Electronic Transactions on Numerical Analysis
Volume 41, 2014

Contents

Abstract.
We consider extensions of Kronrod-type and extensions obtained by generalized averaged Gaussian quadrature formulas for Gauss-Turán quadrature formulas. Existence and uniqueness of these extensions are considered. Their numerical construction is proposed. It is the first general method and is based on a combination of well-known numerical methods for Gauss-Turán, Gauss, Gauss-Kronrod, Anti-Gauss, and generalized averaged Gaussian quadratures. We employ these extensions for estimating the remainder terms in the Gauss-Turán quadratures. Numerical results are presented.

Key Words.
quadrature rule, error estimate

AMS Subject Classifications.
65D32, 65D30

Abstract.
The conjugate gradient and minimal residual methods for the solution of linear systems $Ax = b$ are considered. The operator A is bounded and self-adjoint and maps a Hilbert space X into its dual X^*. This setting is natural for variational problems such as those involving linear partial differential equations. The derivation of the two methods in Hilbert spaces shows that the choice of a preconditioner is equivalent to the choice of the scalar product in X.

Key Words.
Krylov subspace methods, preconditioners, scalar products, Hilbert spaces, Riesz isomorphism

AMS Subject Classifications.
65F10, 65F08

Abstract.
We present a new algorithm for the iterative solution of nonlinear operator eigenvalue problems arising from partial differential equations (PDEs). This algorithm

combines automatic spatial resolution of linear operators with the infinite Arnoldi method for nonlinear matrix eigenproblems proposed by Jarlebring et al. [Numer. Math., 122 (2012), pp. 169–195]. The iterates in this infinite Arnoldi method are functions, and each iteration requires the solution of an inhomogeneous differential equation. This formulation is independent of the spatial representation of the functions, which allows us to employ a dynamic representation with an accuracy of about the level of machine precision at each iteration similar to what is done in the Chebfun system with its chebop functionality although our function representation is entirely based on coefficients instead of function values. Our approach also allows nonlinearity in the boundary conditions of the PDE. The algorithm is illustrated with several examples, e.g., the study of eigenvalues of a vibrating string with delayed boundary feedback control.

Key Words.
Arnoldi's method, nonlinear eigenvalue problems, partial differential equations, Krylov subspaces, delay-differential equations, Chebyshev polynomials

AMS Subject Classifications.
65F15, 65N35, 65N25

42 Multigrid preconditioning of the non-regularized augmented Bingham fluid problem.

Alexis Aposporidis, Panayot S. Vassilevski, and Alessandro Veneziani.

Abstract.
In the numerical solution of visco-plastic fluids, one of the hard problems is the effective detection of *rigid* or *plug* regions. These occur when the strain-rate tensor vanishes and consequently the equations for the fluid region become singular. In order to manage this lack of regularity, different approaches are possible. *Regularization procedures* replace the plug regions with high-viscosity fluid regions, featuring a regularization parameter $\varepsilon > 0$. In Aposporidis et al. [Comput. Methods Appl. Mech. Engrg., 200 (2011), pp. 2434–2446], an augmented formulation for Bingham fluids was introduced to improve the regularity properties of the problem. Results presented there show that the augmented formulation is more effective for numerical purposes and it works also in the non-regularized case ($\varepsilon = 0$) without a significant degradation of the non-linear solver's performance. However, when solving high-dimensional Bingham problems, the augmented formulation leads to more challenging linear systems. In this paper we develop a strategy for preconditioning large non-regularized augmented Bingham systems. We use the regularized problem as a preconditioner for the non-regularized case. Then, we resort to a nonlinear geometric multilevel preconditioner to accelerate the convergence of the flexible Krylov linear solver for the regularized Bingham preconditioner. Results presented here demonstrate the effectiveness of the strategy also in realistic (non-academic) test cases.

Key Words.
multigrid, multilevel flexible GMRES, Bingham flow, mixed finite elements

AMS Subject Classifications.
65F10, 65N30, 65N55

62 Conditional space-time stability of collocation Runge–Kutta for parabolic evolution equations.
Roman Andreev and Julia Schweitzer.

