MATHEMATISCHES FORSCHUNGSINSTITUT OBERWOLFACH

Tagungsbericht 15/1997

Numerical Linear Algebra and Scientific Computing

13.04. - 19.4.1997

The conference, organized by Gene H. Golub (Stanford), Wilhelm Niethammer (Karlsruhe) and Richard S. Varga (Kent), was attended by 46 individuals from 13 countries. In a first attempt to follow the recommendations of the Institute there were fewer lectures in the morning and afternoon sessions, whereas in the evening some problems of numerical algebra and scientific computing have been informally presented and discussed.

One major topic was the iterative solution of large linear systems of equations and — to some extent — eigenvalue problems. Special topics were Lanczos and cg–like methods, especially for non–symmetric systems. Preconditioning, e.g. with approximate inverses was discussed in connection with parallel computing.

Often these methods were examined together with applications such as quantumchromodynamics, impedance tomography, the Oseen problems, connvection–diffusion problems, initial value problems, ill-posed problems and regularization, and the algebraic Riccati equations. Over– and underdetermined systems were considered. Other questions presented were efficient matrix multiplications, multilevel methods and panel clustering in boundary element methods.

Finally, some theoretical questions such as matrix structures, stability radii and inertia of matrices were treated.

An overall impression was that numerical linear algebra is in the center of scientific computing and that a good mixture of experts from both topics were present. This together with the intimate atmosphere of the conference led to many fruitful discussions and initiated forthcoming joint projects.

GREG AMMAR

A Parameterized Implementation of the QR algorithm for Sub-Unitary Hessenberg Matrices

Computing the eigenvalues of unitary Hessenberg matrices is appealing for many of the same reasons as for real symmetric tridiagonal matrices. Each class consists of normal Hessenberg matrices that can be represented using $2n - 1$ parameters, and each form lends itself in several ways to efficient eigenvalue computation. For example, one step of the QR algorithm preserves the structure in each class, which provides the basis for implementations of the QR algorithm using $O(n)$ flops per step.
The characteristic polynomials of the leading principal submatrices of a unitary Hessenberg matrix form a (finite) sequence of Szegő polynomials. Computing the zeros of Szegő polynomials is important in signal processing applications. While significant success has been achieved for the unitary Hessenberg eigenvalue problem, the eigenvalue problem for a leading principal submatrix is less tractable. The Jordan blocks of such matrices can be of arbitrary sizes. Their eigenvalues are inside the unit circle, but are otherwise unconstrained. Although such matrices can also be represented using approximately $2n$ parameters, this parameterization is not preserved by a QR step.
In this talk we will present a new algorithm that efficiently implements the QR algorithm on these sub-unitary Hessenberg matrices. A key observation for the algorithm development is to recognize these matrices as a subset of a class of Hessenberg matrices that can be represented using approximately $4n$ parameters. This larger class of matrices is invariant under the QR iteration, and allows for the implementation of the implicitly shifted QR algorithm in this class using $O(n)$ flops per iteration.
Aspects of this talk represent joint work with William Gragg and Chunyang He.

OWE AXELSSON

On Newton type continuation method

Newton type continuation methods to solve nonlinear systems of equations are considered. In its standard form, when discretized, the resulting step–by–step (or discrete) iteration method converges in general with a superlinear rate but only locally, i.e. for initial values sufficiently close to a solution. To find such sufficiently close approximations various forms of modification of the standard method can be used. Three such methods for which, under mild assumptions on the nonlinear mapping, convergence takes place from any initial point are considered:

(i) "Load increment" method

(ii) Monitoring of stepsized in the damped step version of the Newton method

(iii) Continuation in a meshsize parameter when solving nonlinear boundary value problems and the control of both iteration and discretization errors.

Convergence proofs are given and some aspects in the practical implementations of the methods are discussed, in particular when solving problems with a nearly singular Jacobian matrix.

