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Contents

Abstract.
Our focus is to study constellations of disjoint disks in the hyperbolic space, i.e., the unit disk equipped with the hyperbolic metric. Each constellation corresponds to a set E which is the union of $m > 2$ disks with hyperbolic radii $r_j > 0, j = 1, \ldots, m$. The centers of the disks are not fixed, and hence individual disks of the constellation are allowed to move under the constraints that they do not overlap and their hyperbolic radii remain invariant. Our main objective is to find computational lower bounds for the conformal capacity of a given constellation. The capacity depends on the centers and radii in a very complicated way even in the simplest cases when $m = 3$ or $m = 4$. In the absence of analytic methods, our work is based on numerical simulations using two different numerical methods, the boundary integral equation method and the hp-FEM method, respectively. Our simulations combine capacity computation with minimization methods and produce extremal cases where the disks of the constellation are grouped next to each other. This resembles the behavior of animal colonies minimizing heat flow in arctic areas.

Key Words.
multiply connected domains, hyperbolic geometry, capacity computation

AMS Subject Classifications.
65E05, 31A15, 30C85

Abstract.
We consider radially symmetric capillary surfaces that are described by bounded generating curves. We use the arc-length representation of the differential equations for these surfaces to allow for vertical points and inflection points along the generating curve. These considerations admit capillary tubes, sessile drops, and fluids in annular tubes as well as other examples. We present a multi-scale pseudo-spectral method for approximating solutions of the associated boundary value problems based on interpolation by Chebyshev polynomials. The multi-scale approach is based on a domain decomposition with adaptive refinements within each subdomain.

Key Words.
capillarity, spectral methods

AMS Subject Classifications.
76B45, 65N35, 35Q35, 34B60

40 The stability of split-preconditioned FGMRES in four precisions.
Erin Carson and Ieva Daužickaitė.

Abstract.
We consider the split-preconditioned FGMRES method in a mixed-precision framework, in which four potentially different precisions can be used for computations with the coefficient matrix, application of the left preconditioner, application of the right preconditioner, and the working precision. Our analysis is applicable to general preconditioners. We obtain bounds for the backward and forward errors in the split-preconditioned FGMRES method. Our analysis further provides insight into how the various precisions should be chosen; under certain assumptions, a suitable selection guarantees a backward error of the order of the working precision.

Key Words.
mixed precision, FGMRES, iterative methods, roundoff error, split-preconditioned

AMS Subject Classifications.
65F08, 65F10, 65F50, 65G50, 65Y99

59 Numerical computation of the half Laplacian by means of a fast convolution algorithm.
Carlota M. Cuesta, Francisco de la Hoz, and Ivan Girona.

Abstract.
In this paper we develop a fast and accurate pseudospectral method to numerically approximate the half Laplacian $(-\Delta)^{1/2}$ of a function on $\mathbb{R}$, which is equivalent to the Hilbert transform of the derivative of the function. The main ideas are as follows. Given a twice continuously differentiable bounded function $u \in \mathcal{C}_b^2(\mathbb{R})$, we apply the change of variable $x = L\cot(s)$, with $L > 0$ and $s \in [0, \pi]$, which maps $\mathbb{R}$ into $[0, \pi]$, and denote $(-\Delta)_s^{1/2} u(x(s)) \equiv (-\Delta)^{1/2} u(x)$. Therefore, by performing a Fourier series expansion of $u(x(s))$, the problem is reduced to computing $(-\Delta)_s^{1/2} e^{iks} \equiv (-\Delta)^{1/2}[(x + i)^k/(1 + x^2)^{k/2}]$. In a previous work we considered the case with k even for more general powers $\alpha/2$, with $\alpha \in (0, 2)$, so here we focus on the case with k odd. More precisely, we express $(-\Delta)_s^{1/2} e^{iks}$ for k odd in terms of the Gaussian hypergeometric function ${}_2F_1$ and as a well-conditioned finite sum. Then we use a fast convolution result that enable us to compute very efficiently $\sum_{l=0}^{M} a_l (-\Delta)_s^{1/2} e^{i(2l+1)s}$ for extremely large values of M. This enables us to approximate $(-\Delta)_s^{1/2} u(x(s))$ in a fast and accurate way, especially when $u(x(s))$ is not periodic of period π. As an application, we simulate a fractional Fisher's equation having front solutions whose speed grows exponentially.