Abstract.
We formulate collocation Runge–Kutta time-stepping schemes applied to linear parabolic evolution equations as space-time Petrov–Galerkin discretizations, and investigate their a priori stability for the parabolic space-time norms, that is the operator norm of the discrete solution mapping. The focus is on A-stable Gauß–Legendreand L-stable right-Radau nodes, addressing in particular the implicit midpoint rule, the backward Euler, and the three stage Radau5 time-stepping schemes. Collocation on Lobatto nodes is analyzed as a by-product. We find through explicit estimates that the operator norm is controlled in terms of the parabolic CFL number together with a measure of self-duality of the spatial discretization. Numerical observations motivate and illustrate the results.

Key Words.
Space-time variational formulation, Runge-Kutta collocation method, parabolic evolution equations, space-time stability, Petrov-Galerkin.

AMS Subject Classifications.
35K90, 65M12, 65M20, 65M60

81 On convergence rates for quasi-solutions of ill-posed problems.
Andreas Neubauer and Ronny Ramlau.

Abstract.
Usually, one needs information about the noise level to find proper regularized solutions when solving ill-posed problems. However, for several inverse problems, it is not easy to obtain an accurate estimation of the noise level. If one has information about bounds of the solution in some stronger norm, quasi-solutions are an excellent alternative. Besides existence, stability, and convergence results, it is the major emphasis of this paper to prove convergence rates for quasi-solutions in Hilbert scales.

Key Words.
quasi-solutions, regularization in Hilbert scales, convergence rates

AMS Subject Classifications.
47A52, 65J20

93 The block preconditioned steepest descent iteration for elliptic operator eigenvalue problems.
Klaus Neymeyr and Ming Zhou.

Abstract.
The block preconditioned steepest descent iteration is an iterative eigensolver for subspace eigenvalue and eigenvector computations. An important area of application of the method is the approximate solution of mesh eigenproblems for self-adjoint elliptic partial differential operators. The subspace iteration allows to compute some of the smallest eigenvalues together with the associated invariant subspaces simultaneously. The building blocks of the iteration are the computation of the preconditioned residual subspace for the current iteration subspace and the application of the Rayleigh-Ritz method in order to extract an improved subspace iterate.

The convergence analysis of this iteration provides new sharp estimates for the Ritz values. It is based on the analysis of the vectorial preconditioned steepest descent iteration which appeared in [SIAM J. Numer. Anal., 50 (2012), pp. 3188–3207]. Numerical experiments using a finite element discretization of the Laplacian with up to $5 \cdot 10^7$ degrees of freedom and with multigrid preconditioning demonstrate the near-optimal complexity of the method.

Key Words.
subspace iteration, steepest descent/ascent, Rayleigh-Ritz procedure, elliptic eigenvalue problem, multigrid, preconditioning

AMS Subject Classifications.
65N12, 65N22, 65N25, 65N30

109 Error estimates for a two-dimensional special finite element method based on component mode synthesis.
Ulrich Hetmaniuk and Axel Klawonn.

Abstract.
This paper presents a priori error estimates for a special finite element discretization based on component mode synthesis. The basis functions exploit an orthogonal decomposition of the trial subspace to minimize the energy and are expressed in terms of local eigenproblems. The a priori error bounds state the explicit dependency of constants with respect to the mesh size and the first neglected eigenvalues. A residual-based a posteriori error indicator is derived. Numerical experiments on academic problems illustrate the sharpness of these bounds.

Key Words.
domain decomposition, finite elements, eigendecomposition, a posteriori error estimation

AMS Subject Classifications.
35J20, 65F15, 65N25, 65N30, 65N55

133 Zeros and singular points for one-sided coquaternionic polynomials with an extension to other $\mathbb{R}^4$ algebras.
Drahoslava Janovská and Gerhard Opfer.

Abstract.
For finding the zeros of a coquaternionic polynomial p of degree n, where p is given in standard form $p(z) = \sum c_j z^j$, the concept of a (real) companion polynomial q of degree $2n$, as introduced for quaternionic polynomials, is applied. If z_0 is a root of q, then, based on z_0, there is a simple formula for an element z with the property that $\overline{p(z)}p(z) = 0$, thus z is a singular point of p. Under certain conditions, the same z has the property that $p(z) = 0$, thus z is a zero of p. There is an algorithm for finding zeros and singular points of p. This algorithm will find all zeros z with the property that in the equivalence class to which z belongs, there are complex elements. For finding zeros which are not similar to complex numbers, Newton's method is applied, and a simple technique for computing the exact Jacobi matrix is presented. We also show, that there is no "Fundamental Theorem of Algebra" for coquaternions, but we state a conjecture that a "Weak Fundamental Theorem of Algebra" for coquaternions is valid. Several numerical examples are presented. It