ZHAOJUN BAI

Some Unconventional Numerical Linear Algebra Problems and Their Applications

There are numerous applications in physics, statistics and electrical circuit simulation where it is required to bound or estimate entries and the trace of the inverse and the determinant of a large sparse matrix. In molecular dynamics by tight-binding method, it requires to compute a partial

eigenvalue sum of a large scale symmetric positive definite pair of matrices. All these unconventional numerical linear algebra problems can cast as the problem of computing of the bilinear form $u^T f(A)u$ for a proper defined matrix A and vectors u and function $f(\cdot)$, which is defined on the spectrum of A. We present a numerical method for estimating the bilinear form, where the matrix A is only referenced through matrix-vector multiplications. Therefore it is suitable for large scale problems. The method is based on the Gaussian quadrature for Riemann-Stieltjes integral, and Lanczos process for generating orthogonal polynomials and many other tools. Comparing with approaches which are based on conventional numerical algebra methods, the new approach is generally less accurate, but is much less constrained in memory and computational requirements and is significantly faster. For example, in a tight-binding molecular dynamics study, the accuracy of the new method is acceptable. We are able to tackle problem sizes previously intractable.
This is joint work with Gene Golub.

MICHELE BENZI

A comparision of sparse approximate inverse preconditioners

There exist currently several alternative proposals for constructing sparse approximate inverses, some of which have been compared with standard incomplete factorization techniques. However, there seems to be a lack of direct comparisons between different approximate inverse techniques on a broad range of problems. In this talk, we will survey many of the existing methods and we will present the results of a systematic computational study aimed at assessing the effectiveness of the various methods for different types of problems, with particular attention to their robustness, rates of convergence, and implementation issues. This is joint work with Miroslav Tůma (Czech Academy of Sciences, Prague).

ÅKE BJÖRCK

Solving large sparse or structured total least squares problems

We discuss a class of methods for solving large scale total least squares (TLS) problems: $\min_{E,r} \|(E, r)\|_F$ subject to $(A + E)x = b + r$. The methods are based on the observation that the TLS solution x_{TLS} satisfies the deregularized normal equations $(A^T A - \sigma_{n+1}^2 I)x_{TLS} = A^T b$, where $\sigma_{n+1} = \|(E, r)\|_F$. Together with the equation $\sigma_{n+1}^2 = b^T(b - Ax_{TLS})$ these normal equations form a nonlinear system of equations for x_{TLS} and σ_{n+1}, which can be solved by Newton's method. A suitable starting approximation is the standard least squares solution x_{LS}. If the Rayleigh quotient $\rho(x) = \|b - Ax\|_2^2/\|(x^T, -1)\|_2^2$ is used to approximate σ_{n+1}^2, the local rate of convergence is (almost always) cubic.
In each step two linear systems of the form $(A^T A - \rho I)z = g$ need to be solved for the corrections. These linear systems can be solved by a preconditioned conjugate gradient method as inner iteration. The same preconditioners as developed for the standard least squares problem can be used. Taking the preconditioner to be the Cholesky factor of $A^T A$ typically leads to convergence in two or at most three Rayleigh quotient iterations. Numerical experiments show that taking $(k + 1)$ inner iterations in the kth step suffices. This makes the methods suitable for solving large sparse or structured TLS problems.
Possible generalizations to multidimensional TLS problems are outlined.

MIKHAIL A. BOTCHEV

SSOR-like preconditioning for the Oseen problem

Large sparse systems of linear equations of the form

$$\begin{bmatrix} A & B^T \\ B & -C \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix}, \quad \begin{array}{l} A \neq A^T > 0, \quad n \times n, \\ C = C^T \geq 0, \quad m \times m, \quad m \leq n, \end{array}$$

often arise in numerical solution of the Navier – Stokes equations (the Oseen problem). To solve the system iteratively, we consider indefinite nonsymmetric preconditioning incorporating the SSOR factorization of A. The skew preconditioning (ZAMM vol. 76, suppl. 3, pp. 483–484) is used to analyze convergence for the case when the skew symmetric part of A dominates.
In numerical experiments the introduced technique is compared with the BFBt and the Stokes preconditionings.

CLAUDE BREZINSKI

Multilevel iterative scheme for systems of equations

We introduce generalizations of the linear and nonlinear Richardson iterative methods for solving systems of linear and nonlinear equations. The optimal scalar relaxation parameter of the descent step is replaced by a matrix whose dimension is much lower than the dimension of the original problem. We give generalizations of the $Delta^k$ method introduced for solving fixed point problems. Various numerical examples illustrate the purpose. They concern the solution of partial differential equations by the nonlinear Galerkin method and incremental unknowns.

