MATHEMATISCHES FORSCHUNGSINSTITUT OBERWOLFACH

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Numerical Linear Algebra

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The conference was organized by Gene H. Golub (Stanford), Wilhelm Niethammer (Karlsruhe), Richard S. Varga (Kent); 46 individuals from 12 countries attended. The following topics were emphasized: Iterative solution of nonsymmetric systems of linear equations: Theory, implementation and applications. The 40 contributions offered a broad view in many different directions.

One major topic was the improvement of Lanczos' method for nonsymmetric systems of linear equations, e.g., the detection and explanation of breakdowns and strategies to overcome them. Several talks considered the use of more classical CG-type variants and the design of efficient preconditioners for solving nonsymmetric problems arising in the approximation of partial differential equations arising in fluid dynamics and advection-dispersion problems.

In addition, the convergence properties of polynomial iteration schemes were analyzed in a couple of contexts e.g. for optimality and adaptive improvement. Classical iterative schemes like SOR and ADI were reexamined by several attendees, and included the study of applications to convection diffusion equations and Markov chains.

The spectrum of talks emphasized both, theoretical investigations, e.g. the study of the stability of highly optimized iterative methods, as well as questions of more practical concern such as the efficient implementation of iterative solvers on parallel computers.

As a result of the wide variety of related topics discussed and the good mixture of experts from theory and applications, the intimate atmosphere of the conference led to many fruitful discussions and initiated forthcoming joint projects.

Abstracts

S.F. ASHBY:

(Co–author: M.H. GUTKNECHT)

A matrix analysis of conjugate gradient algorithms

Conjugate gradient methods are powerful techniques for solving the large sparse linear systems that arise in many scientific and engineering applications. To implement a CG method, one must specify an *algorithm*, that is, a sequence of arithmetic operations. Three commonly used CG algorithms are Orthodir, Orthomin, and Orthores. Orthodir is the most robust, and is guaranteed to converge for any nonsingular A. Orthomin and Orthores are more familiar, but less robust: they may "stall" under certain conditions. In this talk we introduce a matrix formulation and use it to explore the relationships between the three algorithms. We first show that Orthodir directly computes a Hessenberg matrix H_k at step k. Orthores also computes a Hessenberg matrix W_k, which in general differs from H_k in the last column, but coincides with H_k at convergence. Orthomin, on the other hand, essentially computes a UL and LU factorization of H_k and W_k, respectively. We will interpret the breakdown of Orthomin and Orthores in terms of these underlying matrix factorizations. Once the breakdown conditions are understood, we can devise new algorithms that avoid these pitfalls. A connection to Lanczos is also discussed. Finally, we consider the special case of B–normal(1) matrices, for which efficient three–term CG algorithms exist.

O. AXELSSON:

(Co–author: P. VASSILEVSKI)

Construction of variable–step preconditioners
for inner–outer iteration methods

The generalized conjugate gradient method was recently applied for the case of variable–step preconditioners, which is in general a nonlinear mapping, and its convergence was analysed.

In a number of practical applications there arise naturally linear algebraic problems with matrices A partioned in a two–by–two block form $A = (A_{i,j})_{i,j=1}^{2}$. For such matrices, a general framework for the construction of variable–step precondi-

tioners utilizing inexact solvers are studied. A particular instance is the use of a conjugate gradient method to compute inner iterations for the first matrix block A_{11} and for the Schur complement matrix $S = A_{22} - A_{21}A_{11}^{-1}A_{12}$.

The disadvantage with this method is that the action of A_{11} is required two or more times during each outer iteration. These actions must be sufficiently accurate, otherwise the rate of convergence can be too slow or even divergence can occur.

In the present paper a modified version of the algorithm is presented where only one accurate action is required per step in addition to an action required only for the computations of the length of a steepest descent step, which can therefore be less accurate. The efficacy of this method will be evident in particular for problems arising in domain decomposition methods.

R. BEAUWENS:

Ordered graphs and numerical linear algebra

We wish, by this talk, to encourage the development of matrix graph concepts that characterize in one or another sense *sparse* matrices and *their ordering* (and that are, therefore, *not* invariant under permutation). We shall give both simple and more sophisticated examples.

As an application of the simple concepts, we shall show that they lead to an elementary and straightforward justification of George and Liu's symbolic factorization algorithm.

As an application of the more elaborate concepts, we shall indicate how they might lead us to a new family of dynamic approximate LU–factorization algorithms where the graphs of the triangular factors would be modified during the factorization process. Such "graph" perturbations would be associated with off–diagonal perturbations (together with diagonal ones). The criterion for controlling their introduction would be to choose them so as to (sufficiently) increase the degree of "S/P consistency" of the upper triangular factor. (NB. By comparison, the presently developed dynamic approximate LU–factorization algorithm uses only diagonal perturbations and controls their introduction by choosing them so as to – sufficiently – increase the diagonal dominance of the upper triangular factor).