Key Words.
half Laplacian, pseudospectral method, Gaussian hypergeometric functions, fast convolution, fractional Fisher's equation

AMS Subject Classifications.
26A33, 33C05, 65T50

99 A review of maximum-norm a posteriori error bounds for time-semidiscretisations of parabolic equations.
Torsten Linss, Natalia Kopteva, Goran Radojev, and Martin Ossadnik.

Abstract.
A posteriori error estimates in the maximum norm are studied for various time-semidiscretisations applied to a class of linear parabolic equations. We summarise results from the literature and present some new improved error bounds. Crucial ingredients are certain bounds in the L_1-norm for the Green's function associated with the parabolic operator and its derivatives.

Key Words.
parabolic problems, maximum-norm a posteriori error estimates, backward Euler, Crank–Nicolson, extrapolation, discontinuous Galerkin–Radau, backward differentiation formulae, Green's function

AMS Subject Classifications.
65M15, 65M60

123 Dimensional reduction for multivariate Lagrange polynomial interpolation problems.
M. Errachid, A. Essanhaji, and A. Messaoudi.

Key Words.
polynomial interpolation, multivariate Lagrange polynomial interpolation problem

AMS Subject Classifications.
65D05, 41A05, 41A63, 41A10, 97N50

136 Convergence analysis of a Krylov subspace spectral method for the 1D wave equation in an inhomogeneous medium.
Bailey Rester, Anzhelika Vasilyeva, and James V. Lambers.

Abstract.
This paper presents a convergence analysis of a Krylov subspace spectral (KSS) method applied to an 1D wave equation in an inhomogeneous medium. It will be shown that for sufficiently regular initial data, this KSS method yields unconditional stability, spectral accuracy in space, and second-order accuracy in time in the case of constant wave speed and a bandlimited reaction term coefficient. Numerical experiments that corroborate the established theory are included along with an investigation of generalizations, such as to higher space dimensions and nonlinear PDEs, that features performance comparisons with other Krylov subspace-based time-stepping methods. This paper also includes the first stability analysis of a KSS method that does not assume a bandlimited reaction term coefficient.

Key Words.
spectral methods, wave equation, convergence analysis, variable coefficients

AMS Subject Classifications.
65M70, 65M12, 65F60

169 Fully algebraic domain decomposition preconditioners with adaptive spectral bounds.
Loïc Gouarin and Nicole Spillane.

Abstract.
In this article a new family of preconditioners is introduced for symmetric positive definite linear systems. The new preconditioners, called the AWG preconditioners

(for Algebraic-Woodbury-GenEO), are constructed algebraically. By this we mean that only the knowledge of the matrix $\mathbf{A}$ for which the linear system is being solved is required. Thanks to the GenEO spectral coarse space technique, the condition number of the preconditioned operator is bounded theoretically from above. This upper bound can be made smaller by enriching the coarse space with more spectral modes.
The novelty is that, unlike in previous work on the GenEO coarse spaces, no knowledge of a partially non-assembled form of $\mathbf{A}$ is required. Indeed, the spectral coarse space technique is not applied directly to $\mathbf{A}$ but to a low-rank modification of $\mathbf{A}$ of which a suitable non-assembled form is known by construction. The extra cost is a second (and to this day rather expensive) coarse solve in the preconditioner. One of the AWG preconditioners has already been presented in a short preprint by Spillane [Domain Decomposition Methods in Science and Engineering XXVI, Springer, Cham, 2022, pp. 745–752]. This article is the first full presentation of the larger family of AWG preconditioners. It includes proofs of the spectral bounds as well as numerical illustrations.

