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programming problems. In this paper we examine the decrease of the convex cost function along the projected-gradient path and extend the earlier estimate given by Joachim Schöberl. The result is an important ingredient in the development of optimal algorithms for the solution of convex quadratic programming problems.

Key Words.
bound-constrained quadratic programming, Euclidean gradient projection, rate of convergence

AMS Subject Classifications.
65K05, 90C20, 49M10

30 Stability results for scattered data interpolation on the rotation group. *Manuel Gräf and Stefan Kunis*.

Abstract.
Fourier analysis on the rotation group $SO(3)$ expands each function into the orthogonal basis of Wigner-D functions. Recently, fast and reliable algorithms for the evaluation of finite expansion of such type, referred to as nonequispaced FFT on $SO(3)$, have become available. Here, we consider the minimal norm interpolation of given data by Wigner-D functions. We prove bounds on the conditioning of this problem which rely solely on the number of Fourier coefficients and the separation distance of the sampling nodes. The reconstruction of N^3 Fourier coefficients from M well separated samples is shown to take only $\mathcal{O}(N^3 \log^2 N + M)$ floating point operations.

Key Words.
scattered data interpolation, iterative methods, FFT

AMS Subject Classifications.
65T50, 65F10, 43A75, 41A05, 15A60

40 On the modeling of entropy producing processes. *Kumbakonam R. Rajagopal*.

Abstract.
A general thermodynamic framework is presented for the study of the response of bodies undergoing entropy producing processes. In general, in such processes the natural configuration of a body, i.e., the configuration that the body would take on the removal of all external stimuli, changes. The fact that material symmetry of the body in these various natural configurations could be different allows one to model the response of bodies that cannot be described by traditional models that are in place. It is assumed that the processes take place in a manner such that the rate at which entropy is produced is maximized. Knowing how the material stores energy, produces entropy, conducts heat, absorbs or emits radiation, etc., allows one to determine the constitutive equation for the stress and other relevant quantities. The fact that the body's natural configuration changes and the form for the stress response from the natural configuration changes, leads to a lot of challenges with regard to the development of analytical as well as numerical methods for the study of the response of bodies.

Key Words.
rate of entropy production, internal energy, Helmholtz potential, rate of dissipation, second law of thermodynamics

AMS Subject Classifications.
80A17, 74C10, 74C15, 74C20, 76A05, 76A10, 76A15

Abstract.
A technique to compute all the possible minors of order $n - j$ of binary Hadamard matrices with entries $(0, 1)$ is introduced. The method exploits the properties of such matrices S and also the symmetry and special block structure appearing when one forms the matrix $D^T D$, where D is a submatrix of S. Theoretically, the method works for every pair of values n and j and provides general analytical formulae. The whole process can be standardized and implemented as a computer algorithm. The usefulness of such a method is justified by the application to the growth problem. This study gives also more insight into some structural properties of these matrices and leads to the formulation of the growth conjecture for binary Hadamard matrices.

Key Words.
binary Hadamard matrices, determinant calculus, symbolic computations, Gaussian elimination, growth problem

AMS Subject Classifications.
15A15, 05B20, 65F40, 65F05, 65G50

Abstract.
Lanczos bidiagonalization is a competitive method for computing a partial singular value decomposition of a large sparse matrix, that is, when only a subset of the singular values and corresponding singular vectors are required. However, a straightforward implementation of the algorithm has the problem of loss of orthogonality between computed Lanczos vectors, and some reorthogonalization technique must be applied. Also, an effective restarting strategy must be used to prevent excessive growth of the cost of reorthogonalization per iteration. On the other hand, if the method is to be implemented on a distributed-memory parallel computer, then additional precautions are required so that parallel efficiency is maintained as the number of processors increases.
In this paper, we present a Lanczos bidiagonalization procedure implemented in SLEPc, a software library for the solution of large, sparse eigenvalue problems on parallel computers. The solver is numerically robust and scales well up to hundreds of processors.