Early experiments ... and difficulties will be described.

C. BREZINSKI:

Avoiding breakdown and near–breakdown in Lanczos method

In Lanczos method, a breakdown occurs when a scalar product in the denominator of a coefficient of some recurrence relation is zero. This is due to the non–existence of some orthogonal polynomial. Avoiding breakdown thus consists in jumping over these non–existing polynomials and computing only those which exist. Thus we obtain a breakdown–free algorithm called the MRZ (method of recursive zoom). If a scalar product in a denominator is small in absolute value then a near–breakdown occurs. It can be avoided similarly and the corresponding algorithm was called the BSMRZ. Similar techniques can be used in the Conjugate Gradient Squared (CGS) algorithm. Numerical results showing the effectiveness of these algorithms were given.

T.F. CHAN:

The interface probing technique in domain decomposition

The interface probing technique is an algebraic technique for constructing interface preconditioners in domain decomposition algorithms. The basic technique is to approximate interface matrices by matrices having a specified sparsity pattern. The construction involves only matrix vector products, and thus the interface matrix need not be known explicitly. A special feature is that the approximations adapt to the variations in the coefficients of the equations and the aspect ratios of the subdomains.

This preconditioner can then be used in conjunction with many standard iterative methods, such as conjugate gradient methods.

In this talk, we summarize some old results and also present some new ones, both algebraic and analytic, about the interface probing technique and its applications to interface operators. Comparisons are made with some optimal preconditioners such as the Golub–Mayer preconditioner.

M. EIERMANN:

(Co–authors: H. DANIELS and A. PETERS)

Symmetric versus non–symmetric CG methods
for solving the advection–dispersion equation

We compare two solution strategies based on different time integration schemes applied to the advection–dispersion equation. The first strategy is based on the classical Crank–Nicolson scheme and leads to a non–symmetric system of linear equations which is solved by the conjugate gradient squared (CGS) method or its variant CGStab. The second strategy — introduced recently by Leismann and Frind (1989) — places the advective component of the equation at the old time level and compensates for the resulting errors by introducing an artificial diffusion term. The scheme of Leismann and Frind yields a symmetric positive definite system which can be solved by the classical conjugate gradient (CGHS) method.

Our aim is to present neither CG–like methods nor discretization procedures, but rather to estimate the performance of different combinations of algorithms. For the one–dimensional model problem, we show that the Leismann–Frind/CGHS approach outperforms Crank–Nicolson/CGS with respect to computational work and storage requirements. These theoretical results are illustrated by an efficiency comparison on an IBM 3090 VF for a 3–D groundwater contamination problem.

H. ELMAN:

Ordering effects and acceleration for line iterative methods
applied to non–self–adjoint problems

We present the results of a theoretical and empirical study of iterative methods for cyclically reduced linear systems arising from discrete convection–diffusion problems. Analytic results show the methods to be effective for a wide class of non–self–adjoint problems. In this talk, we focus on the effects of ordering and acceleration on performance. In particular, we show that red–black line–ordered relaxation operators are less sensitive to direction of flow than naturally–ordered operators, and the red–black operators tend to reduce the error in a pair of neighboring (red and black) lines at each iteration. The addition of acceleration strategies such as GMRES or BiCGSTAB typically enhances convergence speed, although there are problems for which restarted GMRES is actually slower than stationary methods.

B. FISCHER:

Polynomial iteration methods for indefinite symmetric linear systems

We present a Chebyshev–like algorithm for solving sparse symmetric indefinite systems of linear equations. Let E be the union of two disjoint intervals containing the spectrum of the coefficient matrix but not the origin. The scheme is based on (explicitly known) polynomials p that satisfy a certain optimality condition on E. The resulting algorithm shares many properties with the one for positive definite matrices.

In order to compute the set E dynamically we combine the polynomial iteration method with MINRES, which leads to a hybrid type algorithm. It turns out that the optimal polynomials p are also useful to study the convergence behavior of MINRES.

Furthermore we show that the p determine optimum polynomial preconditioners for minimal residual methods. Finally, we indicate that the considered methods (may) also work for nonhermitian matrices.

We demonstrate the effectiveness (or noneffectiveness) of the schemes in a variety of numerical experiments.

