## IP1

# Preconditioning for PDE-constrained Optimization

For many partial differential equations (PDEs) and systems of PDEs efficient preconditioning strategies now exist which enable effective iterative solution of the linear or linearised equations which result from discretization. Few would now argue for the use of Krylov subspace methods for most such PDE problems without effective preconditioners. There are many situations, however, where it is not the solution of a PDE which is actually required, but rather the PDE expresses a physical constraint in an Optimization problem: a typical example would be in the context of the design of aerodynamic structures where PDEs describe the external flow around a body whilst the goal is to select its shape to minimize drag. We will briefly describe the mathematical structure of such PDE-constrained Optimization problems and show how they lead to large scale saddle-point systems. The main focus of the talk will be to present new approaches to preconditioning for such Optimization problems. We will show numerical results in particular for problems where the PDE constraints are provided by the Stokes equations for incompressible viscous flow.

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# IP2

# Exploiting Sparsity in Matrix Functions, with Applications to Electronic Structure Calculations

In this talk, some general results on analytic decay bounds for the off-diagonal entries of functions of large, sparse (in particular, banded) Hermitian matrices will be presented. These bounds will be specialized to various approximations to density matrices arising in Hartree-Fock and Density Functional Theory (assuming localized basis functions are used), proving exponential decay (i.e., 'nearsightedness') for gapped systems at zero electronic temperature and thus providing a rigorous justification for the possibility of linear scaling methods in electronic structure calculations for non-metallic systems. The case of density matrices for disordered systems (Anderson model) and for metallic systems at finite temperature will also be considered. Additional applications, possible extensions to the non-Hermitian case, and some open problems will conclude the talk. This is joint work with Paola Boito and Nader Razouk.

### Michele Benzi

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### IP3

# Matrix Factoriazations and Total Positivity

The concept of a totally positive matrix grew out of three separate applications: Vibrating systems, interpolation, and probability. Since them, this class of matrices continues to garner interest from both applied and theoretical mathematicians. In 1953, a short paper appeared by Anne Whitney in which she established a "reduction" result that may be one of the most powerful results on this topic. My plan for this presentation is to survey the relevant history from Anne's paper to present day, and to discus the resulting impact of her reduction result. Particular attention will be paid to bidiagonal factorizations of totally positive matrices, along with a number of related applications.

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#### IP4

#### Model Reduction for Uncertainty Quantification and Optimization of Large-scale Systems

For many engineering systems, decision-making under uncertainty is an essential component of achieving improved system performance; however, uncertainty quantification and stochastic optimization approaches are generally computationally intractable for large-scale systems, such as those resulting from discretization of partial differential equations. This talk presents recent advances in model reduction methods — which aim to generate lowdimensional, efficient models that retain predictive fidelity of high-resolution simulations — that make possible the characterization, quantification and control of uncertainty in the large-scale setting.

<u>Karen Willcox</u> Massachusetts Institute of Technology kwillcox@mit.edu

## IP5

# Recent Advances in the Numerical Solution of Quadratic Eigenvalue Problems

A wide variety of applications require the solution of a quadratic eigenvalue problem (QEP). The most common way of solving the QEP is to convert it into a linear problem of twice the dimension and solve the linear problem by the QZ algorithm or a Krylov method. Much work has been done to understand the linearization process and the effects of scaling. Structure preserving linearizations have been studied, along with algorithms that preserve the spectral properties in finite precision arithmetic. We present a new class of transformations that preserves the block structure of widely used linearizations and hence does not require computations with matrices of twice the original size. We show how to use these structure preserving transformations to decouple symmetric and nonsymmetric quadratic matrix polynomials.

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# IP6

### Definite versus Indefinite Linear Algebra

Matrices with symmetries with respect to indefinite inner products arise in many applications, e.g., Hamiltonian and symplectic matrices in control theory and/or the theory of algebraic Riccati equations. In this talk, we give an overview on latest developments in the theory of matrices in indefinite inner product spaces and focus on the similarities and differences to the theory of Euclidean inner product spaces. Topics include normality, polar decompositions, and singular value decompositions in indefinite inner product spaces.