ANGELIKA BUNSE–GERSTNER

A Jacobi–like method for solving algebraic Riccati equations on parallel computers

An algorithm to solve continuous-time algebraic Riccati equations through the Hamiltonian Schur form is developed. It is an adaptation of the ideas for an unsymmetric Jacobi method of Eberlein to the case of Hamiltonian matrices. It uses unitary symplectic similarity transformations and preserves the Hamiltonian structure of the matrix. Each iteration step needs only local information about the current matrix, thus admitting efficient parallel implementations on certain parallel architectures. Convergence performance of the algorithm is compared with the recently proposed Hamiltonian–Jacobi algorithm of Byers. The numerical experiments suggest that the method presented here is considerably faster for Hamiltonian matrices which are not near to normality.
This is joint work with Heike Faßbender.

DANIELA CALVETTI

A Lanczos based regularizing iterative method for underdetermined linear systems

We are concerned with the solution of underdetermined linear systems of equations with a very ill-conditioned matrix A, whose dimensions are so large to make solution by direct methods impractical or infeasible. Image reconstruction from projections often gives rise to such systems. In order to facilitate the computation of a meaningful approximate solution, we regularize the linear system, i.e., we replace it by a nearby system that is better conditioned. The amount of regularization is determined by a regularization parameter. Its optimal value is, in most applications, not known a priori. We present a new iterative method based on the Lanczos algorithm for determining a suitable value of the regularization parameter by the discrepancy principle and an approximate solution of the regularized system of equations.

RAYMOND H. CHAN

Iterative Methods for Toeplitz Systems

In this talk, we give some of the latest developments on using the preconditioned conjugate gradient method for solving Toeplitz systems. One of the main advantages of the method is that the complexity of solving a large class of n-by-n Toeplitz systems is reduced to $O(n \log n)$ operations as compared to $O(n \log^2 n)$ operations required by fast direct Toeplitz solvers. Different preconditioners proposed for Toeplitz systems will be reviewed. Applications of the method to Toeplitz-related systems arising from partial differential equations, queuing networks, signal and image processing, integral equations and time series analysis will be given.

TONY F. CHAN

MLBiCGSTAB:A BiCGSTAB Variant Based on Multiple Starting Lanczos Vectors

We present a variant of the popular BiCGSTAB method for solving nonsymmetric linear systems. The method, which we denote by ML (k) BiCGSTAB, is derived from a variant of the BiCG method based on a Lanczos process using multiple ($k > 1$) starting left Lanczos vectors. Compared with the original BiCGSTAB method, our new method produces a residual polynomial which is of lower degree after the same number of steps but which also requires fewer matrix–vector products to generate, on average requiring only $1 + 1/k$ matvec's per step.
Empirically, it also seems to be more stable and faster convergent. The new method can be implemented as a k–term recurrence and can be viewed as a bridge connecting the Arnoldi–based FOM/GMRES methods and the Lanczos–based BiCGSTAB methods.
This is joint work with M.C. Yeung.

PAUL VAN DOOREN

About stability radii

The basic stability radius problem can be defined as follows. Let A be a *stable* matrix with all its eigenvalues in the stability region $\mathcal{S}$ (typically the open left half plane or the open unit disc). The *stability radius* of A is the norm of smallest (complex) perturbation Δ that causes at least one eigenvalue of $A + \Delta$ to become unstable, i.e.

$$r_C = \min \{\|\Delta\|_2, \Delta \in C^{n \times n}, \exists \lambda(A + \Delta) \notin \mathcal{S}\}$$

This problem is well studied by several authors and there exists an analytic formulation for r_C as well as a quadratically convergent algorithm to compute it.
In this talk we discuss several variants and extensions of this standard problem to the generalized eigenvalue problem and to the periodic eigenvalue problem. We also talk about the use of different norms as well as structured perturbations. This is ongoing work with C. Lawrence, C. Oara, J. Sreedhar, A. Tits and V. Vermaut.

ALAN EDELMAN

Recent Progress on Eigenvalue Nearness Problems: Geometrical Analyses and Optimization Approaches

Nearness of a matrix to a multiple eigenvalue is indicated by a small cosine between left and right eigenvectors, as for example is computed by MATLAB's condeig routine or the RCONDE variable in LAPACK. What can we supply the user who wishes to **exactly** obtain the nearest matrix with a multiple eigenvalue or more generally the nearest matrix (or pencil) with a particular canonical form? This is a difficult problem studied in various ways by Boley, Demmel, Golub, Kågström, Ruhe, van Dooren, Wilkinson and many others.
In the first part of this talk, we indicate by which geometrical mechanism current column–at–a–time algorithms such as staircase algorithms fail to obtain the globally closent matrix or pencil.

