Electronic Transactions on Numerical Analysis
Volume 35, 2009

Contents

Abstract.
The recursive zonal equal area (EQ) sphere partitioning algorithm is a practical algorithm for partitioning higher dimensional spheres into regions of equal area and small diameter. Another such construction is due to Feige and Schechtman. This paper gives a proof for the bounds on the diameter of regions for each of these partitions.

Key Words.
sphere, partition, area, diameter, zone

AMS Subject Classifications.
11K38, 31-04, 51M15, 52C99, 74G65

Abstract.
The functions of hypergeometric-type are the solutions $y = y_\nu(z)$ of the differential equation $\sigma(z)y'' + \tau(z)y' + \lambda y = 0$, where σ and τ are polynomials of degrees not higher than 2 and 1, respectively, and λ is a constant. Here we consider a class of functions of hypergeometric type: those that satisfy the condition $\lambda + \nu\tau' + \frac{1}{2}\nu(\nu-1)\sigma'' = 0$, where ν is an arbitrary complex (fixed) number. We also assume that the coefficients of the polynomials σ and τ do not depend on ν. To this class of functions belong Gauss, Kummer, and Hermite functions, and also the classical orthogonal polynomials. In this work, using the constructive approach introduced by Nikiforov and Uvarov, several structural properties of the hypergeometric-type functions $y = y_\nu(z)$ are obtained. Applications to hypergeometric functions and classical orthogonal polynomials are also given.

Key Words.
hypergeometric-type functions, recurrence relations, classical orthogonal polynomials

AMS Subject Classifications.
33C45, 33C05, 33C15

Abstract.
We consider the Stefan-type diffusion boundary-value problem with free boundary and nonlinear Neumann boundary conditions. Such problems describe hydride formation under constant conditions when nonlinear surface processes are taken into

account. We construct the difference numerical method and prove the convergence of the interpolation approximations to the weak solution of the problem. Then we apply the theory of boundary-value problems to show that this weak solution is the classical solution. Thus, the existence of the solution to the problem is proved and the difference method is justified.

Key Words.
Stefan-type problem, free boundary, nonlinear Neumann condition, existence of solution, difference scheme, uniform convergence of approximations

AMS Subject Classifications.
65N06, 65N12, 35K20, 35K60, 35R35, 35A05

57 A full-Newton approach to separable nonlinear least squares problems and its application to discrete least squares rational approximation. *Carlos F. Borges*.

Abstract.
We consider a class of non-linear least squares problems that are widely used in fitting experimental data. A defining characteristic of the models we will consider is that the solution parameters may be separated into two classes, those that enter the problem linearly and those that enter non-linearly. Problems of this type are known as separable non-linear least squares (SNLLS) problems and are often solved using a Gauss-Newton algorithm that was developed in Golub and Pereyra [SIAM J. Numer. Anal., 10 (1973), pp. 413–432] and has been very widely applied. We develop a full-Newton algorithm for solving this problem. Exploiting the structure of the general problem leads to a surprisingly compact algorithm which exhibits all of the excellent characteristics of the full-Newton approach (e.g. rapid convergence on problems with large residuals). Moreover, for certain problems of quite general interest, the per iteration cost for the full-Newton algorithm compares quite favorably with that of the Gauss-Newton algorithm. We explore one such problem, that of discrete least-squares fitting of rational functions.

Key Words.
separable nonlinear least squares, rational approximation

AMS Subject Classifications.
65F20, 65D10, 41A20

69 Spectral approximation of variationally formulated eigenvalue problems on curved domains. *Ana Alonso and Anahí Dello Russo*.

To the memory of Professor Jorge D. Samur

Abstract.
This paper is concerned with the spectral approximation of variationally formulated eigenvalue problems posed on curved domains. As an example of the present theory, convergence and optimal error estimates are proved for the piecewise linear finite element approximation of the eigenvalues and eigenfunctions of a second order elliptic differential operator on a general curved three-dimensional domain.

Key Words.
spectral approximation, eigenvalue problems, curved domains

AMS Subject Classifications.
65N15, 65N25, 65N30

88 On modified asymptotic series involving confluent hypergeometric functions. *Alfredo Deaño and Nico M. Temme*.

Abstract.
A modification of the Poincaré-type asymptotic expansion for functions defined by Laplace transforms is analyzed. This modification is based on an alternative power series expansion of the integrand, and the convergence properties are seen to be superior to those of the original asymptotic series. The resulting modified asymptotic expansion involves a series of confluent hypergeometric functions $U(a, c, z)$, which can be computed by means of continued fractions in a backward recursion scheme. Numerical examples are included, such as the incomplete gamma function $\Gamma(a, z)$ and the modified Bessel function $K_\nu(z)$ for large values of z. It is observed that the same procedure can be applied to uniform asymptotic expansions when extra parameters become large as well.

