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Contents

1 The MR^3-GK algorithm for the bidiagonal SVD. *Paul R. Willems and Bruno Lang*.

Abstract.
Determining the singular value decomposition of a bidiagonal matrix is a frequent subtask in numerical computations. We shed new light on a long-known way to utilize the algorithm of multiple relatively robust representations, MR^3, for this task by casting the singular value problem in terms of a suitable tridiagonal symmetric eigenproblem (via the Golub–Kahan matrix). Just running MR^3 "as is" on the tridiagonal problem does not work, as has been observed before (e.g., by B. Großer and B. Lang [Linear Algebra Appl., 358 (2003), pp. 45–70]). In this paper we give more detailed explanations for the problems with running MR^3 as a black box solver on the Golub–Kahan matrix. We show that, in contrast to standing opinion, MR^3 *can* be run safely on the Golub–Kahan matrix, with just a minor modification. A proof including error bounds is given for this claim.

Key Words.
bidiagonal matrix, singular value decomposition, MRRR algorithm, theory and implementation, Golub–Kahan matrix

AMS Subject Classifications.
65F30, 65F15, 65G50, 15A18

22 Collocation methods based on radial basis functions for the coupled Klein-Gordon-Schrödinger equations. *Ahmad Golbabai and Ali Safdari-Vaighani*.

Abstract.
This paper presents radial basis function (RBF) collocation methods for the coupled Klein-Gordon-Schrödinger equations. Unlike traditional mesh oriented methods, RBF collocation methods require only a scattered set of nodes in the domain where the solution is approximated. For the RBF collocation method in finite difference mode (RBF-FD), weights for the finite difference formula are obtained by solving local RBF interpolation problems set up around each node in the computational domain. We show that the RBF-FD method has good accuracy and a sparse coefficient matrix, as compared to the global form of the RBF collocation method and other methods.

Key Words.
collocation methods, coupled Klein-Gordon-Schrödinger equations, radial basis functions (RBF)

AMS Subject Classifications.
65N06, 65N40, 65D25, 35Q51

32 A combined fourth-order compact scheme with an accelerated multigrid method for the energy equation in spherical polar coordinates. *T. V. S. Sekhar, R. Sivakumar, S. Vimala, and Y. V. S. S. Sanyasiraju*.

Abstract.
A higher-order compact scheme is combined with an accelerated multigrid method to solve the energy equation in a spherical polar coordinate system. The steady forced convective heat transfer from a sphere which is under the influence of an external magnetic field is simulated. The convection terms in the energy equation are handled in a comprehensive way avoiding complications in the calculations. The angular variation of the Nusselt number and mean Nusselt number are calculated and compared with recent experimental results. Upon applying the magnetic field, a slight degradation of the heat transfer is found for moderate values of the interaction parameter N, and for high values of N an increase in the heat transfer is observed leading to a nonlinear behavior. The speedy convergence of the solution using the multigrid method and accelerated multigrid method is illustrated.

Key Words.
higher-order compact scheme, accelerated multigrid method, forced convection heat transfer, external magnetic field

AMS Subject Classifications.
65N06, 65N55, 35Q80

46 Extremal interpolatory problem of Fejér type for all classical weight functions. *Przemysław Rutka and Ryszard Smarzewski*.

Abstract.
Several constructive solutions of interpolating problems of Fejér, Egerváry and Turán, connected with the optimal, most economical and stable interpolation are known for Jacobi, Hermite and Laguerre orthogonal polynomials. In this paper we solve the interpolatory weighted problem of Fejér type for all positive solutions of the Pearson differential equation, which generate finite or infinite sequences of the classical orthogonal polynomials. More precisely, we establish that the Fejér problem is generic in this class of polynomials and present an elementary unified proof of this fact. Next, these results are used to establish a complete solution of the Egerváry and Turán interpolatory problem.

Key Words.
Fejér extremal problem, Pearson differential equation, Sturm-Liouville differential equation, classical orthogonal polynomials, Lagrange optimal interpolation, weighted stability, most economical systems

AMS Subject Classifications.
41A05, 42C05, 65D05, 49K35

60 On domain-robust preconditioners for the Stokes equations. *Manfred Dobrowolski*.

Abstract.
It is well known that the LBB-constant of the Stokes equations and its discrete counterpart degenerate on domains with high aspect ratio. For the solution of the corresponding linear system we propose two preconditioners that are proven to be

independent of the aspect ratio of the underlying domain. Both preconditioners are based on a refined approximation of the Schur complement using a coarser grid.

