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Contents

1 Evaluating matrix functions for exponential integrators via Carathéodory-Fejér approximation and contour integrals. *Thomas Schmelzer and Lloyd N. Trefethen*.

Abstract.
Among the fastest methods for solving stiff PDE are exponential integrators, which require the evaluation of $f(A)$, where A is a negative semidefinite matrix and f is the exponential function or one of the related "φ functions" such as $\varphi_1(z) = (e^z - 1)/z$. Building on previous work by Trefethen and Gutknecht, Minchev, and Lu, we propose two methods for the fast evaluation of $f(A)$ that are especially useful when shifted systems $(A + zI)x = b$ can be solved efficiently, e.g. by a sparse direct solver. The first method is based on best rational approximations to f on the negative real axis computed via the Carathéodory-Fejér procedure. Rather than using optimal poles we approximate the functions in a set of common poles, which speeds up typical computations by a factor of 2 to 3.5. The second method is an application of the trapezoid rule on a Talbot-type contour.

Key Words.
matrix exponential, exponential integrators, stiff semilinear parabolic PDEs, rational uniform approximation, Hankel contour, numerical quadrature

AMS Subject Classifications.
65L05, 41A20, 30E20

19 Homogeneous Jacobi–Davidson. *Michiel E. Hochstenbach and Yvan Notay*.

Abstract.
We study a homogeneous variant of the Jacobi–Davidson method for the generalized and polynomial eigenvalue problem. While a homogeneous form of these problems was previously considered for the subspace extraction phase, in this paper this form is also exploited for the subspace expansion phase and the projection present in the correction equation. The resulting method can deal with both finite and infinite eigenvalues in a natural and unified way. We show relations with the multihomogeneous Newton method, Rayleigh quotient iteration, and (standard) Jacobi–Davidson for polynomial eigenproblems.

Key Words.
homogeneous form, quadratic eigenvalue problem, generalized eigenvalue problem, polynomial eigenvalue problem, infinite eigenvalues, correction equation, subspace method, subspace expansion, large sparse matrices, bihomogeneous Newton, multihomogeneous Newton, Rayleigh quotient iteration, Jacobi–Davidson

AMS Subject Classifications.
65F15, 65F50

31 Preconditioning block Toeplitz matrices. *Thomas K. Huckle and Dimitrios Noutsos*.

Abstract.
We investigate the spectral behavior of preconditioned block Toeplitz matrices with small non-Toeplitz blocks. These matrices have a quite different behavior than scalar or mulitlevel Toeplitz matrices. Based on the connection between Toeplitz and Hankel matrices we derive some negative results on eigenvalue clustering for ill-conditioned block Toeplitz matrices. Furthermore, we identify Block Toeplitz matrices that are easy to solve by the preconditioned conjugate gradient method. We derive some useful inequalities that give information on the location of the spectrum of the preconditioned systems. The described analysis also gives information on preconditioning ill-conditioned Toeplitz Schur complement matrices and Toeplitz normal equations.

Key Words.
Toeplitz, block Toeplitz, Schur complement, preconditioning, conjugate gradient method

AMS Subject Classifications.
65F10, 65F15

46 An SVD approach to identifying metastable states of Markov chains. *David Fritzsche, Volker Mehrmann, Daniel B. Szyld, and Elena Virnik*.

Abstract.
Being one of the key tools in conformation dynamics, the identification of metastable states of Markov chains has been subject to extensive research in recent years, especially when the Markov chains represent energy states of biomo lecules. Some previous work on this topic involved the computation of the eigenvalue cluster close to one, as well as the corresponding eigenvectors and the stationary probability distribution of the associated stoch astic matrix. More recently, since the eigenvalue cluster algorithm may be nonrobust, an optim ization approach was developed. As a possible less costly alternative, we present an SVD approach of identifying metastable states of a stochastic matrix, where we only need the singular vector associated with the second largest singular value. We also introduce a concept of block diagonal dominance on which our algorithm is based. We outline some theoretical background and discuss the advantages of this strategy. Some simulated and real numerical examples illustrate the effectiveness of the proposed algorithm.