Key Words.
partial singular value decomposition, Lanczos bidiagonalization, thick restart, parallel computing

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

Abstract.
This paper presents a modification of Krylov subspace spectral (KSS) methods, which build on the work of Golub, Meurant and others, pertaining to moments and Gaussian quadrature to produce high-order accurate approximate solutions to variable-coefficient time-dependent PDEs. Whereas KSS methods currently use Lanczos iteration to compute the needed quadrature rules, our modification uses block Lanczos iteration in order to avoid the need to compute two quadrature rules for each component of the solution, or use perturbations of quadrature rules. It will be shown that, under reasonable assumptions on the coefficients of the problem, a 1-node KSS method is unconditionally stable, and methods with more than one node are shown to possess favorable stability properties as well. Numerical results suggest that block KSS methods are significantly more accurate than their non-block counterparts.

Key Words.
spectral methods, Gaussian quadrature, variable-coefficient, block Lanczos method, stability, heat equation

AMS Subject Classifications.
65M12, 65M70, 65D32, 65F25

Abstract.
We report on very recent developments concerning the modelling of the complex behaviour of materials within the framework of implicit constitutive theory due to K. R. Rajagopal. In this paper, we restrict ourselves to a hierarchy of power-law-like fluids. For such a class of fluids, we provide an overview of recent results concerning the mathematical analysis of the relevant boundary value problems. Mathematical results are presented for the (Rothe) time discretizations of evolutionary problems. The main purpose of this paper is to emphasize the mathematical tools involved in the theoretical analysis and to initiate the development of numerical methods for the problems presented here.

Key Words.
power-law fluid, incompressible fluid, implicit constitutive theory, Rothe approximation, time discretization, weak solution, existence, regularity

AMS Subject Classifications.
35D05, 35Q30, 35Q35, 76D03, 76D99

Abstract.
We consider the solution of complex symmetric shifted linear systems. Such systems arise in large-scale electronic structure simulations, and there is a strong need of algorithms for their fast solution. With the aim of solving the systems efficiently, we consider a special case of the QMR method for non-Hermitian shifted linear

systems and propose its weighted quasi-minimal residual approach. A numerical algorithm, referred to as shifted QMR_SYM(B), is obtained by the choice of a weight which is particularly cost-effective. Numerical examples are presented to show the performance of the shifted QMR_SYM(B) method.

Key Words.
complex symmetric matrices, shifted linear systems, Krylov methods, COCG, QMR_SYM

AMS Subject Classifications.
65F10

141 Structured low rank approximations of the Sylvester resultant matrix for approximate GCDs of Bernstein basis polynomials. *Joab R. Winkler and John D. Allan.*

Abstract.
A structured low rank approximation of the Sylvester resultant matrix $S(f,g)$ of the Bernstein basis polynomials $f = f(y)$ and $g = g(y)$, for the determination of their approximate greatest common divisors (GCDs), is computed using the method of structured total least norm. Since the GCD of $f(y)$ and $g(y)$ is equal to the GCD of $f(y)$ and $\alpha g(y)$, where α is an arbitrary non-zero constant, it is more appropriate to consider a structured low rank approximation $S(\tilde{f},\tilde{g})$ of $S(f,\alpha g)$, where the polynomials $\tilde{f} = \tilde{f}(y)$ and $\tilde{g} = \tilde{g}(y)$ approximate the polynomials $f(y)$ and $\alpha g(y)$, respectively. Different values of α yield different structured low rank approximations $S(\tilde{f},\tilde{g})$, and therefore different approximate GCDs. It is shown that the inclusion of α allows to obtain considerably improved approximations, as measured by the decrease of the singular values σ_i of $S(\tilde{f},\tilde{g})$, with respect to the approximation obtained when the default value $\alpha = 1$ is used. An example that illustrates the theory is presented and future work is discussed.

Key Words.
Bernstein polynomials, structured low rank approximation, Sylvester resultant matrix

AMS Subject Classifications.
15A12, 65F35

156 Adaptive constraint reduction for training support vector machines. *Jin Hyuk Jung, Dianne P. O'Leary, and André L. Tits.*

Abstract.
A support vector machine (SVM) determines whether a given observed pattern lies in a particular class. The decision is based on prior training of the SVM on a set of patterns with known classification, and training is achieved by solving a convex quadratic programming problem. Since there are typically a large number of training patterns, this can be expensive. In this work, we propose an adaptive constraint reduction primal-dual interior-point method for training a linear SVM with ℓ_1 penalty (hinge loss) for misclassification. We reduce the computational effort by assembling the normal equation matrix using only a well-chosen subset of patterns. Starting with a large portion of the patterns, our algorithm excludes more and more unnecessary patterns as the iteration proceeds. We extend our approach to training nonlinear SVMs through Gram matrix approximation methods. We demonstrate the effectiveness of the algorithm on a variety of standard test problems.