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# IP7

## Beyond the Link-Graph: Analyzing the Content of Pages to Better Understand their Meaning

In recent years the Web link graph has attracted much attention. However once we start analyzing the content Web pages many other fascinating graphs reveal themselves. In my talk I will discuss some of the information structures that we can construct from different Web content analysis sources, such as: anchor text, query and click logs, social tagging, natural language processing of text, and user provided semantic data.

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### IP8

# Numerical Linear Algebra, Data Mining and Image Processing

In this talk, I will present two applications in data mining and image processing. The first application is related to the problem where an instance can be assigned to multiple classes. For example, in text categorization tasks, each document may be assigned to multiple predefined topics, such as sports and entertainment; in automatic image or video annotation tasks, each image or video may belong to several semantic classes, such as urban, building, road, etc; in bioinformatics, each gene may be associated with a set of functional classes. The second application is related to multiple class image segmentation problem. For example, foreground-background segmentation has wide applications in computer vision (scene analysis), computer graphics (image editing) and medical imaging (organ segmentation). Both applications share the concept of semisupervised learning and involve several numerical linear algebra issues. Finally, I will present some matrix computation methods for solving these numerical issues. Experimental results are also given to demonstrate the applications and computation methods.

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# IP9

# Confidence and Misplaced Confidence in Image Reconstruction

Forming the image from a CAT scan and taking the blur out of vacation pictures are problems that are ill-posed. By definition, small changes in the data to an ill-posed problem make arbitrarily large changes in the solution. How can we hope to solve such problems using noisy data and inexact computer arithmetic? In this talk we discuss the use of side conditions and bias constraints to improve the quality of solutions. We discuss their impact on solution algorithms and show their effect on our confidence in the results.

Dianne P. O'Leary

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## IP10

## Sparse Optimization: Algorithms and Applications

Many signal- and image-processing applications seek sparse solutions to large underdetermined linear systems. The basis-pursuit approach minimizes the 1-norm of the solution, and the basis-pursuit denoising approach balances it against the least-squares fit. The resulting problems can be recast as conventional linear and quadratic programs. Useful generalizations of 1-norm regularization, however, involve optimization over matrices, and often lead to considerably more difficult problems. Two recent examples: problems with multiple right-hand sides require jointsparsity patterns among the solutions and involve minimizing the sum of row norms; matrix-completion problems require low-rank matrix approximations, and involve minimizing the sum of singular values. I will survey some of the most successful and promising approaches for sparse optimization, and will show examples from a variety of applications.

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# IP11

## Using Combinatorics to Solve Systems in Mmatrices in Nearly-linear Time

Symmetric M-matrices arise in areas as diverse as Scientific Computing, Combinatorial Optimization, and Machine Learning. In this talk, we survey recently developed combinatorial algorithms for preconditioning these matrices. These algorithms enable one to solve linear equations in these matrices in asymptotically nearly-linear time. The problem of solving equations in symmetric M-matrices leads to questions in graph theory such as: What is the best approximation of a graph by a sparser graph? What about by a tree? And, what is a good decomposition of a graph? We will provide answers and explain their consequences. Finally, we will survey a randomized combinatorial algorithm for scaling a symmetric M-matrix to make it diagonally dominant.

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### CP1

### Preconditioning Systems Arising from Electron Structure Calculations Using the Korringa-Kohn-Rostoker Green Function Method

Electron structure calculations are known to be computationally expensive and arise in different fields of physics. Recently a linear scaling method for metallic systems has been developed by Zeller at Forschungszentrum Jlich. This method uses QMR to solve a linear system with multiple right-hand sides arising from the discretization of the problem. The convergence rate depends on the temperature of the underlying physical problem. We will present first re<u>Matthias Bolten</u> University of Wuppertal bolten@math.uni-wuppertal.de

# $\mathbf{CP1}$

# On Preconditioners for Saddle Point Problems Arising in Implicit Time Stepping of Maxwell's Equations

Time integration of space-discretized Maxwell's equations is often carried out by second-order time integration schemes, treating the curl terms explicitly and obeying the CFL stability restriction. In different applications, for instance, when locally refined unstructured meshes are employed, the CFL restriction can be restrictive, so that unconditionally stable implicit time integration becomes attractive. In implicit time integration of space discretized Maxwell's equations large-scale saddle-point a linear system has to be solved at every time step. As our recent research shows, an powerful preconditioner is then a must. We report on recent results on preconditioning for this type of saddle-point problems.