Key Words.
Stokes equations, LBB constant, finite elements, mixed methods

AMS Subject Classifications.
65N15, 65N30, 35Q30, 76D07

75 The complete stagnation of GMRES for $n \leq 4$. *Gérard Meurant*.

Abstract.
We study the problem of complete stagnation of the generalized minimum residual method for real matrices of order $n \leq 4$ when solving nonsymmetric linear systems $Ax = b$. We give necessary and sufficient conditions for the non-existence of a real right-hand side b such that the iterates are $x^k = 0$, $k = 0, \ldots, n-1$, and $x^n = x$. We illustrate these conditions with numerical experiments. We also give a sufficient condition for the non-existence of complete stagnation for a matrix A of any order n.

Key Words.
GMRES, stagnation, linear systems

AMS Subject Classifications.
15A06, 65F10

102 Trigonometric Gaussian quadrature on subintervals of the period. *Gaspare Da Fies and Marco Vianello*.

Abstract.
We construct a quadrature formula with $n + 1$ angles and positive weights which is exact in the $(2n + 1)$-dimensional space of trigonometric polynomials of degree $\leq n$ on intervals with length smaller than 2π. We apply the formula to the construction of product Gaussian quadrature rules on circular sectors, zones, segments, and lenses.

Key Words.
trigonometric Gaussian quadrature, subintervals of the period, product Gaussian quadrature, circular sectors, circular zones, circular segments, circular lenses

AMS Subject Classifications.
65D32

113 Boundary element collocation method for solving the exterior Neumann problem for Helmholtz's equation in three dimensions. *Andreas Kleefeld and Tzu-Chu Lin*.

Abstract.
We describe a boundary integral equation that solves the exterior Neumann problem for the Helmholtz equation in three dimensions. The unique solution is found by approximating a Fredholm integral equation of the second kind with the boundary element collocation method. We prove superconvergence at the collocation points,

distinguishing the cases of even and odd interpolation. Numerical examples demonstrate the performance of the method solving the integral equation and confirm the superconvergence.

Key Words.
Fredholm integral equation of the second kind, Helmholtz's equation, exterior Neumann problem, boundary element collocation method, superconvergence

AMS Subject Classifications.
35J05, 45B05, 65N35, 65N38

144 Estimations of the trace of powers of positive self-adjoint operators by extrapolation of the moments. *Claude Brezinski, Paraskevi Fika, and Marilena Mitrouli*.

Abstract.
Let A be a positive self-adjoint linear operator on a real separable Hilbert space H. Our aim is to build estimates of the trace of A^q, for $q \in \mathbb{R}$. These estimates are obtained by extrapolation of the moments of A. Applications of the matrix case are discussed, and numerical results are given.

Key Words.
trace, positive self-adjoint linear operator, symmetric matrix, matrix powers, matrix moments, extrapolation

AMS Subject Classifications.
65F15, 65F30, 65B05, 65C05, 65J10, 15A18, 15A45

156 Spectral deflation in Krylov solvers: A theory of coordinate space based methods. *Martin H. Gutknecht*.

Abstract.
For the iterative solution of large sparse linear systems we develop a theory for a family of augmented and deflated Krylov space solvers that are coordinate based in the sense that the given problem is transformed into one that is formulated in terms of the coordinates with respect to the augmented bases of the Krylov subspaces. Except for the augmentation, the basis is as usual generated by an Arnoldi or Lanczos process, but now with a deflated, singular matrix. The idea behind deflation is to explicitly annihilate certain eigenvalues of the system matrix, typically eigenvalues of small absolute value. The deflation of the matrix is based on an either orthogonal or oblique projection on a subspace that is complimentary to the deflated approximately invariant subspace. While an orthogonal projection allows us to find minimal residual norm solutions, the oblique projections, which we favor when the matrix is non-Hermitian, allow us in the case of an exactly invariant subspace to correctly deflate both the right and the corresponding left (possibly generalized) eigenspaces of the matrix, so that convergence only depends on the non-deflated eigenspaces. The minimality of the residual is replaced by the minimality of a quasi-residual. Among the methods that we treat are primarily deflated versions of GMRES, MINRES, and QMR, but we also extend our approach to deflated, coordinate space based versions

of other Krylov space methods including variants of CG and BiCG. Numerical results will be published elsewhere.