Key Words.
constraint reduction, column generation, primal-dual interior-point method, support vector machine

AMS Subject Classifications.
90C20, 90C51, 90C59, 68W01

178 Approximation of the scattering amplitude and linear systems. *Gene H. Golub, Martin Stoll, and Andy Wathen*.

Abstract.
The simultaneous solution of $Ax = b$ and $A^T y = g$, where A is a non-singular matrix, is required in a number of situations. Darmofal and Lu have proposed a method based on the Quasi-Minimal Residual algorithm (QMR). We will introduce a technique for the same purpose based on the LSQR method and show how its performance can be improved when using the generalized LSQR method. We further show how preconditioners can be introduced to enhance the speed of convergence and discuss different preconditioners that can be used. The scattering amplitude $g^T x$, a widely used quantity in signal processing for example, has a close connection to the above problem since x represents the solution of the forward problem and g is the right-hand side of the adjoint system. We show how this quantity can be efficiently approximated using Gauss quadrature and introduce a block-Lanczos process that approximates the scattering amplitude, and which can also be used with preconditioning.

Key Words.
linear systems, Krylov subspaces, Gauss quadrature, adjoint systems

AMS Subject Classifications.
65F10, 65N22, 65F50, 76D07

204 Noise propagation in regularizing iterations for image deblurring. *Per Christian Hansen and Toke Koldborg Jensen*.

Abstract.
We use the two-dimensional discrete cosine transform to study how the noise from the data enters the reconstructed images computed by regularizing iterations, that is, Krylov subspace methods applied to discrete ill-posed problems. The regularization in these methods is obtained via the projection onto the associated Krylov subspace. We focus on CGLS/LSQR, GMRES, and RRGMRES, as well as MINRES and MR-II in the symmetric case. Our analysis shows that the noise enters primarily in the form of band-pass filtered white noise, which appears as "freckles" in the reconstructions, and these artifacts are present in both the signal and the noise components of the solutions. We also show why GMRES and MINRES are not suited for image deblurring.

Key Words.
image deblurring, regularizing iterations, Krylov subspaces, CGLS, LSQR, GMRES, MINRES, RRGMRES, MR-II

AMS Subject Classifications.
65F22, 65F10

Abstract.
Starting from the residual estimates for GMRES formulated by many authors, usually in terms of the quotient of the Hermitian part and the norm of a matrix or by using the field of values of a matrix, we present more general estimates which hold also for restarted and augmented GMRES. Sufficient conditions for convergence are formulated. All estimates are independent on the choice of an initial approximation.

Key Words.
linear equations, restarted and augmented GMRES method, residual bounds, non-stagnation conditions

AMS Subject Classifications.
15A06, 65F10

Abstract.
Schwarz domain decomposition methods are the oldest domain decomposition methods. They were invented by Hermann Amandus Schwarz in 1869 as an analytical tool to rigorously prove results obtained by Riemann through a minimization principle. Renewed interest in these methods was sparked by the arrival of parallel computers, and variants of the method have been introduced and analyzed, both at the continuous and discrete level. It can be daunting to understand the similarities and subtle differences between all the variants, even for the specialist.
This paper presents Schwarz methods as they were developed historically. From quotes by major contributors over time, we learn about the reasons for similarities and subtle differences between continuous and discrete variants. We also formally prove at the algebraic level equivalence and/or non-equivalence among the major variants for very general decompositions and many subdomains. We finally trace the motivations that led to the newest class called optimized Schwarz methods, illustrate how they can greatly enhance the performance of the solver, and show why one has to be cautious when testing them numerically.

