

Electronic Transactions on Numerical Analysis

Volume 46, 2017

Contents

- 1** Efficient evaluation of scaled proximal operators.
Michael P. Friedlander and Gabriel Goh.
- Abstract.**
Quadratic-support functions, cf. Aravkin, Burke, and Pillonetto [J. Mach. Learn. Res., 14 (2013)], constitute a parametric family of convex functions that includes a range of useful regularization terms found in applications of convex optimization. We show how an interior method can be used to efficiently compute the proximal operator of a quadratic-support function under different metrics. When the metric and the function have the right structure, the proximal map can be computed with costs nearly linear in the input size. We describe how to use this approach to implement quasi-Newton methods for a rich class of nonsmooth problems that arise, for example, in sparse optimization, image denoising, and sparse logistic regression.
- Key Words.**
support functions, proximal-gradient, quasi-Newton, interior method
- AMS Subject Classifications.**
90C15, 90C25
- 23** Fast evaluation of real and complex exponential sums.
Stefan Kunis and Ines Melzer.
- Abstract.**
Recently, the butterfly approximation scheme and hierarchical approximations have been proposed for the efficient computation of integral transforms with oscillatory or asymptotically smooth kernels. Combining both approaches, we propose a certain fast Fourier-Laplace transform, which in particular allows for the fast evaluation of polynomials at nodes in the complex unit disk.
- Key Words.**
trigonometric approximation, nonharmonic Fourier series, fast Fourier transform, integral transforms, hierarchical matrices
- AMS Subject Classifications.**
65T50, 42A15, 30E10, 65D05, 65F30
- 36** Sparsity-inducing variational shape partitioning.
Serena Morigi and Martin Huska.
- Abstract.**
We propose a sparsity-inducing multi-channel multiple region model for the efficient partitioning of a mesh into salient parts. Our approach is based on rewriting the Mumford-Shah models in terms of piece-wise smooth/constant functionals

that incorporate a non-convex regularizer for minimizing the boundary lengths. The solution of this optimization problem, obtained by an efficient proximal forward backward algorithm, is used by a simple thresholding/clusterization procedure to segment the shape into the required number of parts. Therefore, it is not necessary to further solve the optimization problem for a different number of partitioning regions. Experimental results show the effectiveness and efficiency of our proposals when applied to both single- and multi-channel (shape characterizing) functions.

Key Words.

mesh decomposition, variational segmentation, non-convex minimization, spectral clustering.

AMS Subject Classifications.

65M10, 78A48.

55 The number of zeros of unilateral polynomials over coquaternions and related algebras.

Drahoslava Janovská and Gerhard Opfer.

Abstract.

We have proved that unilateral polynomials over the nondivision algebras in \mathbb{R}^4 have at most $n(2n - 1)$ zeros, when the polynomial has degree n . Moreover, we have created an algorithm for finding all zeros of polynomials over these algebras using a real polynomial of degree $2n$, called *companion polynomial*. The algebras in question are coquaternions, \mathbb{H}_{coq} , nectarines, \mathbb{H}_{nec} , and conectarines, \mathbb{H}_{con} . Besides the isolated and hyperbolic zeros we introduce a new type of zeros, the *unexpected* zeros. There is a formal algorithm, and there are numerical examples. In a tutorial section on similarity we show how to find the similarity transformation of two algebra elements to be known as similar, where a singular value decomposition of a certain real 4×4 matrix related to the two similar elements has to be applied. We show that there is a strong indication that an algorithm by Serôdio, Pereira, and Vitória [Comput. Math. Appl., 42 (2001), pp. 1229–1237], designed for finding zeros of quaternionic polynomials, is also valid in the nondivision algebras in \mathbb{R}^4 and it produces—though with another technique—the same zeros as those proposed in this paper.

Key Words.

number of zeros of polynomials over nondivision algebras in \mathbb{R}^4 , number of zeros of polynomials over coquaternions, number of zeros of polynomials over nectarines, number of zeros of polynomials over conectarines, unexpected zeros, computation of all zeros of polynomials over nondivision algebras in \mathbb{R}^4

AMS Subject Classifications.