R. FREUND:

(Co–author: N.M. NACHTIGAL)

QMR: a quasi–minimal residual method for non–Hermitian linear systems

The biconjugate gradient (BCG) method is the "natural" generalization of the classical conjugate gradient algorithm for Hermitian positive definite matrices to general non–Hermitian linear systems. Unfortunately, the original BCG algorithm is susceptible to possible breakdowns and numerical instabilities. In this talk, we present a novel BCG–like approach, the quasi–minimal residual (QMR) method, which overcomes the problems of BCG. An implementation of QMR based on a look–ahead version of the nonsymmetric Lanczos algorithm is proposed. It is shown how BCG iterates can be recovered stably from the QMR process. Some further properties of the QMR approach are given and an error bound is presented. Finally, numerical experiments are reported.

A. FROMMER:

A concept of generalized diagonal dominance for nonlinear functions with applications to nonlinear iterative methods

The class of generalized diagonally dominant matrices contains such interesting subclasses as Ω–diagonally dominant, strictly diagonally dominant and M–matrices.

Here we consider nonlinear functions on $\mathbf{R}^n$ and derive a concept of nonlinear generalized diagonal dominance which reduces to the usual one in case of an affine function. As in the linear case, important subclasses are given by strictly or weakly Ω–diagonally dominant functions and certain M–functions. As an application of our concept whe show how one can easily — and in a uniform manner — derive convergence results on global convergence of nonlinear SOR–like iterations such as asynchronous or (nonlinear) SOR–multisplitting iterations.

A. GREENBAUM:

Fast solution of Laplace's equation in multiply connected domains

Recent advances in numerical methods have made the use of integral equations far more attractive for solving many of the problems of mathematical physics. Although integral equation formulations result in dense linear systems, the matrices have highly clustered eigenvalues and are very amenable to solution by iterative methods. The dense matrix need never be formed and the product of the n by n matrix, arising from a suitable integral operator, with an arbitrary vector can be computed in time $O(n)$, using the fast multipole method.

We discuss the use of an integral equation formulation, together with iterative linear system solvers and the fast multipole method, to solve Laplace's equation on multiply connected domains. The approach requires the solution of a single system of linear equations for the unknown density values and the unknown circulations. A preconditioner is introduced, and the GMRES method is shown to be especially effective for such problems.

M.H. GUTKNECHT:

Squared Lanczos methods and product methods

For solving large sparse non–Hermitian linear systems we consider Krylov space methods where the nth residual polynomial is the product of the nth residual polynomials ρ_n of the Lanczos biconjugate gradient method (BiCG) and a second polynomial τ_n of the same degree. One such method is Sonneveld's CGS, where $\tau_n := \rho_n$, another one is van der Vorst's BiCGStab, where τ_n is a product of linear factors which are successively determined by a one–dimensional minimization. We assume that τ_n satisfies a three–term recurrence relation and present in particular an extension of BiCGStab in which τ_n is built up from quadratic factors determined by a two–dimensional minimization. When applied to a real system $Ax = b$, τ_n may have conjugate complex zeros and may thus effectively help to damp the residuals. First numerical experiments are very promising.

M. HANKE:

Iterative methods for ill–conditioned linear systems

Given the linear system $Ax = b$, where A is nonsymmetric, $\|A\| \leq 1$, we consider the Richardson iterative method for the normal equations,

$$x_k = x_{k-1} + A^*(b - Ax_{k-1}), \quad x_0 = 0, \ k = 1, 2, \ldots .$$

We present a convergence analysis which is based on stipulations on the smoothness of the exact solution rather than on the spectrum of A. This is leading to new error bounds which become sharp as the condition number of A tends to infinity: consequently, this kind of analysis is well suited for the study of ill–conditioned problems.

The concept may be generalized to arbitrary semiiterative methods. In this case, the asymptotic speed of convergence becomes almost optimal if certain two–step methods introduced by Stiefel and Brakhage are used to accelerate Richardson's iteration.

As a matter of fact, the solution of an ill–conditioned linear system is rather sensitive to perturbations in the right hand side data. We will show that semiiterative methods may be used to compute stable approximations which are superior in many cases to those of Tikhonov's regularization method with respect to both, efficiency and accuracy.

U. LANGER:

Iterative solvers for the biharmonic equation

The paper is devoted to the numerical solution of the first biharmonic boundary value problem

$$\left.\begin{aligned} \Delta^2 u(x) &= f(x), \quad x \in \Omega \subset \mathbf{R}^2 \\ u(x) = \partial u(x)/\partial n &= 0, \quad x \in \partial\Omega \end{aligned}\right\} \qquad (1)$$

in some plane, bounded domain Ω. One of the most simple discretization methods is the variational finite difference technique proposed by V.G. Korneev (1971) and leading to 5–points finite difference schemes with nodal parameters approximating the unknown function and its first (or mixed second) derivatives at the nodal points. There are several fast direct methods for solving such schemes in rectangular domains under appropriate boundary conditions. These fast direct methods can be utilized within the method of fictitious components and within the domain decomposition method in order to construct efficient and highly parallelizable iterative methods for solving (1) in more complicated domains such as arising in technical applications.

