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*This volume is dedicated to Wilhelm Niethammer
on the occasion of his 60th birthday.*

Contents

- 1 An implicitly restarted Lanczos method for large symmetric eigenvalue problems. *D. Calvetti, L. Reichel, and D.C. Sorensen.*

Abstract. The Lanczos process is a well known technique for computing a few, say k , eigenvalues and associated eigenvectors of a large symmetric $n \times n$ matrix. However, loss of orthogonality of the computed Krylov subspace basis can reduce the accuracy of the computed approximate eigenvalues. In the implicitly restarted Lanczos method studied in the present paper, this problem is addressed by fixing the number of steps in the Lanczos process at a prescribed value, $k + p$, where p typically is not much larger, and may be smaller, than k . Orthogonality of the $k + p$ basis vectors of the Krylov subspace is secured by reorthogonalizing these vectors when necessary. The implicitly restarted Lanczos method exploits that the residual vector obtained by the Lanczos process is a function of the initial Lanczos vector. The method updates the initial Lanczos vector through an iterative scheme. The purpose of the iterative scheme is to determine an initial vector such that the associated residual vector is tiny. If the residual vector vanishes, then an invariant subspace has been found. This paper studies several iterative schemes, among them schemes based on Leja points. The resulting algorithms are capable of computing a few of the largest or smallest eigenvalues and associated eigenvectors. This is accomplished using only $(k + p)n + O((k + p)^2)$ storage locations in addition to the storage required for the matrix, where the second term is independent of n .

Key words. Lanczos method, eigenvalue, polynomial acceleration.

AMS(MOS) subject classification. 65F15.

Files. vol.2.1994/pp1-21.dir/pp1-21.ps, vol.2.1994/pp1-21.dir/pp1-21.pdf.

Forward References.

- 22 Multigrid conformal mapping via the Szegő kernel. *Barry Lee and Manfred R. Trummer.*

Abstract. We introduce a multilevel scheme to solve a second kind integral equation which is important in computing conformal maps. This scheme outperforms conjugate gradient methods previously employed for smooth regions. An analysis of the two-grid scheme is provided.

Key words. conformal mapping, multigrid, Szegő kernel, integral equations.

AMS(MOS) subject classifications. 45L10, 45B05, 65R20, 65F20, 65F10.

Files. vol.2.1994/pp22-43.dir/pp22-43.ps, vol.2.1994/pp22-43.dir/pp22-43.pdf.

Forward References.

- 44 Displacement preconditioner for Toeplitz least squares iterations. *Raymond H. Chan, James G. Nagy, and Robert J. Plemmons.*

Abstract. We consider the solution of least squares problems $\min \|b - Ax\|_2$ by the preconditioned conjugate gradient (PCG) method, for $m \times n$ complex Toeplitz matrices A of rank n . A circulant preconditioner C is derived using the T. Chan optimal preconditioner for $n \times n$ matrices using the displacement representation of A^*A . This allows the fast Fourier transform (FFT) to be used throughout the computations, for high numerical efficiency. Of course A^*A need never be formed explicitly. Displacement-based preconditioners have also been shown to be very effective in linear estimation and adaptive filtering. For Toeplitz matrices A that are generated by 2π -periodic continuous complex-valued functions without any zeros, we prove that the singular values of the preconditioned matrix AC^{-1} are clustered around 1, for sufficiently large n . We show that if the condition number of A is of $O(n^\alpha)$, $\alpha > 0$, then the least squares conjugate gradient method converges in at most $O(\alpha \log n + 1)$ steps. Since each iteration requires only $O(m \log n)$ operations using the FFT, it follows that the total complexity of the algorithm is then only $O(\alpha m \log^2 n + m \log n)$. Conditions for *superlinear convergence* are given and numerical examples are provided illustrating the effectiveness of our methods.

Key words. circulant preconditioner, conjugate gradient, displacement representation, fast Fourier transform (FFT), Toeplitz operator.

AMS(MOS) subject classifications. 65F10, 65F15.

Files. vol.2.1994/pp44-56.dir/pp44-56.ps, vol.2.1994/pp44-56.dir/pp44-56.pdf.

Forward References.

- 57 Minimization properties and short recurrences for Krylov subspace methods. *Rüdiger Weiss.*

Abstract. It is well known that generalized conjugate gradient (cg) methods, fulfilling a minimization property in the whole spanned Krylov space, cannot be formulated with short recurrences for nonsymmetric system matrices. Here, Krylov subspace methods are proposed that do fulfill a minimization property and can be implemented as short recurrence method at the same time. These properties are achieved by a generalization of the cg concept. The convergence and the geometric behavior of these methods are investigated.

Practical applications show that first realizations of these methods are already competitive with commonly used techniques such as smoothed biconjugate gradients or QMR. Better results seem to be possible by further improvements of the techniques. However, the purpose of this paper is not to propagate a special method, but to stimulate research and development of new iterative linear solvers.

Key words. conjugate gradients, convergence, linear systems, Krylov methods.

AMS(MOS) subject classifications. 65F10, 65F50, 40A05.

