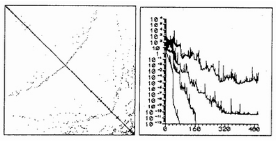

XII GAMM Workshop on Applied and Numerical Linear Algebra

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BOOK OF ABSTRACTS

Contents

KRYLOV SUBSPACE RECYCLING FOR STOCHASTIC COLLOCATION BASED UNCERTAINTY QUANTIFICATION

Kapil Ahuja
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Joint work with Michael L. Parks and Eric de Sturler

Abstract

The stochastic collocation methods transform the PDE with random data to a deterministic problem by using a expansion or polynomial chaos expansion. After discretization, one is required to solve a sequence of linear systems. Krylov subspace recycling is a technique to accelerate the solution of sequences of linear systems. Typically, recycling algorithms are useful when each system in the sequence requires a large number of iterations to converge. When the underlying PDE is an elliptic diffusion equation, then linear systems converge rapidly, and hence, there is not enough "information" generated in one linear system to be recycled to the next (although recycling is needed due to the large number of linear systems in the sequence). We modify existing recycling algorithms such that the recycle space can be built even for rapidly converging linear systems. Recycling algorithms typically use an approximate invariant subspace as the recycle space. We show that another criterion works better here. Experiments show savings of up to 55 percent in time for an uncertainty quantification example.

Acknowledgement: Funding support from Eric T. Phipps and Andrew G. Salinger of Sandia National Labs (Albuquerque) as well as Peter Benner of Max Planck Institute (Magdeburg).

ITERATIVE METHODS FOR SYMMETRIC QUASI-DEFINITE LINEAR SYSTEMS

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Joint work with Dominique Orban

Abstract

We propose generalized versions of LSQR, Craig and LSMR well suited to the solution of symmetric quasi-definite systems of equations such as those arising in regularized interior-point methods for convex optimization or in stabilized control problems. Those methods essentially operate on the normal equations. We establish a connection between the iterates that they generate and those generated by CG and MINRES on the original system.

EFFICIENT PRECONDITIONING TECHNIQUES FOR PHASE-FIELD MODELS

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Abstract

In order to avoid interface conditions and enable the use of a fixed mesh in time-dependent problems, it is shown that a diffusive model of Cahn-Hilliard type can be used. Some numerical examples illustrate the method. A preconditioning method is used that needs no update. Efficient implementation on parallel clusters are shown.

BLOCK FACTORIZATION BASED PRECONDITIONERS WITH APPLICATIONS

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Joint work with Owe Axelsson, Petr Byczanski, and Rostislav Hrtus

Abstract

Approximate block factorization is a basis for construction of many preconditioners. Hierarchical decomposition of standard FEM matrices, saddle point matrices from mixed formulation, multiphysics problems like poroelasticity and PDE-constrained optimization are examples of problems with natural block structures allowing such factorization with approximations to the blocks and the Schur complements. The subsystems can be solved by inner iterations whereas the whole systems are solved iteratively by flexible variants of Krylov space solvers. We will show the general framework and efficiency of various preconditioners of this type for solving the above mentioned problems.

ON SPECIAL GRID TRANSFER OPERATORS FOR MULTIGRID METHODS

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Joint work with Marco Donatelli, Thomas Huckle, and Christos Kravvaritis

Abstract

Based on the theory for Toeplitz matrices we discuss classical sufficient conditions to be satisfied from the grid transfer operators in order to obtain optimal two-grid and V-cycle multigrid methods. Based on this we derive relaxed conditions that allow for the construction of special grid transfer operators that are computationally less expensive while preserving optimality. The new conditions also allow to use rank deficient grid transfer operators, in this case the use of an intermediate iteration as a pre-smoother that is lacking the smoothing property is proposed.

Connected to the use of high-order polynomials as generating symbols for the system matrix and/or the grid transfer operators is the problem that the Toeplitz structure is destroyed on the coarser levels. We discuss some effective and computational cheap coarsening strategies found in the literature. For the case of Toeplitz matrices with a zero of order two (like the Laplacian) we prove the optimality of the V-cycle for these strategies, while for the high-order operators considered before we present numerical results showing near-optimal behavior while keeping the Toeplitz structure on the coarser levels.

CAN RESTARTED GMRES EXHIBIT ANY NONINCREASING CONVERGENCE CURVE?

