of ‘‘thick’’ restarting which keeps more Ritz vectors than needed. The previously proposed dynamic thick restarting has proved very efficient for symmetric non-preconditioned cases, and a competitive technique for preconditioned cases.

Based on the three term recurrence of the Conjugate Gradient algorithm, Murray et al. proposed a different restarting strategy for the preconditioned Davidson method. Assuming the sought Ritz value is sufficiently converged, the Davidson algorithm builds a space similar to that of CG, and thus restarting with two vectors may not hinder convergence. At restart, one keeps the sought Ritz vector from two successive iterations (the current and the previous one). This technique works well when it focuses on one wanted eigenpair, but it impairs convergence for the rest.

We present a theoretical justification for the above scheme, and we address the problem of requiring several eigenpairs by combining the scheme with thick restarting. The resulting technique has proved very efficient and robust. We also present an inexpensive implementation which does not require any additional orthogonalizations or matrix vector multiplications, and can be incorporated to existing (Jacobi-)Davidson codes. Go back. Next abstract.

Variants of the Inverse Iteration Method for Large-Scale Eigenproblems

***Tong Zhang*, Stanford University**

(25 minutes + 5 minutes for questions)

There has been a growing interest in finding preconditioning techniques for eigenvalue problems in the recent years. While most methods have been designed with special iterative procedures, it is also possible to precondition the inverse iteration algorithm directly. A difficulty for this approach is that these inverse iteration systems are often very ill-conditioned. This may be the main reason why little work has been done in this area.

In this talk, I will mention a Newton’s method that avoids the problem of solving an ill-conditioned system, but still gives a quadratic local convergence rate. I will show an algorithm that combines this technique with the conjugate gradient method for computing the extreme eigenpairs of a generalized symmetric eigensystem. I will also relate this algorithm to some existing methods.

The Newton’s method, like the Rayleigh Quotient Iteration method, allows a shift in the inverse iteration. This can cause the problem of missing some desired eigenvalues. If the time permits, I will also talk about the homotopy method, which can be used to remedy this problem. Go back. Next abstract.

Eigenvalue Approaches for Large Scale SVD Computations in Linear Geophysical Inverse Problems

***Osni Marques*, Lawrence Berkeley National Laboratory (joint with Don Vasco)**

(25 minutes + 5 minutes for questions)

Inverse problems arise in many different fields, such as satellite navigation, medical tomography, image enhancement, earthquake location and in the study of the structure of the earth. Basically, given a set of (physical) data, the goal is to estimate model parameters describing the structure of the Earth. For linear problems, the relation between the data and the model parameters is given by a matrix (the 'data kernel'), which represents the physics of the problem. It is important to determine limits on the information we can draw from the data. That is, estimates of model parameter uncertainties and an estimate of the spatial resolution of structure within the Earth. It turns out that a SVD of the data kernel can provide us with the required answers. However, in geophysics applications, the matrices involved can be larger than 10^6 by $2x10^5$. Although sparse, such problems are difficult to deal with since several thousand singular values and singular vectors are required. In this talk we focus on the main issues related to the solution of SVD problems arising in Geophysics by means of an eigenvalue approach on a Cray T3E, comment on tools currently available and strategies to tackle with huge cases. Go back. Next abstract.

A Structural Dynamics Parallel Sparse Eigensolver

***David Day*, Sandia National Laboratory**

(25 minutes + 5 minutes for questions)

Structural dynamics analysis often involves symmetric generalized eigenvalue problems

$K v = s M v$

for symmetric positive semi-definite stiffness and mass matrices K and M. Also rank(M) is approximately equal to the nullity M. The computational task is to compute the smallest (leftmost) modes. These applications are solved using the shift and invert strategy and applying a Lanczos-based solver. Note that the condition number of the ''inversion'' depends on the types of finite elements used to model a structure. Problems that involve plate or shell elements are more challenging. The emphasis of this talk will be on scalable solution methods for linear systems.