Key Words.
linear equations, Krylov space method, Krylov subspace method, deflation, augmented basis, recycling Krylov subspaces, (singular) preconditioning, GMRes, MinRes, QMR, CG, BiCG

186 Spectral analysis of a block-triangular preconditioner for the Bidomain system in electrocardiology. *Luca Gerardo-Giorda and Lucia Mirabella*.

Abstract.
In this paper we analyze in detail the spectral properties of the block-triangular preconditioner introduced by Gerardo-Giorda et al. [J. Comput. Phys., 228 (2009), pp. 3625-3639] for the Bidomain system in non-symmetric form. We show that the conditioning of the preconditioned problem is bounded in the Fourier space independently of the frequency variable, ensuring quasi-optimality with respect to the mesh size. We derive an explicit formula to optimize the preconditioner performance by identifying a parameter that depends only on the coefficients of the problem and is easy to compute. We provide numerical tests in three dimensions that confirm the optimality of the parameter and the substantial independence of the mesh size.

Key Words.
electrocardiology, Bidomain system, preconditioning, finite elements

AMS Subject Classifications.
65M60, 65M12, 65F08

202 Creating domain mappings. *Kendall Atkinson and Olaf Hansen*.

Abstract.
Consider being given a mapping $\varphi : S^{d-1} \underset{onto}{\xrightarrow{1-1}} \partial\Omega$, with $\partial\Omega$ the $(d-1)$-dimensional smooth boundary surface for a bounded open simply-connected region Ω in $\mathbb{R}^d$, $d \geq 2$. We consider the problem of constructing an extension $\Phi : \overline{B}_d \underset{onto}{\xrightarrow{1-1}} \overline{\Omega}$ with B_d the open unit ball in $\mathbb{R}^d$. The mapping is also required to be continuously differentiable with a non-singular Jacobian matrix at all points. We discuss ways of obtaining initial guesses for such a mapping Φ and of then improving it by an iteration method.

Key Words.
domain mapping, multivariate polynomial, constrained minimization, nonlinear iteration

AMS Subject Classifications.
65D99

231 A robust FEM-BEM MinRes solver for distributed multiharmonic eddy current optimal control problems in unbounded domains. *Michael Kolmbauer*.

Abstract.
This work is devoted to distributed optimal control problems for multiharmonic eddy current problems in unbounded domains. We apply a multiharmonic approach to the optimality system and discretize in space by means of a symmetrically coupled finite and boundary element method, taking care of the different physical behavior in

conducting and non-conducting subdomains, respectively. We construct and analyze a new preconditioned MinRes solver for the system of frequency domain equations. We show that this solver is robust with respect to the space discretization and time discretization parameters as well as the involved "bad" parameters like the conductivity and the regularization parameters. Furthermore, we analyze the asymptotic behavior of the error in terms of the discretization parameters for our special discretization scheme.

Key Words.
time-periodic optimization, eddy current problems, finite element discretization, boundary element discretization, symmetric coupling, MinRes solver

AMS Subject Classifications.
49N20, 35Q61, 65M38, 65M60, 65F08

253 Improved predictor schemes for large systems of linear ODEs. *Mouhamad Al Sayed Ali and Miloud Sadkane*.

Abstract.
When solving linear systems of ordinary differential equations (ODEs) with constant coefficients by implicit schemes such as implicit Euler, Crank-Nicolson, or implicit Runge-Kutta, one is faced with the difficulty of correctly solving the repeated linear systems that arise in the implicit scheme. These systems often have the same matrix but different right-hand sides. When the size of the matrix is large, iterative methods based on Krylov subspaces can be used. However, the effectiveness of these methods strongly depends on the initial guesses. The closer the initial guesses are to the exact solutions, the faster the convergence. This paper presents an approach that computes good initial guesses to these linear systems. It can be viewed as an improved predictor method. It is based on a Petrov-Galerkin process and multistep schemes and consists of building, throughout the iterations, an approximation subspace using the previous computations, where good initial guesses to the next linear systems can be found. It is shown that the quality of the computed initial guess depends only on the stepsize of the discretization and the dimension of the approximation subspace. The approach can be applied to most of the common implicit schemes. It is tested on several examples.