X. LI:

An adaptive method for solving nonsymmetric linear systems involving application of SCPACK

An adaptive method for solving large systems of real linear equations $x = T\vec{x} + c$ is developed with the aid of SCPACK. The results from function theory, approximation theory, and conformal mapping theory are used to construct nearly asymptotically optimal semiiterative methods (AOSIMs). GMRES methods are used for eigenvalue estimates of T and for a guess x_0. A polygon Ω is initialized and updated later. The algorithm uses SCPACK to find numerically the conformal mapping ψ from the exterior to the unit disk onto the exterior to Ω. Then, LINPACK and MINPACK are applied to solve the weighted nonlinear least squares problem with small amount of unknowns, say less than 10, to get a rational approximation r to ψ in the ℓ_2–norm. A better SIM w.r.t. Ω can be constructed from r and is performed. The procedure is repeated several times. After a near AOSIM is found, iterates will give the solution of the system.

V. MEHRMANN:

Numerical methods for unsymmetric block structured matrices arising in fluid flow computations

We discuss block matrices of the form $M = [A_{ij}]$, where every A_{ij} is a $k \times k$ matrix, A_{ii} has positive real eigenvalues and A_{ij} has nonpositive real eigenvalues. These matrices are natural block–generalizations of Z–matrices and M–matrices. Matrices of this type arise in the numerical solution of Euler equations in fluid flow computations. We give conditions for the convergence of block iterative methods like block Jacobi or block SOR and also study the spectrum of such matrices in general.

G. MEURANT:

Iterative methods for solving complex linear systems

We are interested in solving the large linear systems

$$Ax = b,$$

A being a matrix with complex entries, that arise from discretization of Maxwell equations. Additionally, we would like to consider the problem when we have many right hand sides

$$Ax_i = b_i \qquad i = 1, \ldots, m.$$

We introduce a general framework for solving these problems.

Let H be a definite complex matrix and let $\tau(r) = (r, Hr)$ be a functional from $\mathbb{C}^n$ to $\mathbb{R}^+$, $(\cdot, \cdot)$ being the usual complex scalar product. τ is strictly convex and has an unique minimum in $r = 0$. We construct a basis $\{d^0, \ldots, d^k\}$ orthogonal in the scalar product defined by the Hermitian matrix $N = A^H H A$ and we minimize τ on $x^0 + < d^0, \ldots, d^k >$ where $x^0 \in \mathbb{C}^n$ is the starting vector. We also introduce a matrix K to relate the gradient of the functional g^k and directions d^k. By proper choices of H and K most of the well known methods are recovered, e.g. CG, Orthomin, BiCG.

To solve the problem with many right hand sides, we choose one system and start building a basis with this system and minimizing $\tau(r_i) = (r_i, Hr_i)$ for the other systems, $r_i = b_i - Ax_i$. When the basis system has converged, we switch to another

system to construct the basis. It can be shown that the new direction can be chosen such that the orthogonality properties are preserved.

We give some numerical examples on simple model problems showing how these different iterative methods compare.

A. MEYER:

Parallel realization of CG–like methods for non–symmetric large sparse FE–systems for local memory/message passing parallel architectures

For symmetric partial differential finite element equations a very natural parallel realization of the preconditioned conjugate gradient method (PCGM) is obtained from subdividing the domain into non–overlapping subdomains along finite element boundaries. On a local memory parallel environment minimal data transfer is achieved (per step of PCGM) from a special vector distribution over the processors following the finite element splitting of the stiffness matrix K. The same can be found of some variants of CG–like algorithms in the non–symmetric case, if the inner product is defined appropriately. We demonstrate that an inner product $< x, y >= y^T P x$ with $P = K^T C^{-1} K$ has some advantages from practical and theoretical points of view, where the hierarchical preconditioning C was used.

N. NACHTIGAL:

(Co–authors: R. FREUND and M.H. GUTKNECHT)

An implementation of the look–ahead Lanczos algorithm for non–Hermitian matrices

The nonsymmetric Lanczos method can be used to compute eigenvalues of large sparse non–Hermitian matrices or to solve large sparse non–Hermitian linear systems. However, the original Lanczos algorithm is susceptible to possible breakdowns and potential instabilities. We present an implementation of a look–ahead version of the Lanczos algorithm which overcomes these problems by skipping over those steps in which a breakdown or near–breakdown would occur in the standard process. The proposed algorithm can handle look–ahead steps of any length and requires the same number of matrix–vector products and inner products as the

standard Lanczos process without look–ahead.