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Joint work with Gerard Meurant

Abstract

This talk continues the work by Arioli, Greenbaum, Ptak and Strakos showing that for full GMRES, any convergence behavior is possible with any spectrum. We will show in what the situation differs if restarted GMRES is considered. We also address prescribing the Ritz values generated during the subsequent restart cycles.

ON SOME ASPECTS OF THE SPACE-TIME DISCONTINUOUS GALERKIN METHOD

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Abstract

The contribution will be concerned with analysis and applications of the space-time discontinuous Galerkin method for the numerical solution of nonlinear convection-diffusion problems and compressible flow. First, we shall discuss the stability and error estimates of this method applied to a scalar model equation. Then the method will be adapted to the simulation of compressible flow in time-dependent domains and fluid-structure interaction. Some results of numerical experiments will be presented.

SOME NEW CLASSES OF MATRICES

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Abstract

We survey results on classes of matrices (CB-matrices, G-matrices, F-matrices) recently introduced and add some new observations. Common features will be emphasized and special cases mentioned.

ITERATIVE METHODS FOR HELMHOLTZ PROBLEMS

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Abstract

In contrast to the positive definite Helmholtz equation, the deceivingly similar looking indefinite Helmholtz equation is difficult to solve using classical iterative methods. Applying directly a Krylov method to the discretized equations without preconditioning leads in general to stagnation and very large iteration counts. Using classical incomplete LU preconditioners can even make the situation worse. Classical domain decomposition and multigrid methods also fail to converge when applied to such systems.

The purpose of this presentation is to investigate in each case where the problems lie, and to explain why classical iterative methods have such difficulties to solve indefinite Helmholtz problems. I will also present remedies that have been proposed over the last decade, for incomplete LU type preconditioners, domain decomposition and also multigrid methods.

DEFLATED MINRES FOR THE GINZBURG-LANDAU PROBLEM

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Joint work with Nico Schlömer

Abstract

We consider the extreme type-II Ginzburg-Landau equations which describe phenomena of superconductivity with a nonlinear PDE model. Newton's method and discretization yield a sequence of ill-conditioned linear algebraic systems. The Jacobian operators are self-adjoint with respect to a special inner product and the linear algebraic systems can thus be solved with the preconditioned MINRES method. However, the operators become singular once the Newton iterate is close to a solution and convergence of MINRES may stagnate. Luckily, additional information can be derived from theoretical properties of the Ginzburg-Landau equation and we show how the "deflated" MINRES method can use this information to improve convergence.

BASIC FACTS AND OPTIONS OF AUGMENTATION AND DEFLATION FOR LINEAR SOLVERS

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Joint work with André Gaul, Jörg Liesen, and Reinhard Nabben

Abstract

The convergence of Krylov space solvers for linear systems is often hampered by a few small eigenvalues of the matrix. A suitable technique for dealing with such problems is to identify an approximately invariant subspace $\mathcal{U}$ that belongs to the set of these small eigenvalues. By using suitable orthogonal or oblique projections along $\mathcal{U}$ (that is, with null space $\mathcal{U}$) the Krylov solver can then be applied to a deflated problem that is restricted to a suitable complementary space. There are various ways to handle and implement this approach. They differ not only algorithmically and numerically, but often also mathematically. Some keywords associated with such methods are (spectral) deflation', 'augmented basis', 'recycling Krylov subspaces', and 'singular preconditioning'.

In this talk we want to review the basic facts, the various options, and some of the literature.

SIMULATION AND CONTROL OF MULTIPHASE FLOWS GOVERNED BY THE CAHN-HILLIARD NAVIER-STOKES SYSTEM (CHNSS)

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Joint work with M. Hintermüller and C. Kahle

Abstract

In the first part of the talk we consider multiphase flow governed by the CHNSS in the phase field approximation with the double obstacle potential, and apply a semi-implicit scheme to its time discretization. We relax the variational inequalities appearing in every time step by a penalization approach and develop reliable and effective residual based a posteriori error estimators for the resulting PDE system along the lines of [1]. In the second part of the talk we develop a model predictive feedback control strategy. Several numerical experiments show the performance of our approach. The work presented in the first part extends the investigations of [1] on adaptivity for the Cahn Hilliard system to the CHNSS.