12D10, 12E10, 15A66, 1604

71 Application of the collocation method with B-splines to the GEW equation.

Halil Zeybek and S. Battal Gazi Karakoç.

Abstract.

In this paper, the generalized equal width (GEW) wave equation is solved numerically by using a quintic B-spline collocation algorithm with two different linearization techniques. Also, a linear stability analysis of the numerical scheme based on the von Neumann method is investigated. The numerical algorithm is applied

to three test problems consisting of a single solitary wave, the interaction of two solitary waves, and a Maxwellian initial condition. In order to determine the performance of the numerical method, we compute the error in the L_2 - and L_∞ - norms and in the invariants I_1 , I_2 , and I_3 of the GEW equation. These calculations are compared with earlier studies. Afterwards, the motion of solitary waves according to different parameters is designed.

Key Words.

GEW equation, finite element method, quintic B-spline, soliton, solitary waves

AMS Subject Classifications.

41A15, 65N30, 76B25

89 Solution of coupled differential equations arising from imbalance problems.

Jenny Niebsch, Ronny Ramlau, and Kirk M. Soodhalter.

Abstract.

We investigate the efficient solution of a set of coupled ordinary differential equations arising from a model describing vibrations of a wind turbine induced by imbalances of its spinning blades. The Forward Problem (computing vibrations from imbalances) admits a coupled integral equation formulation. Each integral equation is solved over the same underlying Hilbert space \mathbb{H} . We observe that these coupled integral equations can be represented as one compact operator acting on the tensor product space $\mathbb{R}^N \otimes \mathbb{H}$, where N is the number of coupled equations. A Galerkin discretization leads to a linear system of dimension nN with corresponding Kronecker product structure, where n is the number of basis elements used to discretize \mathbb{H} . Such systems can be solved using a variety of techniques which exploit the Kronecker structure. We demonstrate the effectiveness of exploiting the tensor structure with numerical experiments and show that our results agree with data recorded from actual wind turbines.

Key Words.

mathematical modeling, couple differential equations, integral equation, Kronecker product, tensor product, Hilbert space

AMS Subject Classifications.

15A69, 34A55, 45D05, 65R20, 65R30

107 Convergence of the cyclic and quasi-cyclic Block Jacobi methods.

Vjeran Hari and Erna Begović Kovač.

Abstract.

This paper studies the global convergence of the block Jacobi method for symmetric matrices. Given a symmetric matrix A of order n , the method generates a sequence of matrices by the rule $A^{(k+1)} = U_k^T A^{(k)} U_k$, $k \geq 0$, where U_k are orthogonal elementary block matrices. A class of generalized serial pivot strategies is introduced, significantly enlarging the known class of weak wavefront strategies, and appropriate global convergence proofs are obtained. The results are phrased in the stronger form: $S(A') \leq cS(A)$, where A' is the matrix obtained from A after one full cycle, $c < 1$ is a constant, and $S(A)$ is the off-norm of A . Hence, using the theory of block Jacobi operators, one can apply the obtained results to prove convergence of block Jacobi methods for other eigenvalue problems such as the generalized eigenvalue problem. As an example, the results are applied to the block J -Jacobi method. Finally, all results are extended to the corresponding quasi-cyclic strategies.

Key Words.

eigenvalues, block Jacobi method, pivot strategies, global convergence

AMS Subject Classifications.

65F15

- 148 A simplification of the stationary phase method: application to the Anger and Weber functions.

José L. López and Pedro J. Pagola.

Abstract.

The main difficulty in the practical use of the stationary phase method in asymptotic expansions of integrals is originated by a change of variables. The coefficients of the asymptotic expansion are the coefficients of the Taylor expansion of a certain function implicitly defined by that change of variables. In general, this function is not explicitly known, and then the computation of those coefficients is cumbersome. Using the factorization of the exponential factor used in previous works of [Tricomi, 1950], [Erdélyi and Wyman, 1963], and [Dingle, 1973], we obtain a variant of the method that avoids that change of variables and simplifies the computations. On the one hand, the calculation of the coefficients of the asymptotic expansion is remarkably simpler and explicit. On the other hand, the asymptotic sequence is as simple as in the standard stationary phase method: inverse powers of the asymptotic variable. New asymptotic expansions of the Anger and Weber functions $\mathbf{J}_{\lambda x}(x)$ and $\mathbf{E}_{\lambda x}(x)$ for large positive x and real parameter $\lambda \neq 0$ are given as an illustration.