Key Words.
alternating and parallel Schwarz methods, additive, multiplicative and restricted additive Schwarz methods, optimized Schwarz methods

AMS Subject Classifications.
65F10, 65N22

Abstract.
Model order reduction (MOR) is common in simulation, control and optimization of complex dynamical systems arising in modeling of physical processes, and in the spatial discretization of parabolic partial differential equations in two or more dimensions. Typically, after a semi-discretization of the differential operator by the finite or boundary element method, we have a large state-space dimension n. In order to accelerate the simulation time or to facilitate the control design, it is often desirable to employ an approximate reduced-order system of order r, with $r \ll n$, instead

of the original large-scale system. We show how to compute a reduced-order system with a balancing-related model reduction method. The method is based on the computation of the cross-Gramian $\mathcal{X}$, which is the solution of a Sylvester equation. As standard algorithms for the solution of Sylvester equations are of limited use for large-scale (possibly dense) systems, we investigate approaches based on the iterative sign function method, using data-sparse matrix approximations (the hierarchical matrix format) and an approximate arithmetic. Furthermore, we use a modified iteration scheme for computing low-rank factors of the solution $\mathcal{X}$. The projection matrices for MOR are computed from the dominant invariant subspace of $\mathcal{X}$. We propose an efficient algorithm for the direct calculation of these projectors from the low-rank factors of $\mathcal{X}$. Numerical experiments demonstrate the performance of the new approach.

Key Words.
model reduction, balanced truncation, cross-Gramian, hierarchical matrices, sign function method

AMS Subject Classifications.
93B11, 93B40, 93C20, 37M05

271 Decompositional analysis of Kronecker structured Markov chains. *Yujuan Bao, İlker N. Bozkurt, Tuğrul Dayar, Xiaobai Sun, and Kishor S. Trivedi*.

Abstract.
This contribution proposes a decompositional iterative method with low memory requirements for the steady-state analysis of Kronecker structured Markov chains. The Markovian system is formed by a composition of subsystems using the Kronecker sum operator for local transitions and the Kronecker product operator for synchronized transitions. Even though the interactions among subsystems, which are captured by synchronized transitions, need not be weak, numerical experiments indicate that the solver benefits considerably from weak interactions among subsystems, and is to be recommended specifically in this case.

Key Words.
Markov chain, Kronecker representation, decomposition, iterative method, multigrid, aggregation, disaggregation

AMS Subject Classifications.
60J27, 15A72, 65F10, 65F50, 65B99

295 A counterexample for characterizing an invariant subspace of a matrix. *Hubert Schwetlick and Kathrin Schreiber*.

Abstract.
As an alternative to Newton's method for computing a simple eigenvalue and corresponding eigenvectors of a nonnormal matrix in a stable way, an approach based on singularity theory has been proposed by Schwetlick/Lösche [Z. Angew. Math. Mech., 80 (2000), pp. 9–25]. In this paper, by constructing a counterexample with a singular linear block operator, it is shown that a straightforward extension of this technique to the computation of invariant subspaces of dimension $p > 1$ will not work, in general. Finding this counterexample required a detailed study of the linear block operator.

Key Words.
eigenvalue problem, simple invariant subspace, block Newton method, block Rayleigh quotient iteration

AMS Subject Classifications.
65F15

306 Structured polynomial eigenproblems related to time-delay systems. *Heike Fassbender, D. Steven Mackey, Niloufer Mackey, and Christian Schröder.*

Abstract.
A new class of structured polynomial eigenproblems arising in the stability analysis of time-delay systems is identified and analyzed together with new types of closely related structured polynomials. Relationships between these polynomials are established via the Cayley transformation. Their spectral symmetries are revealed, and structure-preserving linearizations constructed. A structured Schur decomposition for the class of structured pencils associated with time-delay systems is derived, and an algorithm for its computation, which compares favorably with the QZ algorithm, is presented along with numerical experiments.

Key Words.
polynomial eigenvalue problem, palindromic matrix polynomial, quadratic eigenvalue problem, even matrix polynomial, structure-preserving linearization, matrix pencil, structured Schur form, real QZ algorithm, spectral symmetry, Cayley transformation, involution, time-delay system, delay-differential equation, stability analysis

AMS Subject Classifications.
15A18, 15A21, 15A22, 34K06, 34K20, 47A56, 47A75, 65F15

331 The RCWA method – A case study with open questions and perspectives of algebraic computations. *John J. Hench and Zdeněk Strakoš.*

Abstract.
Diffraction of light on periodic media represents an important problem with numerous physical and engineering applications. The Rigorous Coupled Wave Analysis (RCWA) method assumes a specific form of gratings which enables a straightforward separation of space variables. Using Fourier expansions, the solutions of the resulting systems of ordinary differential equations for the Fourier amplitudes can be written, after truncation, in form of matrix functions, with an elegant formulation of the linear algebraic problem for integrating constants. In this paper, we present a derivation of the RCWA method, formulate open questions which still need to be addressed, and discuss perspectives of efficient solution of the related highly structured linear algebraic problems. A detailed understanding of the RCWA method for the two-dimensional grating is, in our opinion, necessary for the development of a successful generalization of the method to practical problems.