In the second part of this talk, we show how recently derived algorithms for optimization on the Stiefel manifold can provide a "fix" and will describe current software efforts to realize this fix.
This talk represents joint work with Yanyuan Ma and Ross Lippert, and builds upon research with Erik Elmroth and also Jim Demmel and Bo Kågström.

OLIVER ERNST

Minimal Residual Methods for Stabilized Discretizations of Convection–Diffusion Problems

We examine the effect of stabilization techniques for finite element discretization of convection–diffusion problems on the convergence behavior of the minimal residual Krylov subspace iteration method. It is shown that — besides removing non physical oscillation in the discute solution — this also leads to faster convergence of the discrete iteration.
This is shown for the case of additive multilevel preconditioning for some simple model problems.

BERND FISCHER

Towards optimal streamline upwinding for advection–diffusion problems

In this talk we consider the design of robust and efficient finite element approximation methods for solving advection–diffusion equations. The theme of the talk is that stabilization of the discretization is often achieved by "regularizing" the discrete system which typically introduces stability parameters into the solution process. These must be carefully chosen if the resulting methodology is to be effective — it is all too easy to over–stabilize giving smooth but inaccurate solutions.
It turns out that for the advection–diffusion problem the quality of the approximation is largely determined by spectral properties of the underlying discrete opertor. Our aim is to show that it is possible to guarantee good approximation by choosing the parameter value which gives "optimally convergent" Krylov subspace iterative solvers when applied to the regularized equation systems.
The effectiveness of the proposed schemes will be demonstrated in a variety of examples.

ROLAND W. FREUND

Reduced–order modeling of large–scale dynamical systems by Lanczos–type methods

We present an approach for the stable and efficient computation of matrix Padé approximations to the matrix–valued transfer functions of general multi–input multi–output time–invariant linear dynamical systems. The proposed method is based on a variant of a novel Lanczos–type method for multiple starting vectors, which was recently developed by Aliaga, Boley, Freund and Hernández. We establish a connection between the Lanczos process and matrix Padé approximants of multi–input multi–output transfer functions. This result generalizes the well–known Lanczos–Padé connection between the classical Lanczos process and scalar Padé approximants of single–input single–output transfer functions, to the case of matrix–valued transfer functions.

ANDREAS FROMMER

Krylov Subspace Methods for Problems in Quantumchromodynamics

Quantumchromodynamics (QCD) is the fundamental theory of the strong interaction between matter. Calculating physical observables from this theory requires to solve many very large non–hermitian linear systems which arise from a nearest neighbor coupling on a four–dimensional space–time lattice. QCD computations are one of the most important and time consuming supercomputer applications.

We present recent progress with Krylov subspace methods for solving these systems exploiting non-trivial symmetry properties, particular parameter dependences and preconditioning techniques. In particular, we will focus on parallel SSOR type preconditioners and present a general framework to treat shifted systems simultaneously in restarted GMRES and other Krylov subspace methods.

ELDAR GELADI

Iterative solution of elliptic problems by approximate factorization

We analyze a space-time domain decomposition iteration, for a model advection diffusion equation in one and two dimensions. The asymptotic convergence rate is superlinear, and it is governed by the diffusion of the error across the overlap between subdomains. Hence, it depends on both the size of this overlap and the diffusion coefficient in the equation. However, it is independent of the number of subdomains. The convergence rate for the heat equation in a large time window is initially linear and it deteriorates as the number of subdomains increases. The duration of the transient linear regime is proportional to the length of the time window. For advection dominated problems, the convergence rate is initially linear and it improves as the the ratio of advection to diffusion increases. Moreover, it is independent of the size of the time window and of the number of subdomains. In two space dimensions, the iteration possesses the smoothing property: high modes of the error are damped much faster then low modes. This is a result of the natural smoothing property of the heat equation. Numerical calculations illustrate our analysis.

MARTIN H. GUTKNECHT

Look-ahead Lanczos Revisited

The construction of the iterates and residuals of Lanczos-type solvers is based on either a three-term recurrence or a pair of coupled two-term recurrences for the Lanczos vectors that generate two Krylov spaces. However, the Lanczos process for non-Hermitian matrices is well-known to be endangered by breakdowns. These breakdowns and the corresponding near-breakdowns can be circumvented by look-ahead steps in all but very exceptional situations (the so-called incurable breakdowns). Look-ahead means to replace ill-defined or ill-conditioned Lanczos vectors by other, so-called inner vectors, which still expand the Krylov space, but do not satisfy all the biorthogonality conditions. There are various legitimate ways to define these inner vectors. We discuss the pros and cons of several choices and show that the introduction of certain auxiliary vectors reduces the memory overhead in the case of successive look-ahead steps.
This is joint work with Marlis Hochbruck.