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Jan Verwer CWI The Netherlands jan.verwer@cwi.nl

# CP1

## A Two-Level Ilu Preconditioner for Electromagnetism Applications

In this work, we consider the solution of the linear systems arising from electromagentism applications by preconditioned Krylov subspace methods. Sparse approximate inverse preconditioners based on Frobenius norm minimization are quite effective for this type of problems. We experiment with a two-level ILU preconditioner with graph partioning techniques, and discarding small entries which correspond to far field interactions. Preliminary results show that this two-level preconditioner is competitive.

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# CP1

# Preconditioning GMRES(m) for Finite Volume Discretization of Incompressible Navier-Stokes Equation by Hermitian/Skew-Hermitian Sepera-

# tion

Existing papers show that, after finite difference and finite element discretization of incompressible Naiver-Stokes equation, we will get special linear system with structure of saddle point problem. GMRES(m) with newly developed preconditioner Hermitian/Skew-Hermitian Separation (GMRES(m)-HSS) provides an efficient way to solve the saddle point system. In this paper, firstly we discuss saddle point system from finite volume discretization of incompressible Naiver-Stokes equation. Then, we solve the system by GMRES(m)-HSS. Furthermore, if the size of the original PDE model is large, the solution speed of the linear system is still slow. Since large portion of computational effort of GMRES(m)-HSS is spent on building the orthogonalization basis, in this paper, by newly developed highlevel parallel programming language, we develop a method to accelerate convergence of GMRES(m)-HSS by parallel Gram-Schmidt (pGS) process. Theoretical analysis shows that pGS can decrease time complexity of GMRES(m)-HSS from O(m) to O(m). Computational experiments show that pGS can significantly increase solution speed of GMRES(m)-HSS.

## <u>Di Zhao</u>

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## $\mathbf{CP2}$

## On a stable variant of Simpler GMRES and GCR

We propose and analyze a stable variant of Simpler GM-RES and GCR, which is based on an adaptive choice of the Krylov subspace basis at a given iteration step using an intermediate residual norm decrease criterion. The new direction vector is chosen as in the original implementation of Simpler GMRES or it is equal the normalized residual vector as in the GCR method. Such an adaptive strategy leads to a well-conditioned basis of the Krylov subspace, which results in a numerically stable and more robust variant of Simpler GMRES or GCR.

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# $\mathbf{CP2}$

## Progressive Gmres: A Minimum Residual Krylov Method Which Is Equivalent to Minres in the Symmetric Case

We study Beckermann and Reichel's Progressive GM-RES (ProGMRES) algorithm, a minimum residual Krylov method for approximating solutions to  $n \times n$  nearly symmetric linear systems, with skew symmetric part of rank s << n. Generating the Krylov subspace basis requires the storage of only s + 2 vectors. We show that for symmetric, possibly indefinite systems, the algorithm is equivalent in exact arithmetic to MINRES. Experiments imply that, in many cases, ProGMRES is computationally equivalent to MINRES for symmetric systems. However, in some experiments, ProGMRES appears to be less stable.

<u>Kirk M. Soodhalter</u>, Daniel B. Szyld Temple University Department of Mathematics ksoodha@temple.edu, szyld@temple.edu CP2

## GIDR(s,l): IDR(s) with Higher-Degree Stabilization Polynomials

Recently Sleijpen and van Gijzen have proposed IDR(s) with stabilization polynomials of higher degree, named IDRstab, which is an efficient method for solving real large nonsymetric systems of equations. Their derivation of IDRstab is based on a complex version of the so-called IDR principle, although they consider real systems of equations. In the present talk we introduce a generalized real IDR principle, which enables us to incorporate stabilization polynomials of higher degree into IDR(s).

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# $\mathbf{CP2}$

### Notes on the Convergence of the Restarted Gmres.

Our first result concerns the convergence of restarted GM-RES for normal matrices. We prove that the cycleconvergence of the restarted GMRES applied to systems with a normal coefficient matrix is sublinear. The second result concerns the convergence of the restarted GMRES in the general case. In the general case, we prove that any admissible cycle-convergence curve is possible for the restarted GMRES at a certain number of cycles. This result holds for any eigenvalue distribution, therefore eigenvalues alone do not determine the convergence of restarted GMRES.