References

[1] Hintermüller, M., Hinze, M., Kahle, C.: *An adaptive finite element Moreau-Yosida-based solver for a non-smooth Cahn-Hilliard problem.* Optim. Meth. Software 26:777-811 (2011)

MONOLITHIC SOLVER FOR FLUID-STRUCTURE INTERACTION PROBLEMS

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Abstract

We present a monolithic approach for solving the fluid-structure interaction problem with general constitutive laws for the fluid and solid parts. It is based on the ALE formulation of the balance equations for the fluid and solid in the time dependent domain. The discretization is done by the finite element method. The discretized system of nonlinear algebraic equations is solved using approximate Newton method with line-search strategy as the basic iteration and geometric multigrid as linear solver. Since we know the sparsity pattern of the Jacobian matrix in advance, its approximate computation can be done by using finite differences in an efficient way so that the linear solver remains the dominant part in terms of the CPU time.

ADAPTIVE APPROACHES TO ALGEBRAIC MULTIGRID

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Joint work with James Brannick

Abstract

By the time of its development Algebraic Multigrid (AMG) was thought of as a black box solver for systems of linear equations. However, the classical formulation of AMG turned out to lack the robustness to overcome certain challenges encountered in many of today's computational simulations. In recent years several methods have been proposed that try to overcome such difficulties by means of adaptive techniques, such as the framework of smoothed aggregation or bootstrap algebraic multigrid.

In this talk we discuss the general concept of algebraic multigrid and its features that can make it a highly efficient solver. We give examples of the challenges that need to be overcome and give an overview on the techniques and strategies developed in recent years. We try to give an extensive insight into various approaches, discuss their differences and similarities and try to connect them in a common framework.

GENERALIZED GRAM–SCHMIDT-BASED APPROXIMATE INVERSE PRECONDITIONING FOR THE CONJUGATE GRADIENT METHOD

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Joint work with Miroslav Rozložník and Miroslav Tůma

Abstract

This contribution deals with an approximate inverse preconditioning for the conjugate gradient method. In particular, it focuses on the generalized Gram–Schmidt process. Its algorithm is performed incompletely which means that some computed entries (small in some sense) are dropped. Assume a system of linear equations in the form $Ax = b$, where A is symmetric and positive definite. Symmetrically preconditioned system can be written in the form

$$\tilde{Z}^T A\tilde{Z}y = \tilde{Z}^T b, \qquad x = \tilde{Z}y,$$

where $\tilde{Z}$ is the factor of the approximation $\tilde{Z}\tilde{Z}^T$ to A^{-1}, that plays the role of the preconditioner. It seems that the A-orthogonality of the column vectors of the matrix $\tilde{Z}$ measured by the norm $\|\tilde{Z}^T A\tilde{Z} - I\|$ (the loss of A-orthogonality among column vectors of the matrix $\tilde{Z}$) and sparsity of the preconditioner reflected in the number of nonzeros of $\tilde{Z}$ indicate usefulness of the preconditioner.

Exact version of the generalized Gram–Schmidt process provides matrices Z and U, so that $U^T U = (Z^{(0)})^T AZ^{(0)}$, $Z^T AZ = I$, and $ZU = Z^{(0)}$. Columns of the matrix $Z^{(0)}$ are initial vectors that are A-orthogonalized against previously computed vectors. Matrix U is composed from the orthogonalization coefficients. It is clear, that for $Z^{(0)} = I$ the matrix U is equal to the Cholesky factor of the matrix $A = U^T U$. The bounds for the norms $\|\bar{Z}^T A\bar{Z} - I\|$, $\|\bar{Z}\bar{U} - I\|$, $\|\bar{U}^T\bar{U} - (Z^{(0)})^T AZ^{(0)}\|$ for the main orthogonalization schemes, where the quantities with an extra bar are computed in the finite precision arithmetic, can be found in [1]. As for dropping, original schemes for the generalized Gram–Schmidt process have been introduced in [2]. These dropping rules considered magnitudes of matrix entries absolutely or with respect to some intermediate quantities. The rules were successful in practice but they lack theoretical justification. Note that up to now, theory of incomplete decompositions supports mainly their rather special cases.

Construction of an incomplete decomposition supported by theoretical background is the subject of this contribution. The analysis in [1] motivates development of new rules to drop entries in incomplete generalized Gram-Schmidt algorithm such that the computed factors have similar properties as obtained from the standard finite precision algorithm. In our case, the role of the roundoff unit is played by the drop

tolerance. In order to improve numerical properties of the computational schemes, we introduce additional pivotal strategies and demonstrate their usefulness. We hope that the resulting algorithms may extend scope of applicability of the considered type of approximate inverse preconditioning.