Key Words.

asymptotic expansions, oscillatory integrals, method of the stationary phase, Anger and Weber functions

AMS Subject Classifications.

33B15, 41A60

- 162 Stagnation of block GMRES and its relationship to block FOM.

Kirk M. Soodhalter.

Abstract.

We analyze the convergence behavior of block GMRES and characterize the phenomenon of stagnation which is then related to the behavior of the block FOM method. We generalize the block FOM method to generate well-defined approximations in the case that block FOM would normally break down, and these generalized solutions are used in our analysis. This behavior is also related to the principal angles between the column-space of the previous block GMRES residual and the current minimum residual constraint space. At iteration j , it is shown that the proper generalization of GMRES stagnation to the block setting relates to the column space of the j th block Arnoldi vector. Our analysis covers both the cases of normal iterations as well as block Arnoldi breakdown wherein dependent basis vectors are replaced with random ones. Numerical examples are given to illustrate what we have proven, including one built from a small application problem to demonstrate the validity of the analysis in a less pathological case.

Key Words.

block Krylov subspace methods, GMRES, FOM, stagnation

AMS Subject Classifications.

65F10, 65F50, 65F08

- 190 A BDDC preconditioner for a symmetric interior penalty Galerkin method.
Susanne C. Brenner, Eun-Hee Park, and Li-Yeng Sung.

Abstract.

We develop a nonoverlapping domain decomposition preconditioner for the symmetric interior penalty Galerkin method for heterogeneous elliptic problems. The preconditioner is based on balancing domain decomposition by constraints (BDDC). We show that the condition number of the preconditioned system satisfies similar estimates as those for conforming finite element methods. Corroborating numerical results are also presented.

Key Words.

nonoverlapping domain decomposition, BDDC preconditioner, symmetric interior penalty method

AMS Subject Classifications.

65N55, 65N30

- 215 On the approximation of functionals of very large Hermitian matrices represented as matrix product operators.
Moritz August, Mari Carmen Bañuls, and Thomas Huckle.

Abstract.

We present a method to approximate functionals $\text{Tr}f(A)$ of very high-dimensional Hermitian matrices A represented as Matrix Product Operators (MPOs). Our method is based on a reformulation of a block Lanczos algorithm in tensor network format. We state main properties of the method and show how to adapt the basic Lanczos algorithm to the tensor network formalism to allow for high-dimensional computations. Additionally, we give an analysis of the complexity of our method and provide numerical evidence that it yields good approximations of the entropy of density matrices represented by MPOs while being robust against truncations.

Key Words.

tensor decompositions, numerical analysis, Lanczos method, Gauss quadrature, quantum physics

AMS Subject Classifications.

65F60, 65D15, 65D30, 65F15, 46N50, 15A69

- 233 Convergence rates for ℓ^1 -regularization without the help of a variational inequality.
Daniel Gerth.

Abstract.

We show that convergence rates for ℓ^1 -regularization can be obtained in an elementary way without requiring a classical source condition and without the help of a variational inequality. For the specific case of a diagonal operator we improve the convergence rate found in the literature and conduct numerical experiments that illustrate the predicted rate. The idea of the proof is rather generic and might be used in other settings as well.

Key Words.

ℓ^1 -regularization, Tikhonov regularization, variational inequality, convergence rates

AMS Subject Classifications.

