

Report No. 12/2002

**Miniworkshop:
Preconditioning in Eigenvalue Computations**

March 3rd – March 9th, 2002

This workshop was organized by Andrew Knyazev (Denver, USA), Volker Mehrmann (Berlin, Germany), Harry Yserentant and Klaus Neymeyr (both Tübingen, Germany).

Whereas the topic of preconditioning for the iterative solution of linear systems has been an important research area for already more than 20 years, it has still not reached the same attraction for eigenvalue problems. Recently, however, the research on preconditioning for eigenvalue problems has become very active. This is mainly due to an increased interest in preconditioning techniques in application areas such as:

- dynamics of electromagnetic fields;
- electronic structure calculations;
- band structure calculations in photonic crystals;
- vibrations and buckling in mechanics, structural dynamics;
- neutron flow simulations in nuclear reactors.

In these areas eigenvalue problems for partial differential operators are to be solved. Classical multigrid methods, as designed for the solution of the corresponding boundary value problems, can be used as preconditioners. Preconditioned eigensolvers result in conceptually simple, easy-to-implement and computationally cheap schemes, as grid-independent convergence transfers to the multigrid-preconditioned eigensolvers.

The investigation of “Preconditioning for eigenvalue problems” (convergence acceleration for iterative eigenvalue methods is probably a better term) involves research in several different areas, ranging from classical linear algebra to modern numerical treatment of partial differential equations.

Advances in the theory of preconditioned eigensolvers also stimulate research on some nontrivial problems of operator theory, e.g., the ultimate understanding of preconditioned iterative methods will most likely have to be based on a theory of polynomials of two noncommuting operators, which is presently not available.

Major new developments in this area, which have taken place in recent years include the following:

- sharp nonasymptotic convergence estimates for the preconditioned gradient method were obtained;

- inexact Jacobi-Davidson techniques were developed that allow adaptation of the classical shift-and-invert methods, e.g., Rayleigh quotient iterations, to the use of preconditioning;
- the Davidson method, popular in quantum chemistry, was analyzed in the general framework of preconditioned eigensolvers;
- multigrid, domain decomposition and incomplete factorization based preconditioning was developed for eigenproblems.

The main topic of the workshop was the exchange of new ideas concerning several approaches to the analysis of “preconditioned eigensolvers” and their further development.

Part of the meeting was dedicated to preconditioned eigensolvers for mesh discretizations of eigenproblems for self-adjoint and coercive elliptic partial differential operators. Recent results show that these *eigenproblems* can be solved with optimal complexity by using multigrid/multilevel preconditioners as developed for the solution of *boundary value problems*. As a topic of special interest a preconditioned conjugate-gradient-like method for symmetric eigenvalue problems has been discussed. Though hard theoretical problems remain to be solved, stimulating debates on these solvers emerged in several sessions.

As preconditioning for eigenproblems is not restricted to symmetric positive definite problems, further sessions were devoted to preconditioning strategies, to the convergence analysis, to eigenvalue cluster robustness, and last, but not least, to the convergence acceleration for eigensolvers applied to quadratic eigenproblems.

Most talks were followed by extensive discussions, which were in some cases extended to evening sessions. In general, the given talks reflected that major new developments have taken place in recent years. The workshop has given us the chance to indicate new and fruitful directions, to present the state of the art in the area, and to exchange ideas and approaches for further development. Some joint projects have emerged at the workshop - not only on the (convergence) theory of preconditioned eigensolvers, but also on algorithmic improvements in application areas.

To summarize, the workshop confirmed that “preconditioning for eigenproblems” is a rapidly growing area with a considerable impact on several challenging applications.

Abstracts

Efficient computation of eigenpairs of a quadratic operator eigenvalue problem

THOMAS APEL

The stress distribution at the top of a polyhedral corner or at a crack tip has the typical r^α -singularity. Mathematically, the exponent α is an eigenvalue of a quadratic operator eigenvalue problem. The finite element method is sufficiently flexible to solve the problem numerically, such that also anisotropic or composite materials can be treated.