ANNE GREENBAUM

Lanczos Vectors in the Computation of Matrix Functions

The Lanczos algorithm uses a three–term recurrence to construct on orthonormal basis for the Krylov space corresponding to a symmetric matrix A and a nonzero starting vector f. The vectors and recurrence coefficients produced by this algorithm can be used for a number of purposes, including solving linear systems $Au = \varphi$ and computing the matrix exponential $e^{-tA}\varphi$. Although the vectors produced in finite precision arithmetic are **not** orthogonal, we show why they can still be used effectively for these purposes.

MARLIS HOCHBRUCK

On the use of Krylov methods in ODE solvers

In this talk we study the numerical integration of large stiff systems of differential equations by methods that use Krylov approximations for approximating the exponential or a related function of the Jacobian. We first show that Krylov methods for approximating the exponential typically converge faster than those for the solution of the linear systems arising in standard stiff integrators.
The exponential methods offer favorable properties in the integration of differential equations whose Jacobian has large imaginary eigenvalues. The emphasis in this talk lies on the interplay between the construction of an ODE solver and the costs and memory requirements of the involved Krylov processes.
This is joint work with Christian Lubich.

THOMAS K. HUCKLE

Sparse Approximate Inverses

We consider a general sparse matrix A. Computing a sparse approximate inverse matrix M by minimizing $\|AM - E\|$ in the Frobenius norm is very useful for deriving preconditioners in iterative solvers, especially in a parallel environment. First we give an overview over the original SPAI-algorithm for computing such a matrix M.
The problems, that appear in this connection in a distributed memory setting, are the distribution of the data - mainly submatrices of A - on the different processors. An a-priori knowledge of the data that has to be sent to a processor would be very helpful in this connection in order to reduce the communication time. Therefore we compare different strategies for choosing a-priori an approximate sparsity structure of A^{-1}. Such a sparsity pattern can be used as a maximum pattern of allowed entries for the sparse approximate inverse M. Then, with this maximum pattern we are able to distribute the claimed data in one step to each processor. Therefore, communication is necessary only at the beginning and at the end of a subprocess. Using the graphs associated with A, A^T, and A^TA, we develop heuristic methods to find good and sparse approximate patterns for A^{-1}.
Furthermore we suggest the preconditioning of sparse triangular matrices by sparse approximate inverses. If A is well-conditioned then by using the same pattern as in A, a sparse approximate inverse matrix M can be computed very efficiently in a parallel environment and leads to fast convergence in iterative methods like BiCGSTAB.

BO KÅGSTRÖM

Nearby Jordan and Kronecker structures –
a qualitative approach in terms of stratifications and versal deformations

By viewing an n–by–n matrix A as a point in n^2 space instead of an array of numbers or an operator on vectors, and similarly viewing an $m \times n$ matrix pencil $A - \lambda B$ as a point in $2mn$ space, certain numerical computations relating to the Jordan or Kronecker canonical forms can be viewed as moving matrices or matrix pencils from point to point or manifold to manifold in the n^2 and $2mn$ spaces, respectively. Our objective is to make use of the geometry of the matrix and matrix pencil spaces, to improve our knowledge of numerical algorithms and their failures.
We derive *versal deformations* of the Kronecker canonical form by deriving the tangent space and orthonormal bases for the normal space to the orbits of strictly equivalent matrix pencils. These deformations reveal the local perturbation theory of matrix pencils that is related to the Kronecker canonical form. We also obtain a new singular value bound for the distance to the orbits of less generic pencils. The concepts, results and their derivations are mainly expressed in the language of numerical linear algebra. We conclude with experiments and applications.
The problem of *stratification* is to understand how the orbits relate to each other, i.e., to understand the closure hierarchy of Jordan and Kronecker structures. If the clustering of eigenvalues is well–defined

then the only question that may arise is what is the Jordan structure corresponding to an individual eigenvalue. For matrices, it is then enough to consider the stratification of nilpotent matrices, which elegantly can be expressed by dominance orderings of integer partitions. When we are less confident in the clustering, we must consider the stratification of matrix bundles. We use a similar approach for the complete understanding of the stratification problem for orbits and bundles of matrix pencils. As a direct application, since we expect (staircase) algorithms to compute Kronecker structures that are nearby the original structures, algorithms can supply to the user which structures are in the immediate vicinity of the computed structure. This information can also be used in an enhanced staircase algorithm for computing the least (or the most) nearby Kronecker structure with a specific application in mind.
This is ongoing work and in this presentation we review some recent results from joint work with Alan Edelman, MIT and Erik Elmroth, Umeå.