The demand for parallel solution methods in structural dynamics arises because memory limitations restrict the order of problems that can be solved in core using direct linear system solution methods to approximately 100,000 unknowns. Our parallel sparse eigensolver combines three packages:

1. A parallel finite element library (in progress)

2. PARPACK
3. FETI

PARPACK is the parallel version of the well-known ARPACK eigensolver package. The Finite Element Tearing and Interconnecting (FETI) method is a two-level domain decomposition method that extends to plate and shell problems.

This talk will be divided into two parts. First I will review the FETI iterative linear system solver. In the second part of this talk I will discuss model linear systems and eigenvalue problems of size up to 400,000 unknowns solved using this parallel sparse eigensolver. This project is in progress. Go back. Next abstract.

An Iterative Block Method for Compouting a Few Close Eigenvalues of a Large Sparse Symmetric Matrix

***James Baglama*, Kent State University (joint with D. Calvetti, L. Reichel, and A. Ruttan)**

(25 minutes + 5 minutes for questions)

We present an Implicitly Restarted Block Lanczos method designed for the computation of a few extreme or non-extreme multiple or close eigenvalues and associated eigenvectors of a large sparse symmetric matrix. Our method generalizes the Implicitly Restarted Lanczos method introduced by Sorensen. The method requires that certain acceleration parameters, referred to as shifts, be chosen. The storage requirement and convergence rate depends on the choice of shifts. We also present a new strategy for choosing shifts. Numerical examples will illustrate that the Implicitly Restarted Block Lanczos method with shifts chosen in this manner gives rapid convergence, reliably detects extreme multiple or close eigenvalues, and requires little computer storage in addition to the storage used for the desired eigenvectors. These features make the method well suited for applications were it is essential to reliably detect extreme multiple or close eigenvalues. We will also present an application of the method in the tracking of Liquid Crystals. Go back. Next abstract.

Quasi-Leja Shifts in the Implicitly Restarted Lanczos Method

***Lothar Reichel*, Kent State University (joint with J. Baglama and D. Calvetti)**

(25 minutes + 5 minutes for questions)

The implicitly restarted Lanczos method is a truncated QR algorithm for the computation of a few eigenvalues and associated eigenvectors of a large symmetric matrix. Similarly as in the QR algorithm, the choice of shifts is important for rapid convergence. Wilkinson shifts, popular shifts for the QR algorithm, cannot be used for the Implicitly Restarted Lanczos method because the data required to compute these shifts are not available. Instead ‘‘exact shifts’’ and Leja shifts have been proposed for the Implicitly Restarted Lanczos method. Leja shifts have been found to work well when memory limitations only allow the storage of a Krylov subspace basis of low dimension, or when non-extreme

eigenvalues and associated eigenvectors are desired. We introduce new shifts, quasi-Leja shifts, which yield similar convergence as Leja shifts, but are much simpler to compute. Go back. Next abstract.

Computing Guided Waves in Optical Fibers

***Lawrence Cowsar*, Lucent Technologies (joint with Rich Lehoucq)**

(25 minutes + 5 minutes for questions)

A fundamental problem in the design of optical devices is the characterization of the modes that will propagate unattenuated in a fiber. The shapes and propagation constants (speed) of these modes are the eigenfunctions and eigenvalues of a nonsymmetric eigenvalue problem. In this talk, a brief introduction to this problem is given and a new finite element method is presented. The performance of several formulations and software packages will be compared including a new block implicitly restarted Arnoldi method. The integration of the eigenvalue solver with a mesh adaptive strategy for the finite element scheme will also be discussed. Several instances of matrices from this problem will be made available. Go back. Next abstract.

On Computing Eigenvalues of the Discretized Navier Stokes Equation

***Jennifer Scott*, Rutherford Appleton Laboratory (joint with Rich Lehoucq)**

(25 minutes + 5 minutes for questions)

In this talk we are concerned with finding the leftmost eigenvalues of large sparse nonsymmetric generalized eigenvalue problems which arise in stability studies of incompressible fluid flow. The matrices have a block structure that is typical of mixed finite element discretizations for such problems. We compare the use of shift-invert and Cayley transformations in conjuction with subspace iteration and the implicitly restarted Arnoldi method. Numerical results are presented for some model problems arising from the ENTWIFE finite element package. Go back. Next abstract.