Optimal approximation results were derived in [2] on the basis of new local interpolation error estimates. Locally graded meshes were used to treat the corner singularities in the eigenfunctions.

By the finite element approximation, the operator eigenvalue problem is transformed into a quadratic matrix eigenvalue problem. In [1], we suggested to solve this problem with the Skew-Hamiltonian Implicitly Restarted Arnoldi method. Numerical experiments are documented at the end of the talk.

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[1] Th. Apel, V. Mehrmann, D. Watkins: *Structured eigenvalue methods for the computation of corner singularities in 3D anisotropic elastic structures*. Preprint SFB393/01-25, TU Chemnitz, 2001.

[2] Th. Apel, A.-M. Sändig, S. I. Solov'ev: *Computation of 3D vertex singularities for linear elasticity: Error estimates for a finite element method on graded meshes*. Preprint SFB393/01-33, TU Chemnitz, 2001.

Numerical Methods for spectral problems in energy spaces on composed manifolds

EUGENE G. D'YAKONOV

A review of recently obtained results for special types of spectral problems in energy spaces is given (see [1–7] and references therein).

The energy spaces are special Hilbert spaces and can be regarded as generalizations of classical Sobolev spaces $H^1(\Omega)$; they deal not with a domain $\Omega \subset \mathbf{R}^d$ but with a compact set (multistructure) $X \equiv \cup_{k=1}^{k^*} \bar{Q}_k \subset \mathbf{R}^d$ consisting of blocks (substructures) of different dimensionality.

The problems under consideration are reduced to ones in the operator form $\mathbf{M}\mathbf{u} = \mathbf{sL}\mathbf{u}$ with $\mathbf{L} = \mathbf{L}^* \asymp \mathbf{I}$ and a symmetric and compact operator $\mathbf{M} > 0$; for such problems, the classical Hilbert-Schmidt theorem applies.

Concerning the approximation properties of the energy spaces by spline (finite element) subspaces, it is possible to prove that they are essentially the same as those of Sobolev spaces. Moreover, the analogy takes place even in constructing Rayleigh-Ritz approximations and efficient iterative methods for the arising algebraic problems $Mu = sLu$ in an Euclidean space H with very large $\dim H \equiv N$; $s_1 \geq s_2 \geq \dots \geq s_N$; we are interested in finding, say $p \ll N$, of the first eigenvalues $s_1 \geq s_2 \geq \dots \geq s_p$ and corresponding subspaces.

Construction of model operators (preconditioners) B is discussed with special attention to the case when the grid operators L and B are spectrally equivalent uniformly with respect to several important parameters. Model operators make use of multigrid splittings of the spline space with proper estimation of the angles between subspaces.

Natural generalizations of the well-known preconditioned subspace iterations (for $Mu = sLu$) are described; they yield the Rayleigh-Ritz approximations ($s_1^{(n)} \geq \dots \geq s_p^{(n)}$) and the corresponding p -dimensional subspace $S_p^{(n)}$ with a basis $u_i^{(n)}$, $i \in [1, p]$) in an iteration subspace $H^{(n)} \subset H$ ($\dim H^{(n)} \in [p, 3p - 1]$). The new iteration subspace $H^{(n+1)}$ contains $S_p^{(n)}$, the modified residual vectors $w_i^{(n)} \equiv B^{-1}r_i^{(n)}$, $i = 1, \dots, p$ and $p - 1$ vectors $z_i^{(n)} \equiv B^{-1}Lu_i^{(n)}$, $i = 1, \dots, p - 1$ ($\dim H^{(n+1)} \in [p, 3p - 1]$, $\dim H^{(n+1)} \in [p, 2p]$ if $B = L$). Monotonic convergence of all $s_i^{(n)}$, $i \leq p$, $n \rightarrow \infty$ takes place with estimates of the best known type in theory of preconditioned subspace iterations in the case of infinite precision computations. Some estimates dealing with finite precision computations are obtained. The iterations are very attractive from the point of view of parallel computations in situations when solving of given systems with the chosen preconditioner B can be done effectively on separate processors.