179 Polynomial preconditioning for the GeneRank problem.
Davod Khojasteh Salkuyeh, Vahid Edalatpour, and Davod Hezari.

Abstract.
Identifying key genes involved in a particular disease is a very important problem in biomedical research. The GeneRank model is based on the PageRank algorithm and shares many of its mathematical properties. The model brings together gene expression information with a network structure and ranks genes based on the results of microarray experiments combined with gene expression information, for example, from gene annotations (GO). In this study, we present a polynomial preconditioned conjugate gradient algorithm to solve the GeneRank problem and study its properties. Some numerical experiments are given to show the effectiveness of the suggested preconditioner.

Key Words.
gene network, gene ontologies, conjugate gradient, Chebyshev polynomial, preconditioner, M-matrix

AMS Subject Classifications.
65F10, 65F50, 9208, 92D20

190 Collocation for singular integral equations with fixed singularities of particular Mellin type.
Peter Junghanns, Robert Kaiser, and Giuseppe Mastroianni.

Abstract.
This paper is concerned with the stability of collocation methods for Cauchy singular integral equations with fixed singularities on the interval $[-1, 1]$. The operator in these equations is supposed to be of the form $a\mathcal{I} + b\mathcal{S} + \mathcal{B}^{\pm}$ with piecewise continuous functions a and b. The operator $\mathcal{S}$ is the Cauchy singular integral operator and $\mathcal{B}^{\pm}$ is a finite sum of integral operators with fixed singularities at the points ± 1 of special kind. The collocation methods search for approximate solutions of the form $\nu(x)p_n(x)$ or $\mu(x)p_n(x)$ with Chebyshev weights $\nu(x) = \sqrt{\frac{1+x}{1-x}}$ or $\mu(x) = \sqrt{\frac{1-x}{1+x}}$, respectively, and collocation with respect to Chebyshev nodes of first and third or fourth kind is considered. For the stability of collocation methods in a weighted $\mathbf{L}^2$-space, we derive necessary and sufficient conditions.

Key Words.
collocation method, stability, C^*-algebra, notched half plane problem

AMS Subject Classifications.
65R20, 45E05

249 Parameter estimation of monomial-exponential sums.
Luisa Fermo, Cornelis Van der Mee, and Sebastiano Seatzu.

Abstract.
In this paper we propose a matrix-pencil method for the identification of parameters and coefficients of a monomial-exponential sum which can be considered as an extension of existing matrix-pencil methods for the parameter estimation of exponential sums. The technique adopted is based on properties of the finite difference equations and it overcomes the difficulty of their extension via the invertibility of the generalized Vandermonde matrix. As a result, a matrix-pencil method based on the

GSVD or the SVD is proposed which allows us to identify both simple and multiple parameters. Applications of this method to various examples show its effectiveness.

Key Words.
nonlinear approximation, parameter estimation, matrix pencils

AMS Subject Classifications.
41A46, 15A22, 65F15

262 A unified analysis of three finite element methods for the Monge-Ampère equation.
Michael Neilan.

Abstract.
It was recently shown in S. C. Brenner et al. [Math. Comp., 80 (2011), pp. 1979–1995] that Lagrange finite elements can be used to approximate classical solutions of the Monge-Ampère equation, a fully nonlinear second order PDE. We expand on these results and give a unified analysis for many finite element methods satisfying some mild structure conditions in two and three dimensions. After proving some abstract results, we lay out a blueprint to construct various finite element methods that inherit these conditions and show how C^1 finite element methods, C^0 finite element methods, and discontinuous Galerkin methods fit into the framework.

Key Words.
fully nonlinear PDEs, Monge-Ampère equation, finite element methods, discontinuous Galerkin methods

AMS Subject Classifications.
65N30, 65N12, 35J60.

289 Convergence analysis of the operational Tau method for Abel-type Volterra integral equations.
P. Mokhtary and F. Ghoreishi.