Key Words.
confluent hypergeometric functions, asymptotic expansions, saddle point method, convergence and divergence of series and sequences

AMS Subject Classifications.
33C15, 33F99, 34E05, 30E15, 40A05

104 Acceleration of implicit schemes for large systems of nonlinear ODEs. *Mouhamad Al Sayed Ali and Miloud Sadkane*.

Abstract.
Implicit integration schemes for large systems of nonlinear ODEs require, at each integration step, the solution of a large nonlinear system. Typically, the nonlinear systems are solved by an inexact Newton method that leads to a set of linear systems involving the Jacobian matrix of the ODE which are solved by Krylov subspace methods. The convergence of the whole process relies on the quality of initial solutions for both the inexact Newton iteration and the linear systems. To improve global convergence, line search and trust region algorithms are used to find effective initial solutions. The purpose of this paper is to construct subspaces of small dimension where descent directions for line search and trust region algorithms and initial solutions for each linear system are found. Only one subspace is required for each integration step. This approach can be seen as an improved predictor, leading to a significant saving in the total number of integration steps. Estimates are provided that relate the quality of the computed initial solutions to the step size of the discretization, the order of the implicit scheme and the dimension of the constructed subspaces. Numerical results are reported.

Key Words.
nonlinear equations, nonlinear ODE systems, inexact Newton, GMRES, line search, trust region

AMS Subject Classifications.
65H10, 65L05

118 Monotone convergence of the Lanczos approximations to matrix functions of Hermitian matrices. *Andreas Frommer*.

Abstract.
When A is a Hermitian matrix, the action $f(A)b$ of a matrix function $f(A)$ on a vector b can efficiently be approximated via the Lanczos method. In this note we use M-matrix theory to establish that the 2-norm of the error of the sequence of approximations is monotonically decreasing if f is a Stieltjes transform and A is positive definite. We discuss the relation of our approach to a recent, more general monotonicity result of Druskin for Laplace transforms. We also extend the class of functions to certain product type functions. This yields, for example, monotonicity when approximating $\text{sign}(A)b$ with A indefinite if the Lanczos method is performed for A^2 rather than A.

Key Words.
matrix functions, Lanczos method, Galerkin approximation, monotone convergence, error estimates

AMS Subject Classifications.
6530, 65F10, 65F50

129 On the fast reduction of symmetric rationally generated Toeplitz matrices to tridiagonal form. *K. Frederix, L. Gemignani, and M. Van Barel*.

Abstract.
In this paper two fast algorithms that use orthogonal similarity transformations to convert a symmetric rationally generated Toeplitz matrix to tridiagonal form are developed, as a means of finding the eigenvalues of the matrix efficiently. The reduction algorithms achieve cost efficiency by exploiting the rank structure of the input Toeplitz matrix. The proposed algorithms differ in the choice of the generator set for the rank structure of the input Toeplitz matrix.

Key Words.
Toeplitz matrices, eigenvalue computation, rank structures

AMS Subject Classifications.
65F15

148 Spherical quadrature formulas with equally spaced nodes on latitudinal circles. *Daniela Roşca*.

Abstract.
In a previous paper, we constructed quadrature formulas based on some fundamental systems of $(n+1)^2$ points on the sphere ($n+1$ equally spaced points taken on $n+1$ latitudinal circles), constructed by Laín-Fernández. These quadrature formulas are of interpolatory type. Therefore the degree of exactness is at least n. In some particular cases the exactness can be $n+1$ and this exactness is the maximal that can be obtained, based on the above mentioned fundamental system of points. In this paper we try to improve the exactness by taking more equally spaced points at each latitude and equal weights for each latitude. We study the maximal degree of exactness which can be attained with $n+1$ latitudes. As a particular case, we study

the maximal exactness of the spherical designs with equally spaced points at each latitude. Of course, all of these quadratures are no longer interpolatory.

Key Words.
quadrature formulas, spherical functions, Legendre polynomials

AMS Subject Classifications.
65D32, 43A90, 42C10

Abstract.
We define and analyze a linear transformation – the heat transform – that allows to map solutions of hyperbolic equations to solutions of corresponding parabolic equations. The inversion of this mapping can be used to transform an inverse problem for the heat equation to a similar problem for the wave equation. This work is motivated by problems of finding interfaces, boundaries and associated heat conduction parameters in the thermal analysis of electronic circuits when transient data are available. Since the inversion of the transformation is ill-posed, we use a semi-smooth Newton scheme to regularize it enforcing sparsity of the solution. We present some numerical results of this procedure for simulated and measured data, which shows that heat conduction effects due to interfaces and boundaries can be found and classified by an inversion of the heat transform.

Key Words.
inverse problem, heat transform, sparsity, semi-smooth Newton method, electronic circuits

AMS Subject Classifications.
35R30, 35K15, 80A23, 44A15, 46F12

Abstract.
Iterative aggregation/disaggregation (IAD) methods for the computation of stationary probability vectors of large scale Markov chains form efficient practical analysis tools. However, their convergence theory is still not developed appropriately. Furthermore, as in other multilevel methods such as multigrid methods, the number of relaxations on the fine level of the IAD algorithms which is to be executed plays a very important role. To better understand these methods, in this paper we study some new concepts as well as their behavior and dependence on the parameters involved in aggregation algorithms, and establish some necessary and/or sufficient conditions for convergence. The theory developed offers a proof of convergence of IAD algorithms independent of whether the governing iteration matrix is primitive or cyclic as one of its main results. Another important result concerns a comparison of the rates of convergence of two IAD processes. Some examples documenting the diversity of behavior of IAD methods are given.