M. NEUMANN:

(Co–author: L. ELSNER)

Monotonic sequences and rates of convergence of asynchronized iterative methods

We shall consider comparing the rate of convergence of two asynchronized parallel iteration schemes for solving monotone systems. The two iteration schemes differ in that one always computes the current approximation from a more recent iteration than the other. In general relying on more recent approximations does not lead to faster convergence, but when this process does not undergo a certain slowdown, it can always be counted to have a more favorable convergence rate.

Our analysis is based on constructing and comparing monotonic sequences in a higher dimensional space in which the original iterations take place.

O. NEVANLINNA:

How fast can iterations converge?

As of today we understand well what makes cg to converge fast, but general understanding of how to precondition nonsymmetric problems to allow fast acceleration is largely missing. In this talk a general framework is outlined which aims to provide tools for this. We write our problem as a fixed point problem for a bounded linear operator L in a Banach space X:

$$x = Lx + b.$$

Traditionally we have looked at the *spectral radius* of L, say $\rho(L)$ but already for selfadjoint operators in (finite dimensional) Hilbert spaces the acceleration properties of cg have been discussed in other terms. We do it all here in terms of the *spectrum* $\sigma(L)$ by associating to it the *optimal reduction factor* $\eta(L)$ which is a nonnegative constant. Also, to a given polynomial sequence, associated with an acceleration procedure, we associate a generating operator which has a similar relation to $\eta(L)$

as the resolvent operator has to $\rho(L)$. We demonstrate how this generating operator codes the speed of convergence from the fastest to the slowest including finite termination, superlinear, linear and sublinear convergence.

W. NIETHAMMER:

Remarks on scheduling of iterative methods related to SOR

It is well known that Jacobi iterative methods for linear systems of equations are parallelized in a natural way whereas this does not hold for Gauss–Seidel and SOR methods. In [Niethammer, Numer. Math. 56, 247–256 (1989)], using a columnwise procedure, a scheduling of SOR is presented which is — for dense matrices — suited for parallelization nearly as well as Jacobi's method. For banded matrices the algorithm proposed possesses asymptotically maximal speed up. In this talk it is examined how this implementation can be used in iterative methods related to SOR. For Kaczmarz's and de la Garza's method this algorithm is not efficient, but it can be applied in the computation of the stationary distribution of a finite homogeneous Markov chain. The implementation proposed is especially appropriate for the iterative solution of linear complementarity problems, for serial as well as for parallel computation.

D.P. O'LEARY:

(Co–authors: P.C. HANSEN and G.W. STEWART)

Regularizing conjugate gradient iterations for solving discrete ill–posed problems

This work concerns the use of iterative methods of the conjugate gradient (Krylov subspace) family for solving discretizations of ill–posed problems. Out of a large family of mathematically equivalent conjugate gradient methods, we choose to concentrate on LSQR. We analyze and demonstrate the inherent regularization properties of LSQR by theory and examples, present a stopping criterion based on the "L–curve", and investigate conditions under which additional regularization is necessary.

M.L. OVERTON :

(Co–author: G.H. GOLUB)

The convergence of inexact Chebyshev and Richardson methods

The Chebyshev and second–order Richardson methods are classical iterative schemes for solving linear systems. We consider the convergence analysis of these methods when each step of the iteration is carried out inexactly. This has many applications, since a preconditioned iteration requires, at each step, the solution of a linear system which may be solved inexactly using an "inner" iteration. We derive an error bound wich applies to the general nonsymmetric inexact Chebyshev iteration. We show how this simplifies slightly in the case of a symmetric or skew–symmetric iteration, and we consider both the cases of underestimating or overestimating the spectrum. We show that in the symmetric case, it is actually advantageous to underestimate the spectrum when the spectral radius and the degree of inexactness are both large. This is not true in the case of the skew–symmetric iteration. We show how similar results apply to the Richardson iteration. Finally, we describe numerical experiments which illustrate the results and suggest that the Chebyshev and Richardson method, with reasonable parameter choices, may be more effective than the conjugate gradient method in the presence of inexactness.

W. QUECK:

The convergence rate of the Arrow–Hurwicz algorithm for a nonlinear mixed finite element problem

The nonlinear system $A(u) + Bp = f$, $B^T u = g$ to determine $u \in \mathbb{R}^n$ and $p \in \mathbb{R}^m$ can be solved by the preconditioned Arrow–Hurwicz algorithm

$$J\frac{u^{k+1} - u^k}{\omega} + A(u^k) + Bp^k = f,$$
$$-C\frac{p^{k+1} - p^k}{\tau} + B^T u^{k+1} = g,$$

where J and C are some symmetric and positive definite preconditioners that satisfy the spectral equivalence estimates

$$\lambda_1 J \le A'(u) \le \lambda_2 J \quad \text{and} \quad \mu_1 C \le B^T J^{-1} B \le \mu_2 C.$$