Key Words.
Markov chain, stochastic matrix, conformation dynamics, metastable, eigenvalue cluster, singular value decomposition, block diagonal dominance

AMS Subject Classifications.
15A18, 15A51, 60J10, 60J20, 65F15

70 Hierarchical grid coarsening for the solution of the Poisson equation in free space. *Matthias Bolten*.

Abstract.
In many applications the solution of PDEs in infinite domains with vanishing boundary conditions at infinity is of interest. If the Green's function of the particular PDE is known, the solution can easily be obtained by folding it with the right hand side

in a finite subvolume. Unfortunately this requires $\mathcal{O}(N^2)$ operations. Washio and Oosterlee presented an algorithm that rather than that uses hierarchically coarsened grids in order to solve the problem (Numer. Math. (2000) 86: 539–563). They use infinitely many grid levels for the error analysis. In this paper we present an extension of their work. Instead of continuing the refinement process up to infinitely many grid levels, we stop the refinement process at an arbitrary level and impose the Dirichlet boundary conditions of the original problem there. The error analysis shows that the proposed method still is of order h^2, as the original method with infinitely many refinements.

Key Words.
the Poisson equation, free boundary problems for PDE, multigrid method

AMS Subject Classifications.
35J05, 35R35, 65N55

81 Harmonic Rayleigh–Ritz extraction for the multiparameter eigenvalue problem. *Michiel E. Hochstenbach and Bor Plestenjak*.

Abstract.
We study harmonic and refined extraction methods for the multiparameter eigenvalue problem. These techniques are generalizations of their counterparts for the standard and generalized eigenvalue problem. The methods aim to approximate interior eigenpairs, generally more accurately than the standard extraction does. We study their properties and give Saad-type theorems. The processes can be combined with any subspace expansion approach, for instance a Jacobi–Davidson type technique, to form a subspace method for multiparameter eigenproblems of high dimension.

Key Words.
multiparameter eigenvalue problem, two-parameter eigenvalue problem, harmonic extraction, refined extraction, Rayleigh–Ritz, subspace method, Saad's theorem, Jacobi–Davidson

AMS Subject Classifications.
65F15, 65F50, 15A18, 15A69

97 A rank-one updating approach for solving systems of linear equations in the least squares sense. *A. Mohsen and J. Stoer*.

Abstract.
The solution of the linear system $Ax = b$ with an $m \times n$-matrix A of maximal rank $\mu := \min(m, n)$ is considered. The method generates a sequence of $n \times m$-matrices H_k and vectors x_k so that the AH_k are positive semidefinite, the H_k approximate the pseudoinverse of A and x_k approximate the least squares solution of $Ax = b$. The method is of the type of Broyden's rank-one updates and yields the pseudoinverse in μ steps.

Key Words.
linear least squares problems, iterative methods, variable metric updates, pseudoinverse

AMS Subject Classifications.
65F10, 65F20

116 Fourth order time-stepping for low dispersion Korteweg–de Vries and nonlinear Schrödinger equations. *Christian Klein*.

Abstract.
Purely dispersive equations, such as the Korteweg–de Vries and the nonlinear Schrödinger equations in the limit of small dispersion, have solutions to Cauchy problems with smooth initial data which develop a zone of rapid modulated oscillations in the region where the corresponding dispersionless equations have shocks or blow-up. Fourth order time-stepping in combination with spectral methods is beneficial to numerically resolve the steep gradients in the oscillatory region. We compare the performance of several fourth order methods for the Korteweg–de Vries and the focusing and defocusing nonlinear Schrödinger equations in the small dispersion limit: an exponential time-differencing fourth-order Runge–Kutta method as proposed by Cox and Matthews in the implementation by Kassam and Trefethen, integrating factors, time-splitting, Fornberg and Driscoll's 'sliders', and an ODE solver in MATLAB.

Key Words.
exponential time-differencing, Korteweg–de Vries equation, nonlinear Schrödinger equation, split step, integrating factor

AMS Subject Classifications.
Primary, 65M70; Secondary, 65L05, 65M20

136 On the parameter selection problem in the Newton-ADI iteration for large-scale Riccati equations. *Peter Benner, Hermann Mena, and Jens Saak*.

Abstract.
The numerical treatment of linear-quadratic regulator (LQR) problems for parabolic partial differential equations (PDEs) on infinite-time horizons requires the solution of large-scale algebraic Riccati equations (AREs). The Newton-ADI iteration is an efficient numerical method for this task. It includes the solution of a Lyapunov equation by the alternating direction implicit (ADI) algorithm at each iteration step. Here, we study the selection of shift parameters for the ADI method. This leads to a rational min-max problem which has been considered by many authors. Since knowledge about the exact shape of the complex spectrum is crucial for computing the optimal solution, this is often infeasible for the large-scale systems arising from finite element discretization of PDEs. Therefore, several methods for computing suboptimal parameters are discussed and compared on numerical examples.