Abstract.
In this paper, a spectral Tau method based on Jacobi basis functions is proposed and its stability and convergence properties are considered for obtaining an approximate solution of Abel-type integral equations. This work is organized in two parts. First, we present a stable operational Tau method based on Jacobi basis functions that provides an efficient approximate solution for the Abel-type integral equations by using a reduced set of matrix operations. We also provide a rigorous error analysis for the proposed method in the weighted L^2- and uniform norms under more general regularity assumptions on the exact solution. It is shown that the proposed method converges, but since the solutions of these equations have a singularity near the origin, a loss in the convergence order of the Tau method is expected. To overcome this drawback we then propose a regularization process, in which the original equation is changed into a new equation which possesses a smooth solution, by applying a suitable variable transformation such that the spectral Tau method can be applied conveniently. We also prove that after this regularization technique, the numerical solution of the new equation based on the operational Tau method has exponential rate of convergence. Some standard examples are provided to confirm the reliability of the proposed method.

Key Words.
Operational Tau method, Abel-type Volterra integral equations

AMS Subject Classifications.
45E10, 41A25

Abstract.
In this work the problem of a viscoelastic fluid flow in a movable domain is considered. A numerical approximation scheme is developed based on the Arbitrary Lagrangian-Eulerian (ALE) formulation of the flow equations. The spatial discretization is accomplished by the finite element method, and the discontinuous Galerkin method is used for stress approximation. Both first and second order time-stepping schemes satisfying the geometric conservation law (GCL) are derived and analyzed, and numerical experiments that support the theoretical results are presented.

Key Words.
Viscoelastic fluid flow, moving boundary, finite elements, fluid-structure interaction.

AMS Subject Classifications.
65M60, 65M12.

Abstract.
We study discontinuous Galerkin approximations of the p-biharmonic equation for $p \in (1, \infty)$ from a variational perspective. We propose a discrete variational formulation of the problem based on an appropriate definition of a finite element Hessian and study convergence of the method (without rates) using a semicontinuity argument. We also present numerical experiments aimed at testing the robustness of the method.

Key Words.
discontinuous Galerkin finite element method, discrete variational problem, p-biharmonic equation

AMS Subject Classifications.
65N30, 65K10, 35J40

Abstract.
Scattering of time-harmonic electromagnetic plane waves by a doubly periodic surface structure in $\mathbb{R}^3$ can be simulated by a boundary value problem of the time-harmonic curl-curl equation. For a truncated FEM domain, non-local boundary conditions are required in order to satisfy the radiation conditions for the upper and lower half spaces. As an alternative to boundary integral formulations, to approximate radiation conditions and absorbing boundary methods, Huber et al. [SIAM

J. Sci. Comput., 31 (2009), pp. 1500–1517] have proposed a coupling method based on an idea of Nitsche. In the case of profile gratings with perfectly conducting substrate, the authors have shown previously that a slightly modified variational equation can be proven to be equivalent to the boundary value problem and to be uniquely solvable. Now it is shown that this result can be used to prove convergence for the FEM coupled by truncated wave mode expansion. This result covers transmission gratings and gratings bounded by additional multi-layer systems.

Key Words.
electromagnetic scattering, diffraction gratings, convergence analysis, finite element methods, mortar technique

AMS Subject Classifications.
78A45, 78M10, 65N30, 35J20

Abstract.
In this article, we propose a parameter-uniform computational technique to solve singularly perturbed delay parabolic initial-boundary-value problems exhibiting parabolic boundary layers. The domain is discretized by a uniform mesh in the time direction and a nonuniform mesh for the spatial variable obtained via the equidistribution of a monitor function. The numerical scheme consists of the implicit Euler scheme for the time derivative and the classical central difference scheme for the spatial derivative. A truncation error analysis and a stability analysis are carried out. It is shown that the method converges uniformly in the discrete supremum norm with an optimal error bound. Error estimates are derived, and numerical examples are presented.