The Fréchet–derivative $A'(u)$ of A is supposed to be symmetric and positive definite. The final estimate of the error $x^k = (u^k - u, p^k - p)^T$ after k iteration steps has the form $\|x^k\| \leq \rho^k \|x^0\|$, where the convergence rate ρ can be estimated by $\rho \leq \rho_1^{opt} + \varepsilon c$. In the case of an optimal choice of the parameters τ and ω the essential part ρ_1^{opt} of ρ is given by $\rho_1^{opt} = (1 - c_{opt}(\lambda_1/\lambda_2)^2 \mu_1/\mu_2)^{0.5}$, ε can be chosen sufficiently small. If we can choose such preconditioners J and C such that the ratios λ_1/λ_2 and μ_1/μ_2 are independent of the discretization parameter h then the Arrow–Hurwicz algorithm is asymptotically optimal with respect to the operation count.

L. REICHEL :

(Co–author: C. JAGELS)

The isometric Arnoldi process

The Arnoldi process can be applied to compute a few eigenvalues and eigenvectors of a large non–Hermitian matrix, as well as to the iterative solution of non–Hermitian linear systems of equations. When the matrix is Hermitian the Arnoldi process simplifies to the Lanczos process. If the matrix is unitary then the isometric Arnoldi process is obtained. We present a new implementation of the isometric Arnoldi process that requires fewer arithmetic operations and less computer storage than the Arnoldi process when applied to a general matrix. This implementation is applied to the iterative solution of linear systems of equations.

T. RUSTEN:

Preconditioned iterative methods for saddle point problems

A preconditioned iterative method for indefinite linear systems corresponding to saddle point problems of the form

$$\begin{aligned} Mx + By &= b \\ B^T x &= c, \end{aligned}$$

is suggested. Here $M \in \mathbf{R}^{n \times n}$ is symmetric and positive definite, $B \in \mathbf{R}^{n \times m}$ with $m \leq n$ and B has full rank; i.e., $\text{rank} B = m$. The block structure of the systems are utilized in order to design effective preconditioners, while the governing iterative

method is a standard minimum residual method. The method is applied to systems which arise from discretizations of Stokes problem and mixed formulations of second order elliptic problems.

P.E. SAYLOR:

(Co–authors: S.F. ASHBY, S. LEE, L. PETZOLD and R. SKEEL)

Initial value problems and iterative methods

Initial value problems yield linear algebraic equations at each time step. The error due to a predictor approximation to the solution is shown to be such that the Chebyshev method is appropriate. A matrix–free formulation is assumed. Various technical difficulties arise for which a hybrid version (Elman–Saad–Saylor) of the Manteuffel algorithm is well suited. The adaptive feature of the Manteuffel algorithm is also applicable to the Newton iteration in the nonlinear case.

A. SIDI:

Recent developments in convergence acceleration methods for vector sequences and applications to linear and nonlinear systems

In many problems of science and engineering, one is confronted with the task of solving very large scale systems of linear or nonlinear equations. Such systems arise, for example, from discretization of continuum problems. One common way of solution involves the use of iterative techniques. In many cases of interest, however, these techniques suffer from slow convergence rates and hence tend to become expensive timewise. Recently, acceleration (or extrapolation) methods have been used in conjunction with iterative techniques in order to enhance the convergence properties of the latter. In this talk, we review briefly some of the extrapolation methods. We mention some results pertaining to their convergence and stability properties and mention different ways in which they can be implemented. We point out to their connection with known Krylov subspace methods. Finally, we show examples of applications to linear as well as nonlinear systems, including some that arise in computional fluid mechanics problems.

G. STARKE:

Field of values and the ADI method for non–normal matrices

The convergence of an iterative method is usually measured either by the spectral radius or by a matrix norm of the iteration operator. However, for non–normal matrices, each one of these approaches has its drawbacks. The first one only describes the asymptotic rate of convergence, the second usually produces estimates which are much too pessimistic. Recently, M. Eiermann suggested to use the field of values to judge the performance of an iterative method. This will be substantiated in this paper by upper bounds for the error reduction in the ADI method based on the field of values.

Numerical experiments, obtained for a model problem of discretized non–self–adjoint elliptic boundary value problems, show that these estimates for the error reduction in the ADI method — applied to the corresponding symmetrized linear system — are useful for an a priori prediction of the convergence behavior. Moreover, the results suggest the use of the field of values as a basis for the calculation of the optimal ADI parameters if H and V are highly non–normal.