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[2] Benzi, M., Meyer, C. D., Tuma, M: *A sparse approximate inverse preconditioner for the conjugate gradient method.* SIAM Journal on Scientific Computing, 17(5) (1996), 1135–1149.

Acknowledgement: The work of M. Rozložník and M. Tůma was supported by Grant Agency of the Czech Republic under No. P108/11/0853. The work of J. Kopal was supported by the Ministry of Education of the Czech Republic under the project No. 7822/115.

SOME IMPROVEMENTS TO THE FEAST ALGORITHM

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Joint work with Martin Galgon and Bruno Lang

Abstract

The FEAST algorithm was introduced in 2009 by E. Polizzi as a method for the solution of some eigenvalue problems, in particular, $Ax = \lambda Bx$ with A symmetric and B symmetric positive definite.

In a recent publication, we presented results of an extensive numerical study with the method. This study highlighted several numerical issues of the method. In particular, we addressed the size of the search space and the orthogonality of eigenvectors.

In this talk, we present some improvements making the method more robust, especially with regard to the two issues mentioned before.

We then discuss some strategies for parallelization and finally we give some numerical results.

A PRIORI ERROR ESTIMATES FOR NONLINEAR CONVECTIVE PROBLEMS

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Abstract

Standard textbook techniques for deriving a priori error estimates are well suited for problems like the heat equation, which possess a 'nice' structure (e.g. ellipticity, monotonicity). These parabolic techniques however fail for equations lacking such a structure, e.g. convective problems. Usually, one treats the convection-diffusion problem, and dominates the convective terms by the diffusion, which leads to estimates that blow up with respect to the diffusion coefficient going to zero and are not valid in the purely convective case. We shall present new error estimates for the purely convective and singularly perturbed cases, which are derived essentially using the parabolic technique. We build on estimates by Zhang and Shu (2004), which were limited to explicit schemes only. We extend their results to the method of lines using continuous mathematical induction and a nonlinear Gronwall lemma. For an implicit scheme, we show that the desired estimates cannot be obtained by standard arguments. To circumvent this obstacle, we construct a suitable continuation of the discrete solution with respect to time, so that we can again apply continuous mathematical induction. The key estimates can be applied to standard finite elements, as well as the discontinuous Galerkin method.

STRESS LIMITING BEHAVIOR OF A SAMPLE IN THE ANTI-PLANE STRAIN NUMERICAL SIMULATION

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Joint work with Josef Málek and K. R. Rajagopal

Abstract

The determination of the stresses and strains near a crack tip in a body due to loading has important technological ramifications. In the context of classical linearized elastic theory strain has a $1/\sqrt(r)$ singularity, where r is the distance from the crack tip. As the linearized theory is derived under the assumption of infinitesimal strains, the results are at odds with the basic tenet of the theory. K. R. Rajagopal previously proposed new class of elastic models. These nonlinear models allow finite bounded strains even for infinite stresses and might be well suited to describe the fracturing of brittle elastic bodies. Although these models have nonlinear constitutive relation they fit into framework of small strain elasticity as they use linearized strain tensor. We study a plate with a V-notch being subject to anti-plane strain. Using Finite element method (FEM) we compare model of classical linearized material to the material belonging to the new class of elastic materials proposed by K. R. Rajagopal. The constitutive relation for the classical model is described by one parameter and for the new nonlinear model there are three parameters. We can control strain bound in nonlinear model by these parameters. Using Airy stress function we derive weak formulation of boundary value problem for FEM. We study both models in terms of stress and strain fields around the tip of V-notch for various parameters and angles of V-notch. As the resulting stress fields are for both models similar we focus on comparison of the strain tensor components between classical and nonlinear models.

PIEZOVISCOUS INCOMPRESSIBLE FLUIDS AND LUBRICATION PROBLEMS

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Abstract

In certain situations, such as in some hydrodynamic lubrication problems in engineering, an incompressible fluid is considered with a viscosity depending on pressure. This leads to a number of interesting issues in the whole range from engineering and modelling to numerical simulations and analysis. Some of the recent results and open problems will be mentioned before the talk will focus on the numerical simulations of the (planar, steady, and simplified) lubrication flow.