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# $\mathbf{CP3}$

# Interpolation of Reduced-Order Linear Operators on Matrix Manifolds

A new method is presented for interpolating reduced-order models on matrix manifolds. This method relies on the logarithm and exponential mappings to move the interpolation data to a tangent space where standard multivariate interpolation algorithms can be applied and bring it back to the manifold of interest, respectively. The proposed method is illustrated for several engineering applications associated with the orthogonal manifold and non-compact Stiefel manifold.

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# $\mathbf{CP3}$

# A New Algorithm for Computing a Darboux Transformation with Large Shifts

A monic Jacobi matrix is a tridiagonal matrix which contains the parameters of the three-term recurrence relation satisfied by the sequence of monic polynomials orthogonal with respect to a measure. The basic Geronimus transformation with shift  $\alpha$  transforms the monic Jacobi matrix associated with a measure  $d\mu$  into the monic Jacobi matrix associated with  $d\mu/(x-\alpha) + C\delta(x-\alpha)$ , for some constant C. In this paper we examine the algorithms available to compute this transformation and we propose a more accurate algorithm, estimate its forward errors, and prove that it is forward stable. In particular, we show that for C = 0 the problem is very ill-conditioned, and present a new algorithm that uses extended precision.

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### CP3

### Spectral Methods for Parameterized Matrix Equations

We apply polynomial approximation techniques to the vector-valued function that satisfies a linear system of equations where the matrix and the right hand side depend on a parameter. We derive both an interpolatory pseudospectral method and a residual-minimizing Galerkin method, and we show how each can be interpreted as solving a truncated infinite system of equations; the difference between the two methods lies in where the truncation occurs.

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## $\mathbf{CP3}$

# Riemannian Optimization Algorithms for Matrix Completion

We present new algorithms for the problem of recovering a large low-rank matrix from a subset of its entries, known as matrix completion. The methods minimize the least-square error of the projection of a matrix directly on the Riemannian manifold of matrices of fixed rank. The optimization algorithms are the generalization of steepest descent, nonlinear cg and Newton's algorithm to this Riemannian manifold. We will demonstrate the numerical performance in comparison with some recent algorithms.

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# $\mathbf{CP4}$

# Generalized *M*-Matrices

Various classes of generalized M-matrices are discussed including the new class of GM-matrices. The matrices considered are of the form sI - B where B has either the Perron-Frobenius property or the strong Perron-Frobenius property but it is not necessarily nonnegative, I is the identity matrix, and s is a nonnegative scalar not exceeding the spectral radius of B. Results that are analogous to those known for M-matrices are shown for these classes of generalized M-matrices and various splittings of a GM-matrix are studied along with conditions for their convergence.

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## $\mathbf{CP4}$

## Mixed Class of H-Matrices and Schur Complements

It is well-known that there exist nonsingular H-matrices such that their comparison matrix  $\mathcal{M}(A)$  is singular. All equimodular matrices related to this case form the mixed class of H-matrices,  $H_M$ . Here, we study their Schur complements. In particular, it is determined that the Schur complement of a nonsingular matrix in  $H_M$  exists and is an H-matrix, but it can belong to  $H_M$  or to  $H_I$  ( $\mathcal{M}(S)$  is nonsingular). Conditions to distinguish these two cases are given.

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## $\mathbf{CP4}$

# Numerical Approximation of the Minimal Geršgorin Set

One possibility to find a good numerical approximation to the minimal Geršgorin set (MGS) is presented in [Varga, Cvetković, Kostić, Approximation of the minimal Geršgorin set of a square complex matrix, ETNA 30 (2008), 398-405]. Here we will show some improvements of this algiruthm, plotting an area which contains MGS itself, and for which a limited number of boundary points are actual boundary points of MGS.

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### $\mathbf{CP4}$

## **QR** Decomposition of $\mathcal{H}$ -Matrices

The hierarchical ( $\mathcal{H}$ -) matrix format allows storing a variety of dense matrices from certain applications in a special data-sparse way with linear-polylogarithmic complexity. A new algorithm to compute the QR decomposition of an  $\mathcal{H}$ -matrix will be presented. Like other  $\mathcal{H}$ -arithmetic operations the  $\mathcal{H}QR$  decomposition is of linear-polylogarithmic complexity. We will compare our new algorithm with two older ones by using two series of test examples and discuss benefits and drawbacks of the new approach.