65J20, 47A52

245 Variants of IDR with partial orthonormalization.*Jens-Peter M. Zemke.***Abstract.**

We present four variants of $\text{IDR}(s)$ that generate vectors such that consecutive blocks of $s + 1$ vectors are orthonormal. IDR methods are based on tuning parameters: an initially chosen, so-called *shadow space*, and the so-called *seed values*. We collect possible choices for the seed values. We prove that under certain conditions all four variants are mathematically equivalent and discuss possible breakdowns. We give an error analysis of all four variants and a numerical comparison in the context of the solution of linear systems and eigenvalue problems.

Key Words.

IDR, partial orthonormalization, minimum norm expansion, error analysis

AMS Subject Classifications.

65F25 (primary), 65F10, 65F15, 65F50

273 A unified framework for adaptive BDDC.*Clemens Pechstein and Clark R. Dohrmann.***Abstract.**

In this theoretical study, we explore how to automate the selection of weights and primal constraints in BDDC methods for general SPD problems. In particular, we address the three-dimensional case and non-diagonal weight matrices such as the deluxe scaling. We provide an overview of existing approaches, show connections between them, and present new theoretical results: A localization of the global BDDC estimate leads to a reliable condition number bound and to a local generalized eigenproblem on each *glob*, i.e., each subdomain face, edge, and possibly vertex. We discuss how the eigenvectors corresponding to the smallest eigenvalues can be turned into generalized primal constraints. These can be either treated as they are or (which is much simpler to implement) be enforced by (possibly stronger) classical primal constraints. We show that the second option is the better one. Furthermore, we discuss equivalent versions of the face and edge eigenproblem which match with previous works and show an optimality property of the deluxe scaling. Lastly, we give a localized algorithm which guarantees the definiteness of the matrix \tilde{S} underlying the BDDC preconditioner under mild assumptions on the subdomain matrices.

Key Words.

preconditioning, domain decomposition, iterative substructuring, BDDC, FETI-DP, primal constraints, adaptive coarse space, deluxe scaling, generalized eigenvalue problems, parallel sum

AMS Subject Classifications.

65F08, 65N30, 65N35, 65N55

337 Almost optimal convergence of FEM-FDM for a linear parabolic interface problem.*Matthew O. Adewole.*

Abstract.

The solution of a second-order linear parabolic interface problem by the finite element method is discussed. Quasi-uniform triangular elements are used for the spatial discretization while the time discretization is based on a four-step implicit scheme. The integrals involved are evaluated by numerical quadrature, and it is assumed that the mesh cannot be fitted to the interface. With low regularity assumption on the solution across the interface, the stability of the method is established, and an almost optimal convergence rate of $O\left(k^4 + h^2\left(1 + \frac{1}{|\log h|}\right)\right)$ in the $L^2(\Omega)$ -norm is obtained. In terms of matrices arising in the scheme, we show that the scheme preserves the maximum principle under certain conditions. Numerical experiments are presented to support the theoretical results.

Key Words.

finite element method, interface, almost optimal, parabolic equation, implicit scheme

AMS Subject Classifications.

65N06, 65N15, 65N30

- 359 Approximating eigenvalues of boundary value problems by using the Hermite-Gauss sampling method.

Rashad M. Asharabi.

Abstract.

The Hermite-Gauss sampling operator was introduced by Asharabi and Prestin (2015) to approximate a function from a wide class of entire functions, using few samples from the function and its first derivative. This operator converges at the rate $e^{-(2\pi-\sigma h)N}/\sqrt{N}$, and has been applied to construct a new sampling method for approximating the eigenvalues of boundary value problems whose eigenvalues are real and simple. In this paper, we use the first derivative of this operator to approximate non-real and non-simple eigenvalues of boundary value problems. For this task, we estimate two types of errors associated with the first derivative of the Hermite-Gauss operator. These error estimates give us the possibility to establish the error analysis when the eigenvalues are not real or not algebraically simple. Illustrative examples are discussed and show the effectiveness of the proposed method. Our numerical results are compared with the results of sinc-Gaussian sampling method.

Key Words.

sinc methods, approximating eigenvalues, boundary value problems, error bounds, rate of convergence

AMS Subject Classifications.

34L16, 94A20, 65L15, 65N15

- 375 Fine-grain parallel RRB-solver for 5-/9-point stencil problems suitable for GPU-type processors.