Key Words.
convergence acceleration, implicit scheme, predictor, Petrov-Galerkin, GMRES

AMS Subject Classifications.
65L20, 65F10

271 Variational ensemble Kalman filtering using limited memory BFGS. *Antti Solonen, Heikki Haario, Janne Hakkarainen, Harri Auvinen, Idrissa Amour, and Tuomo Kauranne*.

Abstract.
The extended Kalman filter (EKF) is one of the most used nonlinear state estimation methods. However, in large-scale problems, the CPU and memory requirements of EKF are prohibitively large. Recently, Auvinen et al. proposed a promising approximation to EKF called the variational Kalman filter (VKF). The implementation of VKF requires the tangent linear and adjoint codes for propagating error covariances in time. However, the trouble of building the codes can be circumvented by using

ensemble filtering techniques, where an ensemble of states is propagated in time using the full nonlinear model, and the statistical information needed in EKF formulas is estimated from the ensemble. In this paper, we show how the VKF ideas can be used in the ensemble filtering context. Following VKF, we obtain the state estimate and its covariance by solving a minimization problem using the limited memory Broyden-Fletcher-Goldfarb-Shanno (LBFGS) method, which provides low-storage approximations to the state covariances. The resulting hybrid method, the variational ensemble Kalman filter (VEnKF), has several attractive features compared to existing ensemble methods. The model error and observation error covariances can be inserted directly into the minimization problem instead of randomly perturbing model states and observations as in the standard ensemble Kalman filter. New ensembles can be directly generated from the LBFGS covariance approximation without the need of a square root (Cholesky) matrix decomposition. The frequent resampling from the full state space circumvents the problem of ensemble in-breeding frequently associated with ensemble filters. Numerical examples are used to show that the proposed approach performs better than the standard ensemble Kalman filter, especially when the ensemble size is small.

Key Words.
data assimilation, state estimation, Kalman filtering, ensemble filtering, LBFGS

AMS Subject Classifications.
65K10, 15A29

286 Conformal mapping of circular multiply connected domains onto slit domains. *Roman Czapla, Vladimir Mityushev, and Natalia Rylko*.

Abstract.
The method of Riemann–Hilbert problems is used to unify and to simplify construction of conformal mappings of multiply connected domains. Conformal mappings of arbitrary circular multiply connected domains onto the complex plane with slits of prescribed inclinations are constructed. The mappings are derived in terms of uniformly convergent Poincaré series. In the proposed method, no restriction on the location of the boundary circles is assumed. Convergence and implementation of the numerical method are discussed.

Key Words.
Riemann–Hilbert problem, multiply connected domain, complex plane with slits

AMS Subject Classifications.
30C30, 30E25

298 Optimizing Runge-Kutta smoothers for unsteady flow problems. *Philipp Birken*.

Abstract.
We consider the solution of unsteady viscous flow problems by multigrid methods employing Runge-Kutta smoothers. Optimal coefficients for the smoothers are found by considering the unsteady linear advection equation and performing a Fourier analysis, respectively, looking at the spectral radius of the multigrid iteration matrix. The new schemes are compared to using a classic dual time stepping approach, where the scheme for the steady state equation is reused, meaning that

the smoother coefficients are obtained by an optimization based on the steady state equations, showing significant improvements.

Key Words.
multigrid, unsteady flows, finite volume methods, explicit Runge-Kutta methods, linear advection equation

AMS Subject Classifications.
35L04, 35Q35, 65F10, 65L06, 65M08

313 An iterative substructuring algorithm for a C^0 interior penalty method. *Susanne C. Brenner and Kening Wang*.

Abstract.
We study an iterative substructuring algorithm for a C^0 interior penalty method for the biharmonic problem. This algorithm is based on a Bramble-Pasciak-Schatz preconditioner. The condition number of the preconditioned Schur complement operator is shown to be bounded by $C\left(1+\ln(\frac{H}{h})\right)^2$, where h is the mesh size of the triangulation, H represents the typical diameter of the nonoverlapping subdomains, and the positive constant C is independent of h, H, and the number of subdomains. Corroborating numerical results are also presented.