A NEW MINIMAL RESIDUAL METHOD FOR LARGE SCALE LYAPUNOV EQUATIONS

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Joint work with Valeria Simoncini

Abstract

The solution of large scale algebraic Lyapunov equations is important in the stability analysis of linear dynamical systems. We present a projection-based residual minimizing procedure for solving the Lyapunov equation.As opposed to earlier methods (e.g., [I.M. Jiamoukha and E.M. Kasenally, SIAM J. Numer.Anal., 1994]), our algorithm relies on an inner iterative solver, accompanied with a selection of preconditioning techniques that effectively exploit the structure of the problem. The residual minimization allows us to relax the coefficient matrix passivity constraint, which is sometimes hard to meet in real application problems. Numerical experiments with standard benchmark problems will be reported.

IMPLICITLY CONSTITUTED MATERIALS: MODELING, ANALYSIS AND COMPUTATION

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Joint work with J. Hron, J. Stebel, and K. Touška

Abstract

Implicit constitutive theory that is based on the idea of expressing the response of bodies by an implicit relation between the stress and appropriate kinematical variables, is capable of describing some of the material properties that explicit models seem unable to describe. It also provides a less standard interesting structure of the governing equations. We will present several examples emphasizing the advantages of this framework on three levels: modelling of material responses, theoretical analysis of related boundary values problems and computer simulations.

PEFORMING THE GAMMA-ITERATION IN OPTIMAL H-INFINITY CONTROL VIA PERMUTED GRAPH BASES

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Joint work with Federico Poloni

Abstract

We present a new numerical method for the gamma-iteration in robust control based on the extended matrix pencil formulation. The new method bases the iteration on the computation of special subspaces associated with matrix pencils. We introduce a permuted graph representation of these subspaces, which avoids the known difficulties that arise, when the iteration is based on the solution of algebraic Riccati equations but at the same time makes use of the special symmetry structures that are present in the problems. We show that the new method is applicable in many situations where the conventional methods fail.

HIERARCHICALLY ENHANCED ADAPTIVE FINITE ELEMENT METHODS FOR PDE EIGENVALUE/EIGENVECTOR APPROXIMATIONS

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Joint work with Luka Grubišić and Jeffrey S. Ovall

Abstract

Although adaptive approximation methods have gained a recognition and are well-established, they frequently do not meet the needs of real world applications. In this talk we present a hierarchically enhanced adaptive finite element method for PDE eigenvalue problems. Starting from the results of Grubišić and Ovall on the reliable and efficient asymptotically exact a posteriori hierarchical error estimators in the self-adjoint case, we explore the possibility to use the enhanced Ritz values and vectors to restart the iterative algebraic procedures within the adaptive algorithm. Using higher order hierarchical polynomial finite element bases, as indicated by Bank and by Ovall and Le Borne, our method generates discretization matrices whose compressions onto the complement of piecewise linear finite element subspace (in the higher order finite element space) are almost diagonal. This construction can be repeated for the complements of higher (even) order polynomials and yields a structure which is particularly suitable for designing computational algorithms with low complexity. We present some preliminary numerical results for both the symmetric as well as the nonsymmetric eigenvalue problems.

STRESS - DISPLACEMENT FORMULATIONS FOR HYPERELASTIC MATERIALS: LEAST-SQUARES FINITE ELEMENT METHOD AND GAUSS-NEWTON ITERATION

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Joint work with Gerhard Starke

Abstract

Elastic deformation processes with hyperelastic material laws play an important role in solid mechanics. The main objective is to compute the displacement and the stresses, that occur in a given body due to external forces. In this talk we present a least squares finite element method to solve such problems, which are in general nonlinear. Thereby our solution method is based on Gauss - Newton iterations.

At the end of the talk we will demonstrate our solution method for a special material law on some numerical examples. Here we use quadratic Raviart - Thomas elements for the first Piola - Kirchhoff stress tensor $\mathbf{P}$ and continuous quadratic elements for the displacement $\mathbf{u}$. In our numerical simulations adaptive refinement strategies are used.

THE RICCATI METHOD FOR SINGULAR SUBSPACES OF LARGE SPARSE MATRICES

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Abstract

In the case of clusters of singular values, it is sometimes easier to estimate the left and right singular subspaces than the individual singular triplets. Moreover, after estimating the singular subspaces, the singular triplets can be obtained at small additional cost.