W.J. STEWART:

Queueing networks and p–cyclic Markov chains

Queueing network models are introduced and it is shown how p–cyclic Markov chains can be obtained from certain types of queueing models. The block SOR method for the computation of the steady–state distribution of finite Markov chains that possess p–cyclic infinitesimal generators is considered. It is shown that convergence, in a sense more general than the usual, may be obtained, even if the SOR iteration matrix violates the usual conditions for semiconvergence. Necessary and sufficient conditions for convergence in this, extended, sense are derived. They are then applied in the case where the p^{th} power of the associated Jacobi matrix of the system to be solved possesses only nonnegative eigenvalues. Exact convergence intervals and the optimal ω values are derived for this case. In addition to the "usual" optimal ω in the interval $(1, \frac{p}{p-1})$, other ω values, that yield convergence in the extended sense, are found to achieve the same, optimal, convergence rate. Numerical tests indicate that small perturbations of ω around the optimal value affect the convergence factor much less, if these newly introduced optimal ω values are used.

D.B. SZYLD:

Two–stage methods

We discuss the convergence theory of two–stage methods. These are methods for the solution of $Ax = b$, where $A = M - N$ and the usual (outer) step $Mx_{k+1} = Nx_k + b$ is in turn solved iteratively, say using a splitting $M = F - G$.

We discuss in particular block iterative methods and make some comparisons with multisplitting methods. We compare asymptotic rates of convergence and we present numerical experiments on parallel computers.

In addition, we discuss two–stage semiiterative methods, that is, semiiterative methods in which the (outer) step is in turn solved iteratively.

L.N. TREFETHEN:

Spectra and pseudospectra of convection–diffusion operators

Convection–diffusion operators are canonical examples of non–self–adjoint operators; in numerical linear algebra their discretizations are popular test problems for SOR, CGN, GMRES, CGS, QMR, BICGSTAB, etc.. To be specific, consider the operator

$$\mathcal{L}u = \nu u_{xx} + u_x, \qquad u(0) = u(L) = 0$$

acting on a suitable submanifold of $L^2[0, L]$ $(\nu, L > 0)$. The spectrum of L is a discrete subset of the negative real axis, but the *ϵ–pseudospectra* — the subsets of $\mathbb{C}$ with $\|(zI - \mathcal{L})^{-1}\| \geq \epsilon^{-1}$ — approximate the region bounded by the parabola $Re\, z = -\frac{\nu}{2}(Im\, z)^2$.

It follows that for many practical purposes, L behaves as if its spectrum fills a parabola. This has consequences for iterative methods — for example, to directionality effects in Gauss–Seidel and SOR sweeps, where then importance of sweeping in the physically correct direction is explained by the very different pseudospectra in the two cases.

P.S. VASSILEVSKI:

(Co–author: O. AXELSSON)

Multilevel and domain decomposition methods

A recursive way of constructing variable–step of, in general, nonlinear multilevel preconditioners for selfadjoint and coercive second order elliptic problems, discretized by the finite element method is proposed. The preconditioners satisfy certain coercivity and boundedness properties which allow them to be used in generalized conjugate gradient, GCG type iterative methods. The preconditioner is constructed recursively from the coarsest to finer and finer levels. Each preconditioning step requires only block–diagonal solvers at all levels except at every k_0, $k_0 \geq 1$, level where we perform a sufficient number ν, $\nu \geq 1$, of GCG–type variable–step iterations that involve the use again of a variable–step preconditioning for that level.

It turns out that for any sufficiently large k_0 and, asymptotically, for ν sufficiently large, but not too large, the method has both an optimal rate of convergence and an optimal order of computational complexity, both for two and three space dimensional problem domains.

The method requires no parameter estimates and the convergence results do not depend on the regularity of the elliptic problem.

H. VAN DER VORST:

Bi–CGSTAB: background and some observations

CGS is an often faster converging variant of Bi–CG. It's erratic convergence behavior, however, is notorious. We will show that CGS might converge, in the sense that the updated residual has a small norm, but that the finally obtained approximation to the solution may have little or no significance. This problem in CGS can in general not simply be repaired be replacing the updated residual by the real residual in the iteration procedure.

In another variant of Bi–CG, named Bi–CGSTAB, the convergence behavior is observed to be much more smoother and, as an unexpected bonus, Bi–CGSTAB often also outperforms CGS with respect to the required amount of computational work.

Though this looks quite promising, there are also some strange effects in Bi–CGSTAB in the presence of rounding errors. In the presentation we will briefly

discuss how Bi–CGSTAB and CGS are related with Bi–CG (which helps to explain some of the observed effects) and we will give some numerical examples which show the effects of rounding errors to the iteration process for Bi–CGSTAB.

M. WHEELER:

Modeling advection–diffusion–reaction problems

We discuss finite element and finite difference methods for approximating transport–dominated parabolic partial differential equations. We emphasize operator splitting techniques in which first order terms are treated explicitly in time and diffusion implicitly. For the discrete system this approach leads to a symmetric positive definite system of algebraic equations. In our presentation we describe both theoretical and computational results performed on the INTEL RX.