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Preconditioning for large scale eigenvalue problems in electronic structure calculations

JEAN-LUC FATTEBERT

Ab initio electronic structure calculations in Density Functional Theory require the solution of an eigenvalue problem with a nonlinear operator at every step of the molecular dynamics process. The large number of eigenfunctions required in large scale applications is a major computational difficulty.

Iterative eigensolvers based on block inexact inverse iterations, using multigrid preconditioning, appear to be quite efficient in the context of finite difference discretizations. This method, also called preconditioned block steepest descent, can be used to search for the eigensubspace of the electronic wavefunctions represented by a basis of non-orthogonal functions. In this case, the scaling of the algorithm can be improved by limiting the spread of these functions to localized regions. Numerical results on large physical systems illustrate the efficiency and limits of the method.

The mystery of fast convergence of the locally optimal block PCG eigensolver

ANDREW KNYAZEV

Numerical solution of extremely large and ill conditioned eigenvalue problems is attracting a growing attention recently as such problems are of major importance in applications. They arise typically as discretization of continuous models described by systems of partial differential equations. For such problems, preconditioned matrix-free eigensolvers are especially effective as the stiffness and the mass matrices do not need to be assembled, but instead can be only accessed through functions of the corresponding vector-matrix products.

While the mainstream research in the area introduces preconditioning in eigenvalue solvers using preconditioned inner iterations for solving linear systems with shift-and-invert matrices, our approach is to incorporate preconditioning directly into Krylov-based iterations. This results in simple, robust, and efficient algorithms, in many preliminary numerical comparisons superior to inner-outer schemes commonly used at present, e.g., to the celebrated inexact Jacobi-Davidson methods.

Searching for the optimal eigensolver, we describe the Locally Optimal Block Preconditioned Conjugate Gradient (LOBPCG) method for symmetric eigenvalue problems, based on a local Rayleigh-Ritz optimization of a three-term recurrence. LOBPCG can be viewed as a nonlinear conjugate gradient method of minimization of the Rayleigh quotient, which takes advantage of the optimality of the Rayleigh-Ritz procedure.

Numerical results establish that our LOBPCG method may practically be as efficient as the best possible algorithm on the whole class of preconditioned eigensolvers. We discuss several competitors, namely, some inner-outer iterative preconditioned eigensolvers. Direct numerical comparisons with two of them, the inexact Jacobi-Davidson methods JDCG and JDQR, show that our LOBPCG method is faster. A rigorous theoretical explanation of excellent convergence of the LOBPCG remains challenging and needs innovative mathematical ideas. The best presently known theoretical convergence rate estimate is proved in 2001 in an extensive four-parts paper, but it still does not capture some important convergence properties of the LOBPCG.

A MATLAB code of the LOBPCG method and the Preconditioned Eigensolvers Benchmarking are available at <http://www-math.cudenver.edu/~aknyazev/software/CG/>

The talk is partially based on the papers:

[1] A.V. Knyazev, "Toward the Optimal Preconditioned Eigensolver: Locally Optimal Block Preconditioned Conjugate Gradient Method." *SIAM Journal on Scientific Computing* 23 (2001), no. 2, pp. 517-541.

[2] Andrew Knyazev and Klaus Neymeyr, "A geometric theory for preconditioned inverse iteration. III: A short and sharp convergence estimate for generalized eigenvalue problems." To appear in *Linear Algebra and Its Applications*, 2002.

[3] Andrew Knyazev and Klaus Neymeyr, "Efficient solution of symmetric eigenvalue problems using multigrid preconditioners in the locally optimal block conjugate gradient method." To appear in *Copper Mountain Multigrid issue of ETNA*, 2002.