Files. vol.2.1994/pp57-75.dir/pp57-75.ps, vol.2.1994/pp57-75.dir/pp57-75.pdf.

Forward References.

- 76 Efficient iterative solution of linear systems from discretizing singular integral equations. *Ke Chen.*

Abstract. In this paper we study the solution of singular integral equations by iterative methods. We show that discretization of singular integral operators obtained by domain splitting yields a system of algebraic equations that has a structure suitable for iterative solution. Numerical examples of Cauchy type singular integral equations are used to illustrate the proposed approach. This paper establishes a theory for experimental results presented previously.

Key words. singular integral equations, non-compact operators, direct solutions, preconditioning, conjugate gradient iterative methods.

AMS(MOS) subject classifications. 65F10, 65N38, 45E05.

Files. vol.2.1994/pp76-91.dir/pp76-91.ps, vol.2.1994/pp76-91.dir/pp76-91.pdf.

Forward References.

- 92** Modified Specht's plate bending element and its convergence analysis. *T.M. Shih and Junbin Gao.*

Abstract. This paper discusses Specht's plate bending element, shows the relationships between $\int_{F_\rho} w ds$ or $\int_{F_\rho} \frac{\partial w}{\partial n} ds$ and the nodal parameters (or degrees of freedom), further it sheds lights on the construction methods for that element, and finally it introduces a new plate bending element with good convergent properties which passes the F-E-M-Test is derived.

Key words. interpolation, nonconforming finite element, Specht's element

AMS(MOS) subject classifications. 41A05, 65D05, 65N30.

Files. vol.2.1994/pp92-103.dir/pp92-103.ps, vol.2.1994/pp92-103.dir/pp92-103.pdf.

Forward References.

- 104** Look-ahead Levinson- and Schur-type recurrences in the Padé table. *Martin H. Gutknecht and Marlis Hochbruck.*

Abstract. For computing Padé approximants, we present presumably stable recursive algorithms that follow two adjacent rows of the Padé table and generalize the well-known classical Levinson and Schur recurrences to the case of a nonnormal Padé table. Singular blocks in the table are crossed by look-ahead steps. Ill-conditioned Padé approximants are skipped also. If the size of these look-ahead steps is bounded, the recursive computation of an (m, n) Padé approximant with either the look-ahead Levinson or the look-ahead Schur algorithm requires $O(n^2)$ operations. With recursive doubling and fast polynomial multiplication, the cost of the look-ahead Schur algorithm can be reduced to $O(n \log^2 n)$.

Key words. Padé approximation, Toeplitz matrix, Levinson algorithm, Schur algorithm, look-ahead, fast algorithm, biorthogonal polynomials, Szegő polynomials.

AMS(MOS) subject classifications. 41A21, 42A70, 15A06, 30E05, 60G25, 65F05, 65F30.

Files. vol.2.1994/pp104-129.dir/pp104-129.ps, vol.2.1994/pp104-129.dir/pp104-129.pdf.

Forward References.

- 130 The generalizations of Newton's interpolation formula due to Mühlbach and Andoyer. *C. Brezinski*.

Abstract. Newton's formula for constructing the interpolation polynomial is well-known. It makes use of divided differences. It was generalized around 1971–1973 by Mühlbach for interpolation by a linear family of functions forming a complete Chebyshev system. This generalization rests on a generalization of divided differences due to Popoviciu. In this paper, it is shown that Mühlbach's formula is related to the work of Andoyer which goes back to the beginning of the century.

Key words. interpolation, divided differences, biorthogonality.

AMS(MOS) subject classifications. 65D05, 41A05.

Files. vol.2.1994/pp130-137.dir/pp130-137.ps, vol.2.1994/pp130-137.dir/pp130-137.pdf.

Forward References.

- 138 On the periodic quotient singular value decomposition. *J.J. Hench*.

Abstract. The periodic Schur decomposition has been generally seen as a tool to compute the eigenvalues of a product of matrices in a numerically sound way. In a recent technical report, it was shown that the periodic Schur decomposition may also be used to accurately compute the singular value decomposition (SVD) of a matrix. This was accomplished by reducing a periodic pencil that is associated with the standard normal equations to eigenvalue revealing form. If this technique is extended to the periodic QZ decomposition, then it is possible to compute the quotient singular value decomposition (QSVD) of a matrix pair. This technique may easily be extended further to a sequence of matrix pairs, thus computing the "periodic" QSVD.

Key words. singular value decomposition, periodic Schur decomposition, periodic QR algorithm, periodic QZ algorithm, QSVD, SVD.

AMS(MOS) subject classifications. 15A18, 65F05, 65F15.

Files. vol.2.1994/pp138-153.dir/pp138-153.ps, vol.2.1994/pp138-153.dir/pp138-153.pdf.

Forward References.

- 154 Fast iterative methods for solving Toeplitz-plus-Hankel least squares. *Michael K. Ng*.