Martijn de Jong, Auke van der Ploeg, Auke Ditzel, and Kees Vuik.

Abstract.

Preconditioners based on incomplete factorization are very popular for a fast convergence of the PCG-algorithm. However, these preconditioners are hard to parallelize since most operations are inherently sequential. In this paper we present

the RRB-solver, which is a PCG-type solver using an incomplete Cholesky factorization based on the Repeated Red-Black (RRB) method. The RRB-solver scales nearly as well as Multigrid, and in this paper we show that this method can be parallelized very efficiently on modern computing architectures including GPUs. For an efficient parallel implementation a clever storage scheme turns out to be the key. The storage scheme is called $r_1/r_2/b_1/b_2$ and it ensures that memory transfers are coalesced throughout the algorithm, yielding near-optimal performance of the RRB-solver. The $r_1/r_2/b_1/b_2$ -storage scheme in combination with a CUDA implementation on the GPU gives speedup factors of more than 30 compared to a sequential implementation on one CPU core for 5-/9-point stencils problems. A comparison with algebraic Multigrid further shows that the RRB-solver can be implemented very efficiently on the GPU.

Key Words.

repeated red-black, conjugate gradient, incomplete Cholesky, parallelization, CUDA, 2D Poisson

AMS Subject Classifications.

35J05, 65F08, 65F10, 65F50, 65Y05, 68W10

- 394 Topological solvability and DAE-index conditions for mass flow controlled pumps in liquid flow networks.

Ann-Kristin Baum, Michael Kolmbauer, and Günter Offner.

Abstract.

This work is devoted to the analysis of a model for the thermal management in liquid flow networks consisting of pipes and pumps. The underlying model equation for the liquid flow is not only governed by the equation of motion and the continuity equation, describing the mass transfer through the pipes, but also includes thermodynamic effects in order to cover cooling and heating processes. The resulting model gives rise to a differential-algebraic equation (DAE), for which a proof of unique solvability and an index analysis is presented. For the index analysis, the concepts of the *Strangeness Index* is pursued. Exploring the network structure of the liquid flow network via graph-theoretical approaches allow us to develop network topological criteria for the existence of solutions and the DAE-index. The topological criteria are explained by various examples.

Key Words.

differential-algebraic equations, topological index criteria, hydraulic network

AMS Subject Classifications.

65L80, 94C15

- 424 Sharp Ritz value estimates for restarted Krylov subspace iterations.

Ming Zhou and Klaus Neymeyr.

Abstract.

Gradient iterations for the Rayleigh quotient are elementary methods for computing the smallest eigenvalues of a pair of symmetric and positive definite matrices. A considerable convergence acceleration can be achieved by preconditioning and by computing Rayleigh-Ritz approximations from subspaces of increasing dimensions. An example of the resulting Krylov subspace eigensolvers is the generalized Davidson method. Krylov subspace iterations can be restarted in order to limit their

computer storage requirements. For the restarted Krylov subspace eigensolvers, a Chebyshev-type convergence estimate was presented by Knyazev in [Soviet J. Numer. Anal. Math. Modelling, 2 (1987), pp. 371–396]. This estimate has been generalized to arbitrary eigenvalue intervals in [SIAM J. Matrix Anal. Appl., 37 (2016), pp. 955–975]. The generalized Ritz value estimate is not sharp as it depends only on three eigenvalues. In the present paper we extend the latter analysis by generalizing the geometric approach from [SIAM J. Matrix Anal. Appl., 32 (2011), pp. 443–456] in order to derive a sharp Ritz value estimate for restarted Krylov subspace iterations.

Key Words.

Krylov subspace, Rayleigh quotient, Rayleigh-Ritz procedure, polynomial interpolation, multigrid, elliptic eigenvalue problem.

AMS Subject Classifications.

65F15, 65N25

- 447** Computing the eigenvalues of symmetric tridiagonal matrices via a Cayley transformation.

Jared L. Aurentz, Thomas Mach, Raf Vandebril, and David S. Watkins.

Abstract.