Key Words.
preconditioner, domain decomposition, coarse space, algebraic, linear system, Woodbury matrix identity

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

Abstract.
Data assimilation algorithms combine information from observations and prior model information to obtain the most likely state of a dynamical system. The linearised weak-constraint four-dimensional variational assimilation problem can be reformulated as a saddle point problem, which admits more scope for preconditioners than the primal form. In this paper we design new terms that can be used within existing preconditioners, such as block diagonal and constraint-type preconditioners. Our novel preconditioning approaches (i) incorporate model information and (ii) are designed to target correlated observation error covariance matrices. To our knowledge, (i) has not been considered previously for data assimilation problems. We develop a theory demonstrating the effectiveness of the new preconditioners within Krylov subspace methods. Linear and non-linear numerical experiments reveal that our new approach leads to faster convergence than existing state-of-the-art preconditioners for a broader range of problems than indicated by the theory alone. We present a range of numerical experiments performed in serial.

Key Words.
saddle point systems, variational data assimilation, preconditioning

AMS Subject Classifications.
65F08, 65F10, 65N21

Abstract.
We consider the iterative solution of symmetric saddle-point matrices with a singular leading block. We develop a new ideal positive definite block-diagonal preconditioner that yields a preconditioned operator with four distinct eigenvalues. We offer a few techniques for making the preconditioner practical and illustrate the effectiveness of our approach with numerical experiments. The novelty of the paper lies in the generality of the assumptions made: as long as the saddle-point matrix is nonsingular, there is no assumption on the specific rank of the leading block. Current ideal preconditioners typically rely either on invertibility or a high nullity of the leading block, and the new technique aims to bridge this gap. A spectral analysis is offered, accompanied by numerical experiments.

Key Words.
saddle-point systems, preconditioning, augmentation, Schur complement

AMS Subject Classifications.
65F08, 65F10, 65F15

Abstract.
The Eberlein method is a Jacobi-type process for solving the eigenvalue problem of an arbitrary matrix. In each iteration two transformations are applied to the underlying matrix, a plane rotation and a non-unitary core transformation. The paper studies the method under the broad class of generalized serial pivot strategies. We prove global convergence of the Eberlein method under the generalized serial pivot strategies with permutations and present several numerical examples.

Key Words.
Jacobi-type methods, matrix diagonalization, pivot strategies, global convergence

AMS Subject Classifications.
65F15

Abstract.
Within this paper, we introduce and analyze a novel time-stepping scheme for linear poroelasticity. In each time frame, we iteratively solve the flow and mechanics equations with an additional damping step for the pressure variable. Depending on the coupling strength of the two equations, we explicitly quantify the required number of inner iteration steps to guarantee first-order convergence. By a number of numerical experiments we confirm the theoretical results and study the dependence of the inner iteration steps in terms of the coupling strength. Moreover, we compare our method to the well-known fixed-stress scheme.

Key Words.
poroelasticity, semi-explicit time discretization, decoupling, iterative scheme

AMS Subject Classifications.
65M12, 65M20, 65L80, 76S05

Abstract.
We consider certain (real) nonsymmetric matrices in saddle point form, study their general Jordan normal forms, and prove new conditions so that these matrices are diagonalizable with a real spectrum. For matrices satisfying our conditions we show how to construct an inner product in which these matrices are selfadjoint. Our approach generalizes previously published results in this area, which require stronger assumptions on the given saddle point matrices and hence are less widely applicable.

Key Words.
saddle point problems, eigenvalues and eigenvectors, conjugate gradient iterations, Krylov subspace methods

AMS Subject Classifications.
15A18, 65F10

Abstract.
We introduce a new method with spectral accuracy to solve linear non-autonomous ordinary differential equations (ODEs) of the kind $\frac{d}{dt}\tilde{u}(t) = \tilde{f}(t)\tilde{u}(t)$, $\tilde{u}(-1) = 1$, with $\tilde{f}(t)$ an analytic function. The method is based on a new analytical expression for the solution $\tilde{u}(t)$ given in terms of a convolution-like operation, the $\star$-product. We prove that, by representing this expression in a finite Legendre polynomial basis, the solution $\tilde{u}(t)$ can be found by solving a matrix problem involving the Fourier coefficients of $\tilde{f}(t)$. An efficient procedure is proposed to approximate the Legendre coefficients of $\tilde{u}(t)$, and the truncation error and convergence are analyzed. We show the effectiveness of the proposed procedure through numerical experiments. Our approach allows for a generalization of the method to solve systems of linear ODEs.