Resolvent norm approximations and effective stability studies of large matrices

***Valeria Simoncini*, Pavia**

(25 minutes + 5 minutes for questions)

The norm of the resolvent

$R(A,z)=(A-zI)^{-1}$

where z is a complex number can provide some insight in understanding the qualitative behavior of the eigenvalues of a square matrix A under large perturbations. In order to make this a practical approach, the norm of $R(A,z)$ is evaluated approximately. We present relations from Krylov subspace approximation procedures that clarify the properties and applicability of this technique. We show that the qualitative behavior of the eigenvalues of A is not only predicted by inspecting the resolvent norm but by also evaluating the spectral radius of a related matrix. We show how to numerically compute this radius for large matrices and how this information can be used to analyze the quality of the eigenvalue approximation of a Krylov subspace method and to detect the presence of spurious approximate eigenvalues. Go back. Next abstract.

Adaptively Preconditioned GMRES Algorithms

***Daniela Calvetti*, Stephens Institute of Technology (joint with J. Baglama, G. Golub, and L. Reichel)**

(25 minutes + 5 minutes for questions)

The restarted GMRES algorithm proposed by Saad and Schultz is one of the most popular iterative methods for the solution of large linear systems of equations Ax=b with a nonsymmetric and sparse matrix. This algorithm is particularly attractive when a good preconditioner is available. We describe two new methods for determining preconditioners from spectral information gathered by the Arnoldi process during iterations by the restarted GMRES algorithm. These methods seek to determine an invariant subspace of the matrix A associated with eigenvalues close to the origin, and move these eigenvalues so that a higher rate of convergence of the iterative methods is achieved. Go back. Next abstract.

Lanczos Process for Pole and Residual Computations in Large Linear Circuits

***Qiang Ye*, University of Manitoba (joint with Zhaojun Bai)**

(25 minutes + 5 minutes for questions)

Lanczos process has emerged as an efficient model reduction method for computing approximate poles (eigenvalues) and residuals of large linear circuits. We will present a derivation of the so-called moment matching technique and error estimation in the large scale model reduction. The new error bound allows for the development of an automated non-heuristic termination of the Lanczos process and ensures the desired accuracy of the approximate reduced model. A number of implementation issues will also be addressed and numerical examples will be given. Go back. Next abstract.

Lanczos Method for Complex Symmetric Eigenvlaue Problems and Shift-and-Invert Spectral Transformation

***Zhaojun Bai*, University of Kentucky**

(25 minutes + 5 minutes for questions)

In the first half of this talk, we will present a Lanczos procedure for solving eigenvalue problems of complex symmetric matrices. Such problems arise in many applications, such as the solution of Schrodinger equation with complex scaling techniques in quantum chemistry and heavily damped vibration systems in structural dynamics. While the resulting algorithm presents several advantages over the standard non-symmetric Lanczos method, notably the significant reduction of memory and computational requirements, we will identify tradeoffs between these advantages and the potential extra numerical instability. We will discuss a couple of schemes to stabilize the procedure.

In the second half, we address the shift-and-invert spectral transformation technique to compute interior eigenvalues. The shift-and-invert places the desired eigenvalues in the favorite positions for a Krylov subspace method. However, it may result in a very ill-conditioned problem to solve. We will discuss proper termination (convergence) criteria used with shift-and-invert. Go back. Next abstract.

Application of Lanczos and Davidson Methods to Multiple-Well Isomerization

***Kristi Maschhoff*, Rice University**

(25 minutes + 5 minutes for questions)

Isomerization is important in a number of gas phase processes, for example, soot formation within combustion is thought to proceed via a sequence of isomerization steps. The analysis of gas phase isomerization is complicated by two major considerations. First, the relaxation of such systems to equilibrium is, in general, governed by more than one parameter. Second, these parameters can have a complex dependence on pressure and temperature. Both of these considerations are best tackled within the framework of unimolecular theory using master equation (ME) techniques. Here, the lowest few eigenvalues and eigenvectors of the ME matrix are required for modeling the relaxation of the system. Unfortunately, if large sequences of isomerizations are to be investigated the ME description requires significant computational resources.