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# CP5

### **Eigenspaces of Third-Order Tensors**

Building upon a recently described tensor-tensor multiplication [Kilmer, Martin, and Perrone; submitted, October 2008], we show that, on a particular module of n-by-n matrices, every linear transformation can be represented by tensor-matrix multiplication by a third-order tensor. In this context we investigate invariant sub-modules and define tensor *eigenvectors* and their corresponding *eigenmatrices*. In addition, we examine an Arnoldi-like method for computation of tensor eigenvectors and eigenmatrices.

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# CP5

### Combinatorial Applications of Multidimensional Matrix Theory

Recently the multidimensional matrix theory have found series of applications mostly in all areas of mathematics. In our talk we will be constrained only by our own findings concerning some new approaches in solving problems by means of multidimensional matrices, matrix constructions and functions. Moreover, due to time restrictions, we will report only on combinatorial applications explaining our *Matrix Network Method* and its applications in combinatorial enumeration, in graph and hypergraph coloring, in symmetric function theory, and in substructural combinatorics.

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## $\mathbf{CP5}$

### Fourier Basis Regression Against Multicollinearity

Multicollinearity is a long-standing problem in Statistics. This paper presents an alternative solution to deal with multicollinear observations. In this paper, we propose to use orthogonal Fourier bases F to obtain an estimate of  $\beta$ 

from the subspace spanned by the orthogonalized columns of the X matrix. We also demonstrate that the orthogonalized independent variables have research-related physical interpretations which arise not just because of mathematical convenience but because of the inherent information contained in these new bases. Finally, we show the mathematical elegance of using Fourier bases in regression analysis as opposed to the often messy mathematics of ordinary regression. It is demonstrated that the two definitions of multicollinearity, namely, that based on variance inflation factors and condition numbers are in fact equivalent definitions.

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## $\mathbf{CP5}$

# Scalable Implicit Symmetric Tensor Approximation

We describe some algorithms for producing a best multilinear rank r approximation of a symmetric tensor, useful e.g. for working with higher moments and cumulants of a large p-dimensional random vector. Since the approximated dway tensor has  $p^d$  entries, for large p it is critical never to explicitly represent the entire tensor. Working implicitly and approximately where appropriate, this approach enables the use of higher order factor models on large-scale data.

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## CP6

## Combinative Preconditioning Based on Relaxed Nested Factorization and Tangential Filtering Preconditioner

The problem of solving block tridiagonal linear systems arising from the discretization of PDE on structured grid is considered. Nested Factorization preconditioner introduced by Appleyard et. al. is an effective preconditioner for certain class of problems and a similar method is implemented in Schlumerger's widely used Eclipse oil reservoir simulator. In this work, a relaxed version of Nested Factorization preconditioner is proposed. Effective multiplicative/additive preconditioning is achieved in combination with Tangential filtering preconditioner.

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## CP6

# Inverse Sherman-Morrison Factorization and Its Related Preconditioners

We analyze the Inverse Sherman-Morrison factorization of an invertible matrix, in particular its relations with the LDU factorization. Since the ISM factorization is highly parametrizable we analyze also some relations of the factors for different parameter choices. Also the block version of the factorization is studied. The main motivation for introducing the ISM factorization is to use it as a preconditioner. Some existence properties of these preconditioners and some numerical results are shown.

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## $\mathbf{CP6}$

# The Importance of Structure in Algebraic Preconditioners

In recent years, algebraic preconditioners have achieved a considerable degree of efficiency and robustness. Incomplete factorizations represent an important class of such preconditioners. Despite their success, for many problems further tools are required to enhance performance and improve reliability. We propose an approach that is based on forcing the original matrix structure, or an appropriately modified structure of powers of the system matrix, into a value-based incomplete Cholesky decomposition. Our implementation will be included within the HSL mathematical software library.