TOM MANTEUFFEL

Conjugate Gradient Algorithms Using Multiple Recursions

Much is already known about when a conjugate gradient method can be implemented with short recursions for the direction vectors. The work done in 1984 by Faber and Manteuffel [1] gave necessary and sufficient conditions on the iteration matrix A, in order for a conjugate gradient method to be implemented with a single recursion of a certain form. However, this form does not take into account all possible recursions. This became evident when Jagels and Reichel [3, 4] used an algorithm of Gragg for unitary matrices [2] to demonstrate that the class of matrices for which a practical conjugate gradient algorithm exists can be extended to include unitary and shifted unitary matrices. The implementation uses short double recursions for the direction vectors. This motivates the study of multiple recursion algorithms.
In this talk, we show that the conjugate gradient method for unitary and shifted unitary matrices can be implemented using a single short term recursion of a special type called an (ℓ, m) recursion with $\ell, m \leq 1$. We then examine the class of matrices for which a conjugate gradient method can be carried out using a general (ℓ, m) recursion. This class includes the class of normal matrices with rational degree (ℓ, m) as well as low rank perturbations of these matrices.
Under some circumstances, an (ℓ, m) recursion can break down. We also show that any (ℓ, m) recursion can be reformulated as m short recursions that will not break down.
This is joint work with Teri Barth.

References

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G. MEURANT

Matrices, Moments and Quadrature II or
How to compute the norm of the error in iterative methods

In this talk, we study the numerical computation of the errors in linear systems when using iterative methods. This is done by using methods to obtain bounds or approximations of quadratic forms $u^T A^{-1} u$ where A is a symmetric positive definite matrix and u is a given vector. These techniques involve quadrature rules, orthogonal polynomials and the Lanczos algorithm. Numerical examples are given for the Gauss–Seidel algorithm.
Moreover, we show that using a special formula for the A–norm of the error relating this norm to the (1,1) element of the inverse of the tridiagonal matrix of the Lanczos process, very good bounds of the error can be computed almost for free during the iterations of the conjugate gradient method leading to a reliable stopping criteria.
This is joint work with Gene Golub.

ARNOLD NEUMAIER

Solving ill-conditioned and singular linear systems:
A tutorial on regularization

It is shown that the basic regularization procedures for finding meaningful approximate solutions of ill-conditioned or singular linear systems can be phrased in terms of simple linear algebra that can be taught in any numerical analysis course. Apart from rewriting many known results in a simpler form, we also derive a new two-parameter family of merit functions for the determination of the regularization parameter. The traditional merit functions from generalized cross validation (GCV) and generalized maximum likelihood (GML) are recovered as special cases.

LOTHAR REICHEL

Computing a few eigenvalues of a large symmetric matrix

Equilibrium configurations of liquid crystals in a finite containment are minimizers of the thermodynamic free energy of the system. It is important to be able to track an equilibrium configuration as the temperature of the liquid crystals is decreased. The path of the minimal energy configuration at a bifurcation point can be computed from the null space of a sparse symmetric matrix, which typically is very large, e.g., of order 300000. We describe an Implicitly Restarted Block Lanczos method designed for the computation of a few extreme multiple or close eigenvalues and associated eigenvectors of a large sparse symmetric matrix, and apply this method to determine the desired null space. 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 depends on the choice of shifts. We propose a new strategy for choosing shifts. Numerical examples 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 the application of tracking an equilibrium configuration of liquid crystals.
This joint work with J. Baglama, D. Calvetti and A. Ruttan.