Key Words.
algebraic Riccati equation, Newton-ADI, shift parameters, Lyapunov equation, rational min-max problem, Zolotarev problem

AMS Subject Classifications.
15A24, 30E10, 65B99

150 Algebraic multigrid smoothing property of Kaczmarz's relaxation for general rectangular linear systems. *Constantin Popa*.

Abstract.
In this paper we analyze the smoothing property from classical Algebraic Multigrid theory, for general rectangular systems of linear equations. We prove it for Kaczmarz's projection algorithm in the consistent case and obtain in this way a generalization of the classical well-known result by A. Brandt. We then extend this result for the Kaczmarz Extended algorithm in the inconsistent case.

Key Words.
algebraic multigrid, smoothing property, Kaczmarz relaxation, inconsistent least squares problems

AMS Subject Classifications.
65F10, 65F20, 65N55

163 Filter factor analysis of an iterative multilevel regularizing method. *Marco Donatelli and Stefano Serra-Capizzano*.

Abstract.
Recent results have shown that iterative methods of multigrid type are very precise and efficient for regularizing purposes: the reconstruction quality is of the same level or slightly better than that related to most effective regularizing procedures such as Landweber or conjugate gradients for normal equations, but the associated computational cost is highly reduced. Here we analyze the filter features of one of these multigrid techniques in order to provide a theoretical motivation of the excellent regularizing characteristics experimentally observed in the discussed methods.

Key Words.
regularization, early termination, filter analysis, boundary conditions, structured matrices

AMS Subject Classifications.
65Y20, 65F10, 15A12

178 Stopping criteria for mixed finite element problems. *M. Arioli and D. Loghin*.

Abstract.
We study stopping criteria that are suitable in the solution by Krylov space based methods of linear and non linear systems of equations arising from the mixed and the mixed-hybrid finite-element approximation of saddle point problems. Our approach is based on the equivalence between the Babuška and Brezzi conditions of stability which allows us to apply some of the results obtained in [M. Arioli, D. Loghin, and A. Wathen, *Stopping criteria for iterations in finite-element methods,* Numer. Math., 99 (2005), pp. 381–410]. Our proposed criterion involves evaluating the residual in a norm defined on the discrete dual of the space where we seek a solution. We illustrate our approach using standard iterative methods such as MINRES and

GMRES. We test our criteria on Stokes and Navier-Stokes problems both in a linear and nonlinear context.

Key Words.
augmented systems, mixed and mixed-hybrid finite-element, stopping criteria, Krylov subspaces method

AMS Subject Classifications.
65F10, 65F35, 65F50, 65N30

193 Preconditioning of nonsymmetric saddle point systems as arising in modelling of viscoelastic problems. *Maya Neytcheva and Erik Bängtsson*.

Abstract.
In this paper we consider numerical simulations of the so-called glacial rebound phenomenon and the use of efficient preconditioned iterative solution methods in that context. The problem originates from modeling the response of the solid earth to large scale glacial advance and recession which may have provoked very large earthquakes in Northern Scandinavia. The need for such numerical simulations is due to ongoing investigations on safety assessment of radioactive waste repositories. The continuous setting of the problem is to solve an integro-differential equation in a large time-space domain. This problem is then discretized using a finite element method in space and a suitable discretization in time, and gives rise to the solution of a large number of linear systems with nonsymmetric
matrices of saddle point form. We outline the properties of the corresponding linear systems of equations, discuss possible preconditioning strategies, and present some numerical experiments.

Key Words.
viscoelasticity, (in)compressibility, nonsymmetric saddle-point system, preconditioning, Schur complement approximation, algebraic multilevel techniques

AMS Subject Classifications.
65F10, 74D05, 45D05

212 Solving large-scale quadratic eigenvalue problems with Hamiltonian eigenstructure using a structure-preserving Krylov subspace method. *Peter Benner, Heike Fassbender, and Martin Stoll*.

Abstract.
We consider the numerical solution of quadratic eigenproblems with spectra that exhibit Hamiltonian symmetry. We propose to solve such problems by applying a Krylov-Schur-type method based on the symplectic Lanczos process to a structured linearization of the quadratic matrix polynomial. In order to compute interior eigenvalues, we discuss several shift-and-invert operators with Hamiltonian structure. Our approach is tested for several examples from structural analysis and gyroscopic systems.

Key Words.
quadratic eigenvalue problem, Hamiltonian symmetry, Krylov subspace method, symplectic Lanczos process, gyroscopic systems

AMS Subject Classifications.
65F15, 15A24, 47A75, 47H60