Key Words.
stationary probability vector of Markov chain, iterative aggregation/disaggregation

AMS Subject Classifications.
15A15, 15A09, 15A23, 65F05

201 Gaussian Direct Quadrature methods for double delay Volterra integral equations. *Angelamaria Cardone, Ida Del Prete, and Claudia Nitsch*.

Abstract.
In this paper we consider Volterra integral equations with two constant delays. We construct Direct Quadrature methods based on Gaussian formulas, combined with a suitable interpolation technique. We study the convergence and the stability properties of the methods and we carry out some numerical experiments that confirm our theoretical results.

Key Words.
Volterra integral equations, Direct Quadrature method, Gaussian quadrature formulas, convergence, stability

AMS Subject Classifications.
65R20

217 Large-scale Kalman filtering using the limited memory BFGS method. *H. Auvinen, J. M. Bardsley, H. Haario, and T. Kauranne*.

Abstract.
The standard formulations of the Kalman filter (KF) and extended Kalman filter (EKF) require the storage and multiplication of matrices of size $n \times n$, where n is the size of the state space, and the inversion of matrices of size $m \times m$, where m is the size of the observation space. Thus when both m and n are large, implementation issues arise. In this paper, we advocate the use of the limited memory BFGS method (LBFGS) to address these issues. A detailed description of how to use LBFGS within both the KF and EKF methods is given. The methodology is then tested on two examples: the first is large-scale and linear, and the second is small scale and nonlinear. Our results indicate that the resulting methods, which we will denote LBFGS-KF and LBFGS-EKF, yield results that are comparable with those obtained using KF and EKF, respectively, and can be used on much larger scale problems.

Key Words.
Kalman filter, Bayesian estimation, large-scale optimization

AMS Subject Classifications.
65K10, 15A29

234 An efficient generalization of the Rush–Larsen method for solving electro-physiology membrane equations. *Mauro Perego and Alessandro Veneziani*.

Abstract.
In this paper we describe a class of second-order methods for solving ordinary differential systems coming from some problems in electro-physiology. These methods extend to the second order of accuracy a previous proposal by Rush and Larsen [IEEE Trans. Biomed. Eng., 25 (1978), pp. 389–392] for the same problem. The methods can be regarded in the general framework of exponential integrators following the definition of Minchev and Wright [NTNU Tech. Report 2/05 (2005)]. However, they do differ from other schemes in this class for the specific form of linearization we pursue. We investigate the accuracy, stability, and positivity properties of our methods. Under simplifying assumptions on the problem at hand, our methods reduce to classical multi-step methods. However, we show that in general the new

methods have better stability and positivity properties than the classical ones. We present a time-adaptive formulation which is well suited for our electro-physiology problems. In particular, numerical results are presented for the Monodomain model coupled to Luo-Rudy I ionic model for the propagation of the cardiac potential.

Key Words.
nonlinear ordinary differential systems, electro-physiology, Rush-Larsen scheme, time-adaptivity

AMS Subject Classifications.
65M12, 65L05, 35K65

257 Boundary conditions in approximate commutator preconditioners for the Navier–Stokes equations. *Howard C. Elman and Ray S. Tuminaro*.

Abstract.
Boundary conditions are analyzed for a class of preconditioners used for the incompressible Navier-Stokes equations. We consider pressure convection-diffusion preconditioners [SIAM J. Sci. Comput., 24 (2002), pp. 237–256] and [J. Comput. Appl. Math., 128 (2001), pp. 261–279] as well as least-square commutator methods [SIAM J. Sci. Comput., 30 (2007), pp. 290–311] and [SIAM J. Sci. Comput., 27 (2006), pp. 1651–1668], both of which rely on commutators of certain differential operators. The effectiveness of these methods has been demonstrated in various studies, but both methods also have some deficiencies. For example, the pressure convection-diffusion preconditioner requires the construction of a Laplace and a convection–diffusion operator, together with some choices of boundary conditions. These boundary conditions are not well understood, and a poor choice can critically affect performance. This paper looks closely at properties of commutators near domain boundaries. We show that it is sometimes possible to choose boundary conditions to force the commutators of interest to be zero at boundaries, and this leads to a new strategy for choosing boundary conditions for the purpose of specifying preconditioning operators. With the new preconditioners, Krylov subspace methods display noticeably improved performance for solving the Navier-Stokes equations; in particular, mesh-independent convergence rates are observed for some problems for which previous versions of the methods did not exhibit this behavior.

Key Words.
boundary conditions, commutators, preconditioners, Navier-Stokes equations

AMS Subject Classifications.
Primary: 65F10, 65N30, 76D05; Secondary: 15A06, 35Q30