Let A be a given (sparse) matrix A of size $m \times n$. Our task is to find orthonormal (ON) bases $\hat{X} \in \mathbb{R}^{m\times k}$ and $\hat{Y} \in \mathbb{R}^{n\times k}$ of the left and right singular subspace, respectively, corresponding to k largest singular values of A. Starting with random initial matrices with k orthonormal (ON) columns $X \in \mathbb{R}^{m\times k}$ and $Y \in \mathbb{R}^{n\times k}$, let $(X|Z)$ and $(Y|W)$ be unitary. Then the required ON bases $\hat{X}$ and $\hat{Y}$ are given by $\hat{X} = X + ZP$, $\hat{Y} = X + W\tilde{P}$ where the *corrections* P and $\tilde{P}$ satisfy the Riccati algebraic system of two matrix equations. We show how this system is derived and discuss its solution using an orthogonal projection on the direct sum Krylov subspace $\mathcal{K}^{\ell}\left(\begin{bmatrix}0 & A\ A^{\star} & 0\end{bmatrix}, X \oplus Y\right)$ with the growing block dimension ℓ, $1 \leq \ell \leq m$. A fixed parameter m defines the maximum dimension mk of the updated generalized Rayleigh quotient; after reaching it, the block Arnoldi algorithm is restarted with the estimates closest to k largest singular values. The method can be easily adapted to the computations connected with k smallest singular values.

We present first numerical results computed in MATLAB using some sparse matrices from the Matrix Market Collection. It turns out that in the case of tight clusters of singular values our method is more robust than the MATLAB function `svds`.

Keywords: Riccati's correction equations, block Arnoldi algorithm, orthogonal projection, direct sum Krylov subspace

References

[1] Brandts, J.: *The Riccati algorithm for eigenvalues and invariant subspaces of matrices with inexpensive action.* Lin. Alg. Appl., 358 (2003), 335–365.

Acknowledgement: This research was supported by the VEGA grant no. 2/0003/11.

DISTRIBUTION OF THE ALGEBRAIC AND DISCRETIZATION ERROR IN NUMERICAL SOLUTION OF 1D POISSON MODEL PROBLEM

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Joint work with Zdeněk Strakoš

Abstract

On a simple model problem we show some important phenomena which should be taken into account when solving large scale mathematical modelling problems in general. It is demonstrated that the algebraic error in numerical solution of the discretized problem can have large local components and it can therefore significantly dominate the total error in some part of the domain, even if the globally measured algebraic error is comparable to or smaller than the globally measured discretization error. Therefore, the a posteriori error analysis should include the possible algebraic error.

ORTHOGONAL RATIONAL FUNCTIONS AND RATIONAL KRYLOV SUBSPACES

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Joint work with Lothar Reichel

Abstract

We present three types of recurrence relations for orthogonal rational functions, analogous to the three-term recurrence relation for orthogonal polynomials. The number of terms in these recursions depends both on the number of distinct poles and on the order in which the poles enter the sequence of orthogonal rational functions. The matching moment properties of corresponding rational Krylov subspaces, and the link with the rational Gauss quadrature will be discussed.

STABILITY ANALYSIS OF THE SPLIT BREGMAN ALGORITHM FOR DETERMINING OPTIMAL LAGRANGE PARAMETERS

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Joint work with Iveta Hnětynková

Abstract

The split Bregman algorithm for solving the ill-posed least squares problem $\|Ax - b\|^2$ subject to regularization condition $J(x)$, where J is typically an approximation for $\|Lx\|_{TV}$, has received significant attention dur to the work of Goldstein and Osher in 2008. They showed that the split Bregman algorithm provides an efficient approach for obtaining solutions of the regularized problem which is reformulated as $\|Ax-b\|^2 + \lambda\|Lx-d\|^2 + \mu J(d)$ where L is an appropriate operator and parameters λ, μ are regularization parameters, and can be solved by alternating updates over x and d. The former uses standard Tikhonov least squares problems for x and the latter uses a thresholding obtained via solution of a problem of the kind $\|d - c\|_2^2 + \mu J(d)$, for an updated vector c dependent on the x. Although the algorithm has received significant attention, the generation of optimal parameters λ and μ has not been addressed. We show by a suitable reformulation of the algorithm that the optimal λ is independent of the iteration step, and should be chosen as optimal for the Tikhonov problem. This result moreover demonstrates that the optimal value at each step is indeed step independent. This reduces the major question to determination of μ for which our results confirm that it is the ratio of λ to μ which is of most significance and determines the level of the threshold dependent on the level of the noise in the data. Numerical results will also be reported.