The inexact rational Krylov space method for large nonlinear eigenvalue problems

KARL MEERBERGEN

Applications in chemistry and engineering sometimes give rise to large scale (usually sparse) eigenvalue problems. The most popular method for solving Hermitian problems in engineering is probably the spectral transformation Lanczos method. In this talk, we will discuss three different aspects of the method.

First, the method computes the eigenvalues near a point, called the pole, fairly easily. When a relatively large number of eigenvalues is wanted, it is desirable to alter the pole. Changing poles, however, may lead to a loss of efficiency in the method. We suggest and discuss the use of the rational Krylov (Lanczos) method instead, which is more efficient in this situation.

Second, the method requires the solution of linear systems. Usually direct methods are employed, but iterative methods are considered as well. The Lanczos method requires linear systems to be solved fairly accurately. This is not necessarily the case with the rational Krylov method. We discuss how the Cayley transform can be used to make the use of iterative linear system solvers more effective.

Finally, we consider the case where the Lanczos method uses a semi-inner product. Rounding errors may turn this into an indefinite inner product which may lead to breakdown of the method. We propose the combination of the pseudo-Lanczos method and an implicit restart using nested Lanczos to reduce the instabilities that may arise.

On a “Schur” form for quadratic matrix polynomials

CHRISTIAN MEHL

Quadratic matrix polynomials appear in the context of the quadratic eigenvalue problem. In this talk, we discuss an approach that can be considered as a first step towards a Schur-like form for quadratic matrix polynomials. A step-wise algorithm that computes this form will be presented. However, this algorithm involves nonunitary similarity transformations and requires the solution of a system of nonlinear equations in each step.

‘Preconditioning’ for variable parameter structured quadratic eigenvalue problems

VOLKER MEHRMANN

Numerical methods for the solution of large scale structured quadratic eigenvalue problems that depend on a parameter are discussed. To determine a desired small number of eigenvalues in the interior of the spectrum and the associated eigenvectors or invariant subspaces, ‘preconditioning’ tasks, such as structure preserving spectral transformations, have been performed to achieve reasonably good convergence to physically meaningful results. We describe the use of the structure preserving Skew-Hamiltonian isotropic implicitly restarted Arnoldi method (SHIRA) together with a new extraction procedure for invariant subspaces as ‘preconditioner’ for the Jacobi-Davidson method.

As an application we discuss gyroscopic systems. An approach is presented, that first solves the eigenvalue problem for the undamped system using the structure preserving method followed by the quadratic Jacobi-Davidson as a correction iteration.

Preconditioning in eigenvalue computations

KLAUS NEYMEYR

In this introductory talk we start with a critical discussion of several ideas motivating the concept of preconditioning for eigenvalue problems. Mainly eigenvalue problems for mesh discretizations of coercive, self-adjoint and elliptic differential operators are considered, for which multigrid/level and domain decomposition preconditioners are available. New convergence estimates for a basic preconditioned eigensolver are presented. A theoretical framework for a larger class of preconditioned eigensolvers is suggested, which can serve as a basis for the analysis of preconditioned eigensolvers for more general eigenproblems. Finally, several open problems are pointed out. As a topic of special importance for our workshop some links are worked out between preconditioning for symmetric positive definite eigenproblems and those for nonsymmetric matrices.

Convergence of inexact Rayleigh quotient iterations and of the Jacobi-Davidson method

YVAN NOTAY

We consider the computation of the smallest eigenvalue and associated eigenvector of an Hermitian positive definite pencil.

Rayleigh quotient iterations (RQI) are known to converge cubically and we first analyze how this convergence is affected when the arising linear systems are solved only approximately. We obtain an upper bound on the convergence factor which we show to be sharp for a wide set of error vectors, indicating that the analysis takes properly the errors into account.