Key Words.
diffraction of electromagnetic waves, Maxwell's equations, periodic gratings, RCWA, truncated Fourier expansions, matrix functions, structured matrices, scattering amplitude

AMS Subject Classifications.
78A45, 42A20, 42A85, 35Q60, 65L10, 65F10, 65F30

358 Algorithms for the matrix sector function. *Beata Laszkiewicz and Krystyna Ziętak*.

Abstract.
In this paper we consider algorithms for the matrix sector function, which is a generalization of the matrix sign function. We develop algorithms for computing the matrix sector function based on the (real) Schur decompositions, with and without reordering and the Parlett recurrence. We prove some results on the convergence regions for the specialized versions of Newton's and Halley's methods applied to the matrix sector function, using recent results of Iannazzo for the principal matrix pth root. Numerical experiments comparing the properties of algorithms developed in this paper illustrate the differences in the behaviour of the algorithms. We consider the conditioning of the matrix sector function and the stability of Newton's and Halley's methods. We also prove a characterization of the Fréchet derivative of the matrix sector function, which is a generalization of the result of Kenney and Laub for the Fréchet derivative of the matrix sign function, and we provide a way of computing it by Newton's iteration.

Key Words.
matrix sector function, matrix sign function, matrix pth root, Schur algorithm, Parlett recurrence, Newton's method, Halley's method, stability, conditioning, Fréchet derivative

AMS Subject Classifications.
65F30

384 On the equivalence of primal and dual substructuring preconditioners. *Bedřich Sousedík and Jan Mandel*.

Abstract.
After a short historical review, we present four popular substructuring methods: FETI-1, BDD, FETI-DP, BDDC, and derive the primal versions to the two FETI methods, called P-FETI-1 and P-FETI-DP, as proposed by Fragakis and Papadrakakis. The formulation of the BDDC method shows that it is the same as P-FETI-DP and the same as a preconditioner introduced by Cros. We prove the equality of eigenvalues of a particular case of the FETI-1 method and of the BDD method by applying a recent abstract result by Fragakis.

Key Words.
domain decomposition methods, iterative substructuring, finite element tearing and interconnecting, balancing domain decomposition, BDD, BDDC, FETI, FETI-DP, P-FETI-DP

AMS Subject Classifications.
65N55, 65M55, 65Y05

403 On a multilevel Krylov method for the Helmholtz equation preconditioned by shifted Laplacian. *Yogi A. Erlangga and Reinhard Nabben*.

Abstract.
In Erlangga and Nabben [SIAM J. Sci. Comput., 30 (2008), pp. 1572–1595], a multilevel Krylov method is proposed to solve linear systems with symmetric and nonsymmetric matrices of coefficients. This multilevel method is based on an operator which shifts some small eigenvalues to the largest eigenvalue, leading to a spectrum which is favorable for convergence acceleration of a Krylov subspace method.

This shift technique involves a subspace or coarse-grid solve. The multilevel Krylov method is obtained via a recursive application of the shift operator on the coarse-grid system. This method has been applied successfully to 2D convection-diffusion problems for which a standard multigrid method fails to converge.
In this paper, we extend this multilevel Krylov method to indefinite linear systems arising from a discretization of the Helmholtz equation, preconditioned by shifted Laplacian as introduced by Erlangga, Oosterlee and Vuik [SIAM J. Sci. Comput. 27 (2006), pp. 1471–1492]. Within the Krylov iteration and the multilevel steps, for each coarse-grid solve a multigrid iteration is used to approximately invert the shifted Laplacian preconditioner. Hence, a multilevel Krylov-multigrid (MKMG) method results.
Numerical results are given for high wavenumbers and show the effectiveness of the method for solving Helmholtz problems. Not only can the convergence be made almost independent of grid size h, but also linearly dependent on the wavenumb er k, with a smaller proportional constant than for the multigrid precondition ed version, presented in the aforementioned paper.

Key Words.
multilevel Krylov method, GMRES, multigrid, Helmholtz equation, shifted-Laplace preconditioner

AMS Subject Classifications.
65F10, 65F50, 65N22, 65N55