G. WITTUM:

A new class of fast solvers for large systems of equations

We present a new class of fast solvers based on a special sequence of incomplete decompositions, the so–called frequence–filtering decompositions. The corresponding smoothing correction method is based on the multi–grid idea, i.e. successively filtering out certain frequencies from the error, without using coarse grids. Thus there are no basic problems with robustness as in multi–grid. The corresponding method has an asymptotic complexity of $O(n \log n)$, on grids of intermediate size, however, it is quite efficient and competes quite well with multi–grid.

After presenting the algorithms we give a convergence proof and finally several examples on the performance of the new method applied to linear and non–linear equations.

H. WOŹNIAKOWSKY:

Optimality results of the solution of large linear systems

Consider a large linear system $Ax = b$, where $A \in F$ and b is an $n \times 1$ vector. Here F

is a class of $n \times n$ nonsingular matrices which represents a priori information about A. We also assume that we can compute $Ay, A^T z$ for any $n \times 1$ vectors y and z.

We address the following problem: What is the minimal number of matrix vector multiplications needed to compute $x = x(A, b)$ such that

$$\|Ax - b\| \leq \varepsilon \|b\|, \ \forall A \in F, \ \forall b.$$

Here $\|\cdot\|$ stands for the 2–norm and $\varepsilon \in [0, 1)$.

The answer to our problem depends, obviously, on the class F. Assume that F is orthogonally invariant, i.e., $A \in F \Rightarrow Q^T A Q \in F$ for any $n \times n$ orthogonal Q. Then using the recent results of Nemirovsky (1990, 1991), to be published in J. of Complexity, one can show that:

1° Symmetric case, i.e., $A \in F \Rightarrow A = A^T$.
Krylov information is optimal as long as the needed number of steps $\leq 1/2(n-3)$.

2° Nonsymmetric case. Let
$$F = \{A : \|A\|^{-1} spect((A^T A)^{1/2}) \subset X \subset \mathbf{R}\},$$
where X is compact. Then Krylov information is optimal within a factor of 2.

Krylov information for the symmetric case is given by $b, Ab, \ldots, A^k b$, and for the nonsymmetric case by $b, A^T Ab, \ldots, (A^T A)^k b$.

Although it may happen that the optimal algorithm using Krylov information is hard (or even impossible) to implement, one can show that the classical MINRES algorithm is optimal to within one (additive) step.

We also mention known results on rounding error analysis without and with iterative refinement. The talk is ended by presenting two open problems on the minimal number of inner products and linear functionals needed to compute the approximate solution.

A.YU. YEREMIN:

Incomplete BSSOR preconditionings for solving unsymmetric linear systems

Let $A = L + D + U$ be a nonsingular positive definite matrix and L and U are its strictly lower and upper block triangular parts, while D is the block diagonal. We consider the so called incomplete BSSOR (IBSSOR) preconditionings based on using

instead of exact direct solvers for D incomplete triangular splittings $D = \tilde{D}_L \tilde{D}_U + Q$. It is shown that the multiplication of the IBSSOR preconditioned matrix requires $nz(L) + nz(U) + 2(nz(\tilde{D}_L) + nz(\tilde{D}_u)) + nz(Q)$, where $nz(X)$ stands for the number of nonzeros of a matrix X. We also derive estimates of the deterioration of quality when passing from BSSOR to the corresponding IBSSOR preconditioning.

D.M. YOUNG:

(Co–authors: P.O. FREDERICKSON and B. VONA)

Multilevel methods for solving large sparse linear systems resulting from the use of discretization methods for solving partial differential equations

The numerical solution of a partial differential equation by finite difference methods frequently leads to the problem of solving a large system of linear algebraic equations where the coefficient matrix, A, is sparse. Iterative methods are often used to solve such a system. A typical iterative procedure involves the use of a polynomial acceleration procedure to speed up the convergence of a basic iterative method, such as the Jacobi method or the incomplete Cholesky method. Frequently–used polynomial acceleration procedures include Chebyshev acceleration and conjugate gradient acceleration. In this talk we describe how improved iterative procedures can often be constructed by the use of special preconditioners. Examples of such preconditioners include: the use of a five–point difference equation as a preconditioner for a nine–point equation; the use of a skewed five–point difference equation as a preconditioner for the regular five–point equation; and a two–level parallel multigrid procedure developed by Frederickson and McBryan for solving difference equations in one and two dimensions. To accelerate the convergence special polynomials can be used which are related to the special preconditioners and which can be constructed analytically or numerically to have certain optimization properties.

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