Key Words.
Legendre polynomials, spectral accuracy, ordinary differential equations

AMS Subject Classifications.
65F60, 65L05, 35Q41

Abstract.
Motivated by the aggregation method, we present an iterative method for finding approximate solutions of least-squares problems for linear ill-posed problems over (mixed) rational Krylov spaces. The mixed rational Krylov spaces where the solution is sought consist of Tikhonov-regularized solutions mixed with usual Krylov space elements from the normal equations. We present an algorithm based on the Arnoldi–Lanczos iteration, and, as main result, derive the rational CG method, a short-term iteration that, similar as the usual conjugate gradient method, does not requires orthogonalization or saving of the Krylov basis vectors. Some numerical experiments illustrate the performance of the method.

Andreas Frommer, Gustavo Ramirez-Hidalgo, Marcel Schweitzer, and Manuel Tsolakis.

Abstract.
While preconditioning is a long-standing concept to accelerate iterative methods for linear systems, generalizations to matrix functions are still in their infancy. We go a further step in this direction, introducing polynomial preconditioning for Krylov subspace methods that approximate the action of the matrix square root and inverse square root on a vector. Preconditioning reduces the subspace size and therefore avoids the storage problem together with—for non-Hermitian matrices—the increased computational cost per iteration that arises in the unpreconditioned case. Polynomial preconditioning is an attractive alternative to current restarting or sketching approaches since it is simpler and computationally more efficient. We demonstrate this for several numerical examples.

Key Words.
polynomial preconditioning, matrix square root, inverse square root, Krylov space, matrix functions

AMS Subject Classifications.
65F60, 65F08, 65F50, 15A16

405 Analysis of a one-dimensional nonlocal thermoelastic problem.
Noelia Bazarra, José R. Fernández, and Ramón Quintanilla.

Abstract.
In this paper we study a one-dimensional dynamic thermoelastic problem assuming that the elastic coefficient is negative. Following the ideas proposed by Eringen in the 80s, a nonlocal term is introduced into the constitutive equation for the displacements, leading to a hyperbolic problem. Then, we consider the numerical approximation of the problem by using the classical finite element method to approximate the spatial variable and the implicit Euler scheme to discretize the time derivatives. A discrete stability property is proved, and an a priori error analysis is done, from which we can conclude the linear convergence of the approximations under suitable regularity for the continuous solution. Finally, some numerical simulations are presented, including the demonstration of the numerical convergence and the behavior of the discrete energy for several choices of the constitutive parameters.

Key Words.
nonlocal thermoelasticity, finite elements, discrete stability, a priori error estimates, numerical simulations

AMS Subject Classifications.
65M15, 65M60, 65M12

421 Near-optimal convergence of the full orthogonalization method.
Tyler Chen and Gérard Meurant.

Abstract.
We establish a near-optimality guarantee for the full orthogonalization method (FOM), showing that the *overall* convergence of FOM is nearly as good as GMRES. In particular, we prove that at every iteration k, there exists an iteration $j \leq k$ for which the FOM residual norm at iteration j is no more than $\sqrt{k+1}$ times

larger than the GMRES residual norm at iteration $\boldsymbol{k}$. This bound is sharp, and it has implications for algorithms for approximating the action of a matrix function on a vector.

Key Words.
Full Orthogonalization Method, GMRES

AMS Subject Classifications.
65F10

Abstract.
We show that product Chebyshev polynomial meshes can be used, in a fully discrete way, to evaluate with rigorous error bounds the Lebesgue constant, i.e., the maximum of the Lebesgue function, for a class of polynomial projectors on cube, simplex, and ball, including interpolation, hyperinterpolation, and weighted least-squares approximation. Several examples are presented and possible generalizations outlined. A numerical software package implementing the method is freely available online.