Key Words.
biharmonic problem, iterative substructuring, domain decomposition, C^0 interior penalty methods, discontinuous Galerkin methods

AMS Subject Classifications.
65N55, 65N30

333 Cascadic multigrid preconditioner for elliptic equations with jump coefficients. *Zhiyong Liu and Yinnian He*.

Abstract.
This paper provides a proof of robustness of the cascadic multigrid preconditioner for the linear finite element approximation of second order elliptic problems with strongly discontinuous coefficients. As a result, we prove that the convergence rate of the conjugate gradient method with cascadic multigrid preconditioner is uniform with respect to large jumps and mesh sizes.

Key Words.
jump coefficients, conjugate gradient, condition number, cascadic multigrid

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

340 Fejér orthogonal polynomials and rational modification of a measure on the unit circle. *Juan-Carlos Santos-León*.

Abstract.
Relations between the monic orthogonal polynomials associated with a measure on the unit circle and the monic orthogonal polynomials associated with a rational modification of this measure are known. In this paper we deal with some generalization in order to give an explicit expression of the Fejér orthogonal polynomials on the unit

circle. Furthermore we give a simple and efficient algorithm to compute the monic orthogonal polynomials associated with a rational modification of a measure.

Key Words.
Fejér kernel, orthogonal polynomials, rational modification of a measure

AMS Subject Classifications.
42C05

353 Locally supported eigenvectors of matrices associated with connected and unweighted power-law graphs. *Van Emden Henson and Geoffrey Sanders*.

Abstract.
We identify a class of graph substructures that yields locally supported eigenvectors of matrices associated with unweighted and undirected graphs, such as the various types of graph Laplacians and adjacency matrices. We discuss how the detection of these substructures gives rise to an efficient calculation of the locally supported eigenvectors and how to exploit the sparsity of such eigenvectors to coarsen the graph into a (possibly) much smaller graph for calculations involving multiple eigenvectors. This preprocessing step introduces no spectral error and, for some graphs, may amount to considerable computational savings when computing any desired eigenpair. As an example, we discuss how these vectors are useful for estimating the commute time between any two vertices and bounding the error associated with approximations for some pairs of vertices.

Key Words.
graph Laplacian, adjacency matrix, eigenvectors, eigenvalues, sparse matrices

AMS Subject Classifications.
05C50, 05C82, 65F15, 65F50, 94C15

379 A survey and comparison of contemporary algorithms for computing the matrix geometric mean. *Ben Jeuris, Raf Vandebril, and Bart Vandereycken*.

Abstract.
In this paper we present a survey of various algorithms for computing matrix geometric means and derive new second-order optimization algorithms to compute the Karcher mean. These new algorithms are constructed using the standard definition of the Riemannian Hessian. The survey includes the ALM list of desired properties for a geometric mean, the analytical expression for the mean of two matrices, algorithms based on the centroid computation in Euclidean (flat) space, and Riemannian optimization techniques to compute the Karcher mean (preceded by a short introduction into differential geometry). A change of metric is considered in the optimization techniques to reduce the complexity of the structures used in these algorithms. Numerical experiments are presented to compare the existing and the newly developed algorithms. We conclude that currently first-order algorithms are best suited for this optimization problem as the size and/or number of the matrices increase.

Key Words.
matrix geometric mean, positive definite matrices, Karcher mean, Riemannian optimization

AMS Subject Classifications.
15A24, 53B21, 65K10

403 Integrating Oscillatory Functions in MATLAB, II. *L. F. Shampine*.

Abstract.
In a previous study we developed a MATLAB program for the approximation of $\int_a^b f(x)\, e^{i\omega x}\, dx$ when ω is large. Here we study the more difficult task of approximating $\int_a^b f(x)\, e^{ig(x)}\, dx$ when $g(x)$ is large on $[a, b]$. We propose a fundamentally different approach to the task— backward error analysis. Other approaches require users to supply the location and nature of critical points of $g(x)$ and may require $g'(x)$. With this new approach, the program `quadgF` merely asks a user to define the problem, i.e., to supply $f(x)$, $g(x)$, $[a, b]$, and specify the desired accuracy. Though intended only for modest relative accuracy, `quadgF` is very easy to use and solves effectively a large class of problems. Of some independent interest is a vectorized MATLAB function for evaluating Fresnel sine and cosine integrals.