We next consider the Jacobi-Davidson method. It acts as an inexact RQI method in which the use of iterative solvers is made easier because the arising linear systems involve a projected matrix that is better conditioned than the shifted matrix arising in classical RQI. We show that our general convergence result straightforwardly applies in this context and permits to trace the convergence of the eigenpair in function of the number of inner iterations performed at each step. We also establish a relation between the residual norm reduction during the course of inner iterations and the norm of the residual associated to the next approximate eigenpair. From a practical point of view, this allows to set up a proper stopping strategy, exiting precisely at the moment where further progress would be useless with respect to the convergence of the outer process. beginitemize

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Cluster Robustness of Preconditioned Gradient Subspace Iteration Eigensolvers

EVGUENI OVTCHINNIKOV

The role of preconditioning in iterative methods is to accelerate the convergence of iterations without increasing considerably the computational cost per iteration. In the case of parameter-dependent problems preconditioning often serves as an antidote to the negative influence of certain parameters, such as the mesh size parameter of a discretized problem. Nowadays, various preconditioning techniques are available which make the convergence of iterative methods for solving linear systems, such as the steepest descent or conjugate gradient methods, *robust* with respect to the parameters of the problem, i.e. unaffected by those parameters in their whole range of legitimate values. The case of eigenvalue problems is somewhat more difficult, as the convergence of respective iterative methods (often referred to as *eigensolvers*) generally depends on the distances between consecutive eigenvalues, which, in turn, may depend on the parameters. For some methods, however, there appears to be no dependence on those distances. A familiar example is the inverse *subspace iteration* method, for which convergence estimates are available that do not involve distances between the computed eigenvalues. Hence one may conclude that the inverse subspace iterations are *cluster robust*, i.e. their convergence is not adversely affected by the presence of clustered (i.e. closely situated) eigenvalues. The same kind of robustness so far has not been theoretically established for methods involving preconditioning (referred to as *preconditioned eigensolvers*). The present talk uses a novel approach of studying the convergence of *groups* of eigenvalues, rather than individual ones, to fill the above gap in the convergence theory of preconditioned eigensolvers. The main result is new non-asymptotic convergence estimates for a class of methods combining the subspace iteration technique with the preconditioned steepest descent (here referred to as preconditioned gradient subspace iteration eigensolvers). The new estimates are cluster robust and, furthermore, lead to the smallest proven upper estimates for the asymptotic convergence factors for computed eigenvalues.

Real Symmetric Matrices with multiple Eigenvalues

BERESFORD PARLETT

We describe "avoidance of crossing" and its explanation by von Neumann and Wigner. We show Lax's criterion for degeneracy and discover matrices whose determinants give the discriminant of a given matrix. This yields a simple proof of the bound given by Ilyushechkin on the number of terms in the expansion of the discriminant as a sum of squares. We present the 3×3 case in detail.

Rational Krylov for nonlinear eigenvalues

AXEL RUHE

This is a rather intricate algorithm that I described in a volume dedicated to my academic mother Vera Nikolaevna Kublanovskaya on the occasion of her 80 th birthday on September 21, 2000.

An eigenvalue problem that is nonlinear in the eigenvalue parameter is solved by successive linearizations with Lagrange interpolation. Each such generalized linear eigenproblem is solved with a rational Krylov approach. An interesting difference, compared to linear

eigenproblems, is that now both the numerator and the denominator of the rational function are of interest. The numerators are the matrix evaluated at a sequence of shifts which are updated in each iteration step, in order to converge to the latent roots one by one. When the shift is at a latent root, the solution of a standard eigenvalue problem gives the corresponding latent vector. The denominators are chosen at poles and are changed much more seldom, since each new pole needs a new matrix factorization.

I will describe the algorithm and give some examples from nonlinear mechanical systems. It has been implemented by Patrik Hager in his thesis in Structural Mechanics at Chalmers.

Sylvester type preconditioner for eigenvalue computations

MILOUD SADKANE

(joint work with M. Robbé from Louvain-la-Neuve.)