TOWARDS A GPU ADD-ON FOR THE MESS LIBRARY

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Joint work with Alfredo Remón and Martin Köhler

Abstract

The omnipresence of graphics processing units (GPUs), and their remarkable computational power, in modern desktop computers has made it unavoidable to support those devices in any computational software that claims to be efficiently using the hardware. CUDA and OpenCL have, on the other hand, made programming GPUs much easier and more attractive to a wide range of scientists. Here we present first steps towards an add-on to the MESS library that combines the multicore capabilities of the existing software on the CPU with the manycore features provided by the GPU. We exploit specialized data structures that lower the memory consumption while at the same time increasing the throughput of the GPU computations. The hybrid nature of the implementation offloads the expensive linear system solves to the GPU while in parallel the CPU computes minor operations like evaluation of stopping criteria and solution updates in each step.

The proof of concept implementation is demonstrated in numerical experiments showing what the advantages and drawbacks of the current implementation and the GPUs as high performance computation devices in general are.

THE PARALLEL MULTISHIFT QR ALGORITHM WITH AGGRESSIVE EARLY DEFLATION

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Joint work with Robert Granat, Bo Kågström, and Daniel Kressner

Abstract

The QR algorithm which computes the Schur decomposition of a matrix is by far the most important approach for solving dense nonsymmetric eigenvalue problems. Recently a novel parallel QR algorithm has been developed by incorporating some modern techniques such as small-bulge multishift and aggressive early deflation (AED). The novel parallel approach significantly outperforms the pipelined QR algorithm in ScaLAPACK v1.8.0 and earlier versions. But AED becomes a computational bottleneck in the new parallel QR algorithm. We develop multilevel AED algorithms which indeed decrease the total amount of communications and further improve the performance of the parallel QR algorithm. The improved version is now available as a part of ScaLAPACK version 2.0. Both performance models and numerical experiments demonstrate the efficiency of the new approach.

KRYLOV SUBSPACE RECYCLING FOR FAMILIES OF SHIFTED LINEAR SYSTEMS

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Joint work with Daniel B. Szyld and Fei Xue

Abstract

We address the solution of a sequence of families of linear systems. For each family, there is a base coefficient matrix A_i, and the coefficient matrices for all systems in the family differ from A_i by a multiple of the identity, e.g.,

$$A_i x_i = b_i \quad \text{and} \quad (A_i + \sigma_i^{(\ell)} I) x_i^{(\ell)} = b_i \quad \text{for} \quad \ell = 1 \ldots L_i,$$

where L_i is the number of shifts at step i. This is an important problem arising in various applications. We extend the method of subspace recycling to solve this problem by introducing a GMRES with subspace recycling scheme for families of shifted systems. This new method solves the base system using GMRES with subspace recycling while constructing approximate corrections to the solutions of the shifted systems at each cycle. These corrections improve the solutions of the shifted system at little additional cost. At convergence of the base system solution, GMRES with subspace recycling is applied to further improve the solutions of the shifted systems to tolerance. We present analysis of this method and numerical results involving systems arising in lattice quantum chromodynamics.

STRESS-DISPLACEMENT FORMULATIONS FOR HYPERELASTIC MATERIALS: ADAPTIVE MIXED FE APROXIMATION

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Joint work with Benjamin Müller

Abstract

First-order system formulations for nonlinear elasticity with hyperelastic material models are studied in this talk. The novelty of this approach is that, in addition to the displacements, the full Piola-Kirchhoff stress tensor is approximated in suitable finite element spaces, e.g. using Raviart-Thomas elements. The performance of an adaptive implementation of the method is illustrated as well as the behavior of the nonlinear solution strategies for some examples of finite strain elasticity. In particular, the computation of critical load values is investigated.

KRYLOV SUBSPACE METHODS, MODEL REDUCTION AND ERROR EVALUATION

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Abstract

The current state-of-the art of iterative solvers is the outcome of the tremendous algorithmic development over the last few decades. In this contribution we focus on Krylov subspace methods and view them as matching moments model reduction. This will lead to a possibly new view to several questions on their behaviour and on interpretation of the computed approximate solutions.