Key Words.
quadrature, oscillatory integrand, regular oscillation, irregular oscillation, backward error analysis, Filon, Fresnel integrals, MATLAB

AMS Subject Classifications.
65D30, 65D32, 65D07

414 Computation of the matrix pth root and its Fréchet derivative by integrals. *João R. Cardoso*.

Abstract.
We present new integral representations for the matrix pth root and its Fréchet derivative and then investigate the computation of these functions by numerical quadrature. Three different quadrature rules are considered: composite trapezoidal, Gauss-Legendre and adaptive Simpson. The problem of computing the matrix pth root times a vector without the explicit evaluation of the pth root is also analyzed and bounds for the norm of the matrix pth root and its Fréchet derivative are derived.

Key Words.
matrix pth root, Fréchet derivative, quadrature, composite trapezoidal rule, Gauss-Legendre rule, adaptive Simpson rule

AMS Subject Classifications.
65F60, 65D30

437 Gradient descent for Tikhonov functionals with sparsity constraints: Theory and numerical comparison of step size rules. *Dirk A. Lorenz, Peter Maass, and Pham Q. Muoi*.

Abstract.
In this paper, we analyze gradient methods for minimization problems arising in the regularization of nonlinear inverse problems with sparsity constraints. In particular, we study a gradient method based on the subsequent minimization of quadratic approximations in Hilbert spaces, which is motivated by a recently proposed equivalent method in a finite-dimensional setting. We prove convergence of this method employing assumptions on the operator which are different compared to other approaches. We also discuss accelerated gradient methods with step size control and

present a numerical comparison of different step size selection criteria for a parameter identification problem for an elliptic partial differential equation.

Key Words.
nonlinear inverse problems, sparsity constraints, gradient descent, iterated soft shrinkage, accelerated gradient method

AMS Subject Classifications.
65K10, 46N10, 65M32, 90C48

464 A multiparameter model for link analysis of citation graphs. *Enrico Bozzo and Dario Fasino*.

Abstract.
We propose a family of Markov chain-based models for the link analysis of scientific publications. The PageRank-style model and the dummy paper model discussed in [Electron. Trans. Numer. Anal., 33 (2008), pp. 1–16] can be obtained by a particular choice of its parameters. Since scientific publications can be ordered by the date of publication it is natural to assume a triangular structure for the adjacency matrix of the citation graph. This greatly simplifies the updating of the ranking vector if new papers are added to the database. In addition by assuming that the citation graph can be modeled as a fixed degree sequence random graph we can obtain an explicit estimation of the behavior of the entries of the ranking vector.

Key Words.
link analysis, citation graph, random graph, Markov chain, ranking

AMS Subject Classifications.
15B51, 60J20, 65C40

476 On the minimization of a Tikhonov functional with a non-convex sparsity constraint. *Ronny Ramlau and Clemens A. Zarzer*.

Abstract.
In this paper we present a numerical algorithm for the optimization of a Tikhonov functional with an ℓ_p-sparsity constraints and $p < 1$. Recently, it was proven that the minimization of this functional provides a regularization method. We show that the idea used to obtain these theoretical results can also be utilized in a numerical approach. In particular, we exploit the technique of transforming the Tikhonov functional to a more viable one. In this regard, we consider a surrogate functional approach and show that this technique can be applied straightforwardly. It is proven that at least a critical point of the transformed functional is obtained, which directly translates to the original functional. For a special case, it is shown that a gradient based algorithm can be used to reconstruct the global minimizer of the transformed and the original functional, respectively. Moreover, we apply the developed method to a deconvolution problem and a parameter identification problem in the field of physical chemistry, and we provide numerical evidence for the theoretical results and the desired sparsity promoting features of this method.

Key Words.
sparsity, surrogate functional, inverse problem, regularization

AMS Subject Classifications.
65L09, 65J22, 65J20, 47J06, 94A12