Abstract. In this paper, we consider the impulse responses of the linear-phase filter whose characteristics are determined on the basis of an observed time series, not on a prior specification. The impulse responses can be found by solving a least squares problem $\min \|\mathbf{d} - (X_1 + X_2)\mathbf{w}\|_2$ by the fast Fourier transform (FFT) based preconditioned conjugate gradient method, for $(M + 2n - 1)$ -by- n real Toeplitz-plus-Hankel data matrices $X_1 + X_2$ with full column rank. The FFT-based preconditioners are derived from the spectral properties of the given input stochastic process, and their eigenvalues are constructed by the Blackman-Tukey spectral estimator with Bartlett window which is commonly used in signal processing. When the stochastic process is stationary and when its spectral density function is positive and differentiable, we prove that with probability 1, the spectra of the preconditioned normal equations is $O(M \log n)$ operations and each iteration requires $O(n \log n)$ operations, the total complexity of our algorithm is of order $O(M \log n + (2\alpha + 1)n \log^2 n + n \log n)$ operations. Finally, numerical results are reported to illustrate the effectiveness of our FFT-based preconditioned iterations.

Key words. least squares estimations, linear-phase filter, Toeplitz-plus-Hankel matrix, circulant matrix, preconditioned conjugate gradient method, fast Fourier transform.

AMS(MOS) subject classifications. 65F10, 65F15, 43E10.

Files. vol.2.1994/pp154-170.dir/pp154-170.ps, vol.2.1994/pp154-170.dir/pp154-170.pdf.

Forward References.

- 171 Domain decomposition and multigrid algorithms for elliptic problems on unstructured meshes. *Tony F. Chan and Barry F. Smith.*

Abstract. Multigrid and domain decomposition methods have proven to be versatile methods for the iterative solution of linear and nonlinear systems of equations arising from the discretization of partial differential equations. The efficiency of these methods derives from the use of a grid hierarchy. In some applications to problems on unstructured grids, however, no natural multilevel structure of the grid is available and thus must be generated as part of the solution procedure.

In this paper, we consider the problem of generating a multilevel grid hierarchy when only a fine, unstructured grid is given. We restrict attention to problems in two dimensions. Our techniques generate a sequence of coarser grids by first forming a maximal independent set of the graph of the grid or its dual and then applying a Cavendish type algorithm to form the coarser triangulation. Iterates on the different levels are combined using standard interpolation and restriction operators. Numerical tests indicate that convergence using this approach can be as fast as standard multigrid and domain decomposition methods on a structured mesh.

Key words. domain decomposition, grid refinement, multigrid, numerical partial differential equations.

AMS(MOS) subject classifications. 65N30, 65F10.

Files. vol.2.1994/pp171-182.dir/pp171-182.ps, vol.2.1994/pp171-182.dir/pp171-182.pdf.

Forward References.

- 183 Convergence of infinite products of matrices and inner–outer iteration schemes. *Rafael Bru, L. Elsner, and M. Neumann.*

Abstract. We develop conditions under which a product $\prod_{i=0}^{\infty} T_i$ of matrices chosen from a possibly infinite set of matrices $\mathcal{S} = \{T_j | j \in J\}$ converges. We obtain the following conditions which are sufficient for the convergence of the product: There exists a vector norm such that all matrices in \mathcal{S} are nonexpansive with respect to this norm and there exists a subsequence $\{i_k\}_{k=0}^{\infty}$ of the sequence of the nonnegative integers such that the corresponding sequence of operators $\{T_{i_k}\}_{k=0}^{\infty}$ converges to an operator which is paracontracting with respect to this norm. We deduce the continuity of the limit of the product of matrices as a function of the sequences $\{i_k\}_{k=0}^{\infty}$. But more importantly, we apply our results to the question of the convergence of inner–outer iteration schemes for solving **singular** consistent linear systems of equations, where the outer splitting is regular and the inner splitting is weak regular.

Key words. iterative methods, infinite products, contractions.

AMS(MOS) subject classification. 65F10.

Files. vol.2.1994/pp183-193.dir/pp183-193.ps, vol.2.1994/pp183-193.dir/pp183-193.pdf, vol.2.1994/pp183-193.dir/pp183-193orig.ps.

Forward References. vol.3.1995/pp24-38.dir/pp24-38.ps, vol.3.1995/pp24-38.dir/pp24-38.pdf.

- 194** Reducibility and characterization of symplectic Runge-Kutta methods. *Peter Görtz and Rudolf Scherer.*

Abstract. Hamiltonian systems arise in many areas of physics, mechanics, and engineering sciences as well as in pure and applied mathematics. To their symplectic integration certain Runge–Kutta–type methods are profitably applied (see Sanz–Serna and Calvo [10]). In this paper Runge–Kutta and partitioned Runge–Kutta methods are considered. Different features of symmetry are distinguished using reflected and transposed methods. The property of DJ–irreducibility ensures symplectic methods having nonvanishing weights. A characterization of symplectic methods is deduced, from which many attributes of such methods and hints for their construction follow. Order conditions up to order four can be checked easily by simplifying assumptions. For symplectic singly–implicit Runge–Kutta methods the order barrier is shown to be two.

Key words. Hamiltonian system, symplectic method, Runge–Kutta and partitioned Runge–Kutta method, DJ–reducibility.

AMS(MOS) subject classification. 65L06.

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Forward References.