Key Words.
singularly perturbed delay parabolic problem, boundary layers, uniform convergence, equidistribution grid, monitor function

AMS Subject Classifications.
65M06, 65M12

Abstract.
In this paper, a structure-preserving algorithm is developed for the computation of a semi-stabilizing solution of a Generalized Algebraic Riccati Equation (GARE). The semi-stabilizing solution of GAREs has been used to characterize the solvability of the (J, J')-spectral factorization problem in control theory for general rational matrices which may have poles and zeros on the extended imaginary axis. The main difficulty in solving such a GARE lies in the fact that its associated Hamiltonian/skew-Hamiltonian pencil has eigenvalues on the extended imaginary axis. Consequently, it is not clear which eigenspace of the associated Hamiltonian/skew-Hamiltonian pencil can characterize the desired semi-stabilizing solution. That is, it is not clear which eigenvectors and principal vectors corresponding to the eigenvalues on the

extended imaginary axis should be contained in the eigenspace that we wish to compute. Hence, the well-known generalized eigenspace approach for the classical algebraic Riccati equations cannot be employed directly. The proposed algorithm consists of a structure-preserving doubling algorithm (SDA) and a postprocessing procedure to determine the desired eigenvectors and principal vectors corresponding to the purely imaginary and infinite eigenvalues. Under mild assumptions, linear convergence of rate $1/2$ for the SDA is proved. Numerical experiments illustrate that the proposed algorithm performs efficiently and reliably.

Key Words.
Generalized Algebraic Riccati Equation, structure-preserving doubling algorithm, semi-stabilizing solution

AMS Subject Classifications.
15A15, 15A09, 15A23

Abstract.
This article is devoted to the development of a constructive approach to constrained interpolation problems from a fractal perspective. A general construction of an α-fractal function $s^\alpha \in \mathcal{C}^p$, the space of all p-times continuously differentiable functions, by a fractal perturbation of a traditional function $s \in \mathcal{C}^p$ using a finite sequence of base functions is introduced. The construction of smooth α-fractal functions described here allows us to embed shape parameters within the structure of differentiable fractal functions. As a consequence, it provides a unified approach to the fractal generalization of various traditional non-recursive rational splines studied in the field of shape preserving interpolation. In particular, we introduce a class of α-fractal rational cubic splines $s^\alpha \in \mathcal{C}^1$ and investigate its shape preserving aspects. It is shown that s^α converges to the original function $\Phi \in \mathcal{C}^2$ with respect to the $\mathcal{C}^1$-norm provided that a suitable mild condition is imposed on the scaling vector α. Besides adding a layer of flexibility, the constructed smooth α-fractal rational spline outperforms its classical non-recursive counterpart in approximating functions with derivatives of varying irregularity. Numerical examples are presented to demonstrate the practical importance of the shape preserving α-fractal rational cubic splines.

Key Words.
iterated function system, α-fractal function, rational cubic spline, convergence, convexity, monotonicity, positivity

AMS Subject Classifications.
28A80, 26A48, 26A51, 65D07, 41A20, 41A29, 41A05

Abstract.
Stable high-order linear interpolation schemes are well suited for the accurate approximation of antiderivatives and the construction of efficient quadrature rules. In this paper we utilize for this purpose the family of linear barycentric rational interpolants by Floater and Hormann, which are particularly useful for interpolation with

at each iteration during the block Arnoldi procedure and reduce computational expense. Moreover, by analyzing its main mathematical properties, we show that the vector deflation procedure arises from the non-increasing behavior of the singular values of the block residual. In addition, the new approach also inherits the property of deflating small eigenvalues to mitigate convergence slowdown. Finally, the effectiveness of the proposed method is illustrated by some numerical experiments.

Key Words.
deflated BFGMRES-DR, block Krylov subspace, modified block Arnoldi vector deflation, harmonic Ritz vectors, deflated block flexible Arnoldi procedure, multiple right-hand sides

AMS Subject Classifications.
65F10,65F50

497 An exponential integrator for non-autonomous parabolic problems.
David Hipp, Marlis Hochbruck, and Alexander Ostermann.

Abstract.
For the time integration of non-autonomous parabolic problems, a new type of exponential integrators is presented and analyzed. The construction of this integrator is closely related to general construction principles of the continuous evolution system. The proximity to the continuous problem allows one to obtain a third-order method that does not suffer from order reduction. The stated order behavior is rigorously proved in an abstract framework of analytic semigroups. The numerical behavior of the integrator is illustrated with an example that models a diffusion process on an evolving domain. Comparisons with an implicit Runge-Kutta method of order three and a standard fourth-order Magnus integrator are given.

Key Words.
exponential integrators, parabolic problems, time-dependent operators, evolving domains

AMS Subject Classifications.
65M12, 65L06