Key Words.
multivariate polynomial meshes, cube, simplex, ball, polynomial projectors, interpolation, least-squares, hyperinterpolation, polynomial optimization, Lebesgue constant

AMS Subject Classifications.
65D05, 65D10, 65K05

Abstract.
The paper proposes polynomial-based projection-type and modified projection-type methods to solve weakly singular Volterra–Hammerstein integral equations of the second kind. Jacobi polynomials are used as basis functions. This type of equations often exhibits singular behavior at the left endpoint of the integration interval, and the exact solutions are typically nonsmooth. In the method under consideration, the independent variable is first transformed to provide a new integral equation with a smoother solution, allowing the Jacobi spectral method to be easily applied to the transformed equation and a full convergence analysis of the method to be performed. In different numerical tests, the effectiveness of the proposed approach is demonstrated.

Key Words.
Volterra–Hammerstein integral equations, Jacobi polynomials, weakly singular kernels, orthogonal projection, interpolatory projection, superconvergence

AMS Subject Classifications.
45B05, 45G10, 65R20

471 Structured condition numbers for a linear function of the solution of the generalized saddle point problem.
Sk. Safique Ahmad and Pinki Khatun.

Abstract.
This paper addresses structured normwise, mixed, and componentwise condition numbers (*CNs*) for a linear function of the solution to the generalized saddle point problem (*GSPP*). We present a general framework that enables us to measure structured *CNs* of the individual components of the solution. Then, we derive their explicit formulae when the input matrices have symmetric, Toeplitz, or some general linear structures. In addition, compact formulae for unstructured *CNs* are obtained, which recover previous results on *CNs* for *GSPPs* for specific choices of the linear function. Furthermore, applications of the derived structured *CNs* are provided to determine the structured *CNs* for the weighted Toeplitz regularized least-squares problems and Tikhonov regularization problems, which recovers some previous studies in the literature.

Key Words.
generalized saddle point problems, condition number, perturbation analysis, weighted Toeplitz regularized least-squares problem, Toeplitz matrices

AMS Subject Classifications.
65F35, 65F20, 65F99, 15A12

501 A single shooting method with approximate Fréchet derivative for computing geodesics on the Stiefel manifold.
Marco Sutti.

Abstract.
This paper shows how to use the shooting method, a classical numerical algorithm for solving boundary value problems, to compute the Riemannian distance on the Stiefel manifold $\mathrm{St}(n,p)$, the set of $n \times p$ matrices with orthonormal columns. The proposed method is a shooting method in the sense of the classical shooting methods for solving boundary value problems; see, e.g., Stoer and Bulirsch, 1993. The main feature is that we provide an approximate formula for the Fréchet derivative of the geodesic involved in our shooting method. Numerical experiments demonstrate the algorithm's accuracy and performance. Comparisons with existing state-of-the-art algorithms for solving the same problem show that our method is competitive and even beats several algorithms in many cases.

Key Words.
Stiefel manifold, shooting methods, endpoint geodesic problem, Riemannian distance, Newton's method, Fréchet derivative

AMS Subject Classifications.
65L10, 65F45, 65F60, 65L05, 53C22, 58C15

520 Efficient third-order tensor-oriented directional splitting for exponential integrators.
Fabio Cassini.

Abstract.
Suitable discretizations of popular multidimensional operators (for instance of diffusion or diffusion-advection type) by tensor product formulas lead to matrices with

d-dimensional Kronecker sum structure. For evolutionary partial differential equations containing such operators and when integrating in time with exponential integrators, it is then of paramount importance to efficiently approximate the actions of φ-functions of the arising matrices. In this work we show how to produce directional split approximations of third order with respect to the time step size. These approximations conveniently employ tensor-matrix products (the so-called μ-mode product and the related Tucker operator, realized in practice with high-performance level 3 BLAS operations) and allow for the effective usage of exponential Runge–Kutta integrators up to order three. The technique can also be efficiently implemented on modern computer hardware such as Graphic Processing Units. This approach is successfully tested against state-of-the-art techniques on two well-known physical models that lead to Turing patterns, namely the 2D Schnakenberg and the 3D FitzHugh–Nagumo systems, on different hardware and software architectures.