We discuss an algorithm for approximating invariant subspaces of a large not necessarily diagonalizable matrix A . The construction of the algorithm is rather simple. From a rectangular matrix X , the idea is to augment the subspace $\text{Span}\{X, AX\}$ by a rectangular matrix $K(X)$ that, if computed exactly, it renders the space $\text{Span}\{X + K(X)\}$ invariant by A . The matrix $K(X)$ is constructed from a linearization of an algebraic Riccati equation, i.e. a Sylvester equation, and can be seen as a block version of the correction used in the Jacobi-Davidson method. The approximation of the operator K may lead to a convergence with quasi-quadratic rate. This is confirmed by the numerical experiments where K is constructed with multigrid techniques.

Preconditioners for Jacobi-Davidson

GERARD SLEIJPEN

We discuss approaches for an efficient handling of the correction equation in the Jacobi-Davidson method. The correction equation is effective in the space orthogonal to the current eigenvector approximation. The operator in the correction equation is composed from three factors that allow for a sparse representation. If the given matrix eigenproblem is sparse then one often aims for the construction of a preconditioner for that matrix. We discuss how to restrict this preconditioner effectively to the space orthogonal to the current eigenvector.

In case of excellent preconditioners, the obvious approach may introduce instabilities that may hamper convergence. For preconditioners of multilevel type, we show how such instabilities can be avoided. We explain also that such preconditioners can efficiently and effectively be updated when better approximations to the eigenvalues of interest become available. The approach also leads to good initial guesses for the eigenvectors.

We argue that explicit right preconditioning can have advantages when, for instance, using domain decomposition.

In order to avoid misconvergence one has to make the right selection for the approximations, and this aspect is discussed as well.

Fixed Polynomial Approximate Shift Invert Preconditioning for Large Eigenvalue Problems

SORENSEN

A technique is developed for approximating the shift invert spectral transformation with a fixed degree polynomial operator. A given preconditioner for an iterative linear solver is used to construct the transformation in an automatic way. The fixed polynomial is obtained by applying the iterative method (e.g. GMRES, BiCGstab, or QMR) to a single linear system solved to a specified accuracy and then taking the (preconditioned) matrix polynomial defined by the solver as an approximate inverse.

The advantage of such a scheme is that the resulting polynomial operator is fixed throughout. Thus, the Krylov theory is retained without requiring the highly accurate solves that would be needed if an iterative solve were to be performed anew at each step to approximate the shift invert spectral transformation. Initial experiments indicate that a fairly low degree polynomial approximation will often suffice. Experimental results indicate that the degree will depend on the quality of the initial linear system preconditioner. If the quality of the linear system preconditioner is independent of dimension, then the number of matrix-vector products required to solve a problem will remain nearly constant as the dimension increases. Thus, in some cases, linear scaling may be achieved.

One of the primary motivations for this approach is to extend the range of problems that a given Krylov method might be able to solve (such as the implicitly restarted Arnoldi method in ARPACK). The effectiveness of this approach to Preconditioning for eigenvalue problems was demonstrated using ARPACK to solve a large 2-D Laplacian and also to conduct a linear stability analysis for an ocean circulation model. The latter was a fairly difficult nonsymmetric problem and a simple ILU preconditioner was sufficient to obtain near linear scaling with this problem.

Structure-Preserving Spectral Transformations of Hamiltonian Eigenvalue Problems

DAVID S. WATKINS

The study of singularities in stress fields of anisotropic elastic structures leads to large Hamiltonian eigenvalue problems. In the interest of efficiency and stability, such problems should be solved by methods that exploit either the Hamiltonian structure itself or some related structure. On the other hand, it is often necessary to apply a spectral transformation to expose the eigenvalues of interest. Any such transformation should respect the structure. In this talk a variety of spectral transformations that transform the problem to either a symplectic, a skew-Hamiltonian, or a Hamiltonian form are discussed. For each of these structures, implicitly-restarted Krylov subspace methods that exploit the structure are developed.

Edited by Klaus Neymeyr

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