In this talk I will first discuss the development of a diffusion equation (DE) approximation to the full master equation. This approximation coupled with matrix rearrangement results in a narrow banded form whose lowest eigenpairs can be determined using a shift-invert Lanczos approach (ARPACK). This truncated model is shown to be a valid approximation to the long term behavior of the isomerization process. For isomerization reactions where the DE approximation is not valid or if the data and model require a more accurate approach, we can then refine the initial estimates obtained using the DE approximation by returning to the full ME operator. In these situations we can still take advantage of the DE approximation by using it as a preconditioner within a generalized block Davidson method with the initial (DE) eigenvector estimates as starting vectors. Go back. Next abstract.

A Block Inverse Iteration Method Using Multigrid for Electronic Structure

Calculations

***Jean-Luc Fattebert*, DMA-EPFL**

(25 minutes + 5 minutes for questions)

We are interested in the numerical resolution of an eigenvalue problem with a nonlinear operator, the Kohn-Sham equations, when computing the electronic structure of a molecule enclosed in a cubic box, for given atomic positions. We work in the context of the local density approximation (LDA) model and replace the singular atomic potentials by pseudopotentials.

The discretization of the 3D problem is done on regular meshes or composite meshes refined in the center of the domain. The Laplacian is approximated by a "Mehrstellenverfahren" finite difference scheme of order 4. The nonlinearity of the operator in the Kohn-Sham equations is treated by a fixed point algorithm in which, at every step, we look for the smallest eigenvalues and the corresponding eigenvectors solutions of a discretized stationary Schrodinger equation with a linear operator.

We propose an iterative scheme to determine the searched solutions of these symmetric eigenvalue problems with linear operators, starting from approximations given by the solutions obtained at the previous step. The method is a block generalization of the Rayleigh Quotient Iteration which uses Petrov-Galerkin approximations. Its convergence is quadratic in an alternative case very close to the used one. The algorithm is adapted to a multigrid resolution of the linear systems obtained in the inverse iterations.

The algorithm has been numerically tested on problems coming from the computation of the electronic structure of some atoms and molecules (Si, O, CO, furan), showing its applicability to non-academic problems. Go back. Next abstract.

Conjugate-gradient based electronic structure calculations

***Bernd Pfrommer*, University of California at Berkeley**

(25 minutes + 5 minutes for questions)

Electronic structure calculations based on Density Functional Theory (DFT) are an important branch of computational physics. We present a convergence analysis for the conjugate-gradient minimization of a Kohn-Sham energy functional, using a functional with implicit orthonormality constraints. We discuss the effects of preconditioning, and show with a numerical example that preconditioning makes the rate of convergence sensitive to the choice of the shift η. We also present performance numbers for the 3d-FFT and matrix-matrix multiplies which are involved in the conjugate-gradient minimization within a pseudopotential/plane-wave approach. We compare the application performance of the SGI PowerChallenge as a typical symmetric multiprocessor to the one of the scalable Cray T3E at NERSC. Go back. Next abstract.

Eigenvalue Test Problems in The Rutherford-Boeing Sparse Matrix Collection

***John G. Lewis*, Boeing Information Services (joint with Roger G. Grimes and Iain S. Duff)**

(25 minutes + 5 minutes for questions)

The Rutherford-Boeing Sparse Matrix Collection will extend the Harwell-Boeing Sparse Matrix Collection in number and size of test matrices and particularly in representing more of the eigenproblem and its solutions. Have we got it right? Can we include the data you would like to see?

I will describe the directions we have been taking with the collection and our plans for a new release in the very near future. This will be your opportunity to give us feedback to ensure that we have a useful collection of test eigenproblems. Go back.