Key Words.
exponential integrators, μ-mode product, directional splitting, φ-functions, Kronecker sum, Turing patterns, Graphic Processing Units

AMS Subject Classifications.
65F60, 65L04, 65L05, 65M20

Abstract.
This paper deals with a new boundary integral equation method for the numerical solution of the exterior Neumann problem for the Laplace equation in planar domains with corners. Using the single layer representation of the potential, the differential problem is reformulated in terms of a boundary integral equation (BIE) whose solution has singularities at the corners. A "modified" Nyström-type method based on a Gauss–Jacobi–Lobatto quadrature formula is proposed for its approximation. Convergence and stability results are proved in proper weighted spaces of continuous functions. Moreover, the use of a smoothing transformation allows one to increase the regularity of the solution and, consequently, the order of convergence of the method. The efficiency of the proposed method is illustrated by some numerical tests.

Key Words.
boundary integral equations, Neumann problem, domains with corners, Nyström method

AMS Subject Classifications.
65R20, 45E99, 45F15

Abstract.
In this study, we consider the development of tailored quasi-Monte Carlo (QMC) cubatures for non-conforming discontinuous Galerkin (DG) approximations of elliptic partial differential equations (PDEs) with random coefficients. We consider both the affine and uniform and the lognormal models for the input random field

and investigate the use of QMC cubatures to approximate the expected value of the PDE response subject to input uncertainty. In particular, we prove that the resulting QMC convergence rate for DG approximations behaves in the same way as if continuous finite elements were chosen. Notably, the parametric regularity bounds for DG, which are developed in this work, are also useful for other methods such as sparse grids. Numerical results underline our analytical findings.

Key Words.
diffusion equation, discontinuous Galerkin, quasi-Monte Carlo, random coefficient

AMS Subject Classifications.
65C05, 65N30

618 LSEMINK: a modified Newton–Krylov method for Log-Sum-Exp minimization.
Kelvin Kan, James G. Nagy, and Lars Ruthotto.

Abstract.
This paper introduces LSEMINK, an effective modified Newton–Krylov algorithm geared toward minimizing the log-sum-exp function for a linear model. Problems of this kind arise commonly, for example, in geometric programming and multinomial logistic regression. Although the log-sum-exp function is smooth and convex, standard line-search Newton-type methods can become inefficient because the quadratic approximation of the objective function can be unbounded from below. To circumvent this, LSEMINK modifies the Hessian by adding a shift in the row space of the linear model. We show that the shift renders the quadratic approximation to be bounded from below and that the overall scheme converges to a global minimizer under mild assumptions. Our convergence proof also shows that all iterates are in the row space of the linear model, which can be attractive when the model parameters do not have an intuitive meaning, as is common in machine learning. Since LSEMINK uses a Krylov subspace method to compute the search direction, it only requires matrix-vector products with the linear model, which is critical for large-scale problems. Our numerical experiments on image classification and geometric programming illustrate that LSEMINK considerably reduces the time-to-solution and increases the scalability compared to geometric programming and natural gradient descent approaches. It has significantly faster initial convergence than standard Newton–Krylov methods, which is particularly attractive in applications like machine learning. In addition, LSEMINK is more robust to ill-conditioning arising from the nonsmoothness of the problem. We share our MATLAB implementation at a GitHub repository (https://github.com/KelvinKan/LSEMINK).

Key Words.
log-sum-exp minimization, Newton–Krylov method, modified Newton method, machine learning, geometric programming

AMS Subject Classifications.
65K10

A1 Application of the Schur–Cohn Theorem to the precise convergence domain for a p-cyclic SOR iteration matrix.
Apostolos Hadjidimos, Xiezhang Li, and Richard S. Varga.

Abstract.
Assume that $A \in C^{n \times n}$ is a block p-cyclic consistently ordered matrix and that its

associated Jacobi iteration matrix B, which is weakly cyclic of index p, has eigenvalues μ whose pth powers are all real nonpositive (resp. nonnegative). Usually, one is interested only in the relaxation parameter ω that minimizes the spectral radius of the iteration matrix of the associated SOR iterative method, but here we are interested in all real values for the relaxation parameter ω for which the SOR iteration matrix is convergent. This will be achieved for the values of $p = 2, 3, 4, \ldots,$ and for $p \to \infty$.

Key Words.
block p-cyclic matrix, weakly cyclic of index p matrix, block Jacobi and SOR iteration matrices, Schur–Cohn Algorithm

AMS Subject Classifications.
65F10