THE NUMERICAL SOLUTION OF RICCATI EQUATIONS

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Joint work with Marlliny Monsalve and Valeria Simoncini

Abstract

We compare experimentally the two most common approaches for the solution of Riccati equations: variants of Newton's method, and Krylov subspace projection. We conclude that, with the appropriate choice of subspace, the latter is computationally superior. As part of an explanation of why this is so, we prove several results. Consider the projection of a Riccati and a Lyapunov equation (with the same coefficient matrices) onto the same subspace (using a Galerkin approach), and lift the solutions of the projected systems to the larger space. Our new results compare the two solutions and the two residuals, and bound the norm of their difference. We also present a new formula which allows us to compute the norm of the Riccati residual without explicitly computing it.

COMPUTABLE UPPER BOUNDS ON FRIEDRICHS' AND TRACE CONSTANTS

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Joint work with Ivana Šebestová

Abstract

We present computable upper bounds on the optimal constants in Friedrichs' and trace inequalities. Since the optimal constants are equal to the reciprocal values of the smallest eigenvalues of the corresponding differential operators, we actually compute lower bounds on the spectrum of these operators. The results are applicable to a wide class of elliptic operators and are based on the idea of [1].

References

[1] Kuttler, J. R., Sigillito, V. G.: *Bounding eigenvalues of elliptic operators.* SIAM J. Math. Anal. 9 (1978), 768–778.

ADAPTIVE INEXACT NEWTON METHODS WITH A POSTERIORI STOPPING CRITERIA FOR NONLINEAR DIFFUSION PDES

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Joint work with Alexandre Ern

Abstract

We consider nonlinear algebraic systems arising from numerical discretizations of nonlinear partial differential equations of diffusion type. In order to solve them, some iterative nonlinear solver, and, on each step of this solver, some iterative linear solver are used. We propose an adaptive choice of the number of steps of both the linear and nonlinear solvers. Both stopping criteria are based on an a posteriori error estimate which distinguishes the different error components, namely the algebraic error, the linearization error, and the discretization error; we stop whenever the corresponding error does not affect the overall error significantly. Our estimates also give a gua ranteed upper bound on the overall error at each step of the nonlinear and linear solvers. We prove the (local) efficiency and robustness of our estimates with respect to the size of the nonlinearity. This is achieved thanks to the choice of the error measure, the dual norm of the residual augmented by a jump seminorm. Our developments are carried at an abstract level, yielding a general framework. We apply this framework to the fixed point and Newton linearizations and to most common discretization methods: the finite element, the nonconforming finite element, the discontinuous Galerkin, and finite volume and mixed finite element ones. All iterative linear solvers are covered. Numerical experiments illustrate the tight overall error control and important computational savings achieved by our approach.

IMPROVING EIGENPAIRS FROM AMLS WITH SUBSPACE ITERATIONS

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Joint work with Jiacong Yin

Abstract

Automated Multi-Level Sub-structuring (AMLS) is a very efficient condensation method for determining a large number of eigenmodes and frequency responses for quite large and complex structures. Compared to the classical block Lanczos method AMLS reduces computational resources in terms of time and hardware requirements. However, the accuracy of AMLS is often not very high. In this talk we discuss how to improve the obtained eigenpairs with subspace iteration taking advantage of transformed stiffness matrix from AMLS.

PRECONDITIONING OF LARGE-SCALE SADDLE POINT SYSTEMS ARISING IN RICCATI FEEDBACK CONTROL OF FLOW PROBLEMS

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Joint work with Peter Benner, Jens Saak, and Martin Stoll

Abstract

In order to explore boundary feedback control of flow problems we consider the (Navier-) Stokes equations that describe instationary, incompressible flows for low and moderate Reynolds numbers. After a standard finite element discretization we get a differential-algebraic system of differential index two. We show how to reduce this index with a projection method to get a generalized state space system, where a linear quadratic control approach can be applied. This leads to large-scale saddle point systems which have to be solved. For obtaining a fast iterative solution of those systems we derive efficient preconditioners based on the approaches due to Wathen et al. [Elamn/Silvester/Wathen 2005, Stoll/Wathen 2011]. Finally we show recent numerical results regarding the arising nested iteration.