In this paper we present a new algorithm for solving the symmetric tridiagonal eigenvalue problem that works by first using a Cayley transformation to convert the symmetric matrix into a unitary one and then uses Gragg’s implicitly shifted unitary QR algorithm to solve the resulting unitary eigenvalue problem. We prove that under reasonable assumptions on the symmetric matrix this algorithm is backward stable. It is comparable to other algorithms in terms of accuracy. Although it is not the fastest algorithm, it is not conspicuously slow either. It is approximately as fast as the symmetric tridiagonal QR algorithm.

Key Words.

eigenvalue, unitary QR, symmetric matrix, core transformations, rotations

AMS Subject Classifications.

65F15, 65H17, 15A18, 15B10,

- 460** The block Hessenberg process for matrix equations.

M. Addam, M. Heyouni, and H. Sadok.

Abstract.

In the present paper, we first introduce a block variant of the Hessenberg process and discuss its properties. Then, we show how to apply the block Hessenberg process in order to solve linear systems with multiple right-hand sides. More precisely, we define the block CMRH method for solving linear systems that share the same coefficient matrix. We also show how to apply this process for solving discrete Sylvester matrix equations. Finally, numerical comparisons are provided in order to compare the proposed new algorithms with other existing methods.

Key Words.

Block Krylov subspace methods, Hessenberg process, Arnoldi process, CMRH, GMRES, low-rank matrix equations.

AMS Subject Classifications.

65F10, 65F30

- 474 An optimization-based multilevel algorithm for variational image segmentation models.
Abdul K. Jumaat and Ke Chen.

Abstract.

Variational active contour models have become very popular in recent years, especially global variational models which segment all objects in an image. Given a set of user-defined prior points, selective variational models aim at selectively segmenting one object only. We are concerned with the fast solution of the latter models. Time marching methods with semi-implicit schemes (gradient descents) or additive operator splitting are used frequently to solve the resulting Euler-Lagrange equations derived from these models. For images of moderate size, such methods are effective. However, to process images of large size, urgent need exists in developing fast iterative solvers. Unfortunately, geometric multigrid methods do not converge satisfactorily for such problems. Here we propose an optimization-based multilevel algorithm for efficiently solving a class of selective segmentation models. It also applies to the solution of global segmentation models. In a level-set function formulation, our first variant of the proposed multilevel algorithm has the expected optimal $O(N \log N)$ efficiency for an image of size $n \times n$ with $N = n^2$. Moreover, modified localized models are proposed to exploit the local nature of the segmentation contours, and consequently, our second variant—after modifications—practically achieves super-optimal efficiency $O(\sqrt{N} \log N)$. Numerical results show that a good segmentation quality is obtained, and as expected, excellent efficiency is observed in reducing the computational time.

Key Words.

active contours, image segmentation, level-set function, multilevel, optimization methods, energy minimization

AMS Subject Classifications.

62H35, 65N22, 65N55, 74G65, 74G75

- 505 A block Lanczos method for the linear response eigenvalue problem.
Zhongming Teng and Lei-Hong Zhang.

Abstract.

In the linear response eigenvalue problem arising from computational quantum chemistry and physics one needs to compute a small portion of eigenvalues around zero together with the associated eigenvectors. Lanczos-type methods are particularly suitable for such a task. However, single-vector Lanczos methods can only find one copy of any multiple eigenvalue and can be very slow when the desired eigenvalues form a cluster. In this paper, we propose a block Lanczos-type implementation for the linear response eigenvalue problem, which is able to compute a cluster of eigenvalues much faster and more efficiently than the single-vector version. Convergence results are established and reveal the accuracy of the approximations of eigenvalues in a cluster and of the eigenspace. A practical thick-restart procedure is introduced to alleviate the increasing numerical difficulties of the block Lanczos method in computational costs, memory demands, and numerical stability. Numerical examples are presented to support the effectiveness of the thick-restart block Lanczos method.

Key Words.

linear response eigenvalue problems, block Lanczos methods, convergence analysis,
thick-restart

AMS Subject Classifications.

65F15, 15A18