GERHARD STARKE

Field-of-values analysis of multilevel methods for convection-diffusion-problems

The convergence rate of Krylov subspace methods such as GMRES for the solution of discretized nonsymmetric elliptic problems using multilevel preconditioners is studied. Bounds on the convergence rate are presented which are based on the smallest real part of the field of values of the coefficient matrix and of its inverse. Estimates for these quantities are available during the iteration from the underlying Arnoldi process. Moreover, these bounds arise naturally in the finite element analysis of multilevel preconditioning. The second part of the talk is concerned with a coarsening procedure for convection-dominated problems discretized by the streamline diffusion method. The coarse space operators are constructed based on local solutions along the edges of the corresponding one-dimensional variational problems with respect to the streamline diffusion bilinear form.

ZDENĚK STRAKOŠ

The Role of Orthogonality in the Nonsymmetric Krylov Space Methods

In the symmetric case, the loss of orthogonality among the vectors of the Lanczos basis and its role in slowing down the convergence of the conjugate gradient method has been thoroughly studied. Some questions still remain open, but the essence of the problem seems to be reasonably well understood. In the nonsymmetric case, the situation is different. Potential breakdowns complicate stability analysis of the methods based on three–term recurrences. The loss of orthogonality in the Arnoldi process is not as dramatic as in the Lanczos process. In order to maintain a good level of orthogonality, Householder or iterated Gram–Schmidt orthogonalization schemes have been used and the modified Gram–Schmidt orthogonalization has been strictly preferred over the classical one. Until very recently, the loss of orthogonality among the Arnoldi vectors has not been related to the decrease of the residual in the corresponding Krylov space methods.
In our contribution we present recent results on the subject suggesting that the role of orthogonality in the nonsymmetric Krylov space methods should be carefully re–examined.

EUGENE TYRTYSHNIKOV

Skeleton Approximations and Mosaic Ranks

The fact that nonsingular coefficient matrices can be covered by blocks close to low–rank matrices is well known probably for years. It was used in some cost–effective matrix–vector multiplication algorithms. However, it has been never paid a proper attention in the matrix theory. To fill in this gap we propose a notion of mosaic ranks of a matrix which reduces a description of block matrices with low–rank blocks to a single number. A general algebraic framework will be presented that allows one to obtain some theoretical estimates on the mosaic ranks. We also discuss some practical algorithms and approaches based on interrelations with some concepts of the rank–revealing framework.

G.W. STEWART

A Gap–Revealing Matrix Decomposition

In this paper it is observed that if the R–factor of a pivoted QR decomposition of a matrix A is reduced by postmultiplication by an orthogonal matrix to a lower triangular matrix L then the diagonals of L track the singular values of A much better than to those of the R–factor. Thus the resulting decompositon, which we call a PLQ–decomposition, can be used to find gaps in the singular values, say for rank determination. The decomposition can be computed for no more than twice the work of the original QR–decomposition and furnishes orthonormal bases for the row and null space of A. The approach also leads to a 2–norm estimator for a general matrix.

HENK VAN DER VORST

The main effects of rounding errors in Krylov solvers for symmetric linear systems

The three-term Lanczos process leads, for a symmetric matrix, to bases for Krylov subspaces of increasing dimension. The Lanczos basis, together with the recurrence coefficients, can be used for the solution of linear systems, by solving the reduced system in one way or another. This leads to well-known methods: MINRES (GMRES), CR, CG, and SYMMLQ. We will discuss in what way and to what extent the various approaches are sensitive to rounding errors.
In our analysis we will assume that the Lanczos basis is generated in exactly the same way for the different methods (exept CR), and we will not consider the errors in the Lanczos process itself. These errors may lead to large perturbations with respect to the exact process, but convergence takes still place. Our attention is focused to what happens in the solution phase. We will show that the way of solution may lead, under circumstances, to large additional errors, that are not corrected by continuing the iteration process. Our findings are supported and illustrated by numerical examples.

In the evening the following problems in scientific computing have been presented and discussed:

D. Boley : Algebraic Kronecker structure of matrix pencils and block Toeplitz matrices
M. Brühl/M. Hanke : Electrical impedance tomography
H. Bulgak : A doubling algorithm in scientific computing
M. Eiermann : Field of values and iterative methods
K. Giebermann : Aspects of the boundary element method for Helmholtz equation
N. Higham : Modifying the inertia of matrices arising in optimization
R. Nabben : Decay rates on the inverse of nonsymmetric tridiagonal and band matrices
M. Neumann : Cut edge decoupling and first mean passage times for random walks on graphs
A. Krautstengl : Gerschgorin on the blocks

Berichterstatter: Martin Brühl und Klaus Giebermann

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