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# CP6

## Optimal Block Method and Preconditioner for Banded Matrices

Optimized Schwarz methods (OSMs) for PDEs use Robin (or higher order) transmission conditions in the artificial interfaces between subdomains, and the Robin parameter can be optimized. We present a completely algebraic version of the OSM, including an algebraic approach to find the optimal operator or a sparse approximation thereof. We can thus apply this method to any banded or block banded linear system of equations, and in particular to discretizations of PDEs on irregular domains. With the computable optimal operator, we prove that both the OSM and GMRES with OSM preconditioning converge in no more than two iterations for the case of two subdomains. Very fast convergence is attained even when the optimal operator is approximated by a sparse transmission matrix. Numerical examples illustrating these results are presented.

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# $\mathbf{CP7}$

# Sublinearly Fast Solvers for Finite Difference Operators on Mostly Structured Grids

For boundary value problems associated with constant coefficient finite difference operators on structured grids without body loads, we will demonstrate there exists solvers whose complexity is lower than O(N), where N denotes the number of grid points. We analytically construct the fundamental solution for the difference operator, then use fast techniques for computing convolutions involving the fundamental solution. The resulting methods scale on the order of the number of grid points on the boundary.

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## $\mathbf{CP7}$

# Linear Systems with Large Off-Diagonal Elements and Discontinuous Coefficients

Previous work showed that "geometric" scaling of the equations is useful for handling nonsymmetric systems with discontinuous coefficients. It is shown that after such scaling,  $AA^T$  contains relatively large diagonal elements. These two operations are inherent in the sequential CGMN and the block-parallel CARP-CG algorithms, making them very effective for systems with large off-diagonal elements and discontinuous coefficients. Examples involving heterogeneous media include convection-diffusion equations with large convection and the Helmholtz equation with large wave numbers.

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#### $\mathbf{CP7}$

## Fast Iterative Solver for Incompressible Navier-Stokes Equations with Spectral Elements

We introduce a block preconditioning technique for spectral element discretization of the steady Navier-Stokes equations. This method is built from subsidiary Domain Decomposition solvers which use the Fast Diagonalization Method to eliminate degrees of freedom on subdomain interiors. We demonstrate the effectiveness of this preconditioner in numerical simulations of several benchmark ?ows including Kovasznay ?ow, ?ow in a lid-driven cavity and ?ow over a backward-facing step.

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## CP7

## Numerical Linear Algebra Applied to the Simulation of the Dynamic Interaction between a Railway Track and a High Speed Train

In the simulation of the dynamic interaction between a railway track and a high speed train, many useful linear algebra techniques have to be applied effectively in order to execute it as efficiently and accurately as possible. At first, in the eigenvalue analysis of the large model consisting of two subsystems of the vehicles and the track, it is an interesting problen how we should deal with the interface of contact between a wheel and a rail. Contact points of the interaction move along the track and therefore the characteristic of the system depends on the time. An appropriate methodology of eigenvalue analysis of these dynamically interacting system is needed. Secondly, for railway engineers it is very important to know the influence of the system structural components on a variation of contact force between a wheel and a rail. Because a large variation of contact force causes the early deterioration of the track geometry. In this study, including the investigation of the above problems, an application of numerical linear algebra and related techniques such as singular value decomposition, inverse analysis method are described.

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# CP8

## Cyclic Reduction and Multigrid

Given a discretized PDE on a uniform mesh, one step of cyclic reduction amounts to ordering the gridpoints in red/black fashion and eliminating the ones that correspond to one of the colors. The resulting operator is spectrally better than its original (unreduced) counterpart, but a drawback of this approach is that implementation is not easy, in particular in three dimensions, due to the irregular structure of the associated mesh. In this talk we examine cyclic reduction in the context of multigrid, analyze the smoothing properties of cyclically reduced operators, and discuss ways of efficiently implementing solvers based on this approach.

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## $\mathbf{CP8}$

# Adaptive Algebraic Block Iterative Methods

This talk will present a new method of adaptively constructing block iterative methods based on Local Sensitivity Analysis (LSA). The main application is the development of adaptive smoothers for multigrid methods. Given a linear system, Ax = b, LSA is used to identify blocks of the matrix, A, which are strongly connected in a sense similar to the traditional measure of strength in algebraic multigrid methods. Block iterative Gauss-Seidel or Jacobi methods can then be constructed based on the identified blocks. The size of the blocks can be varied adaptively allowing for the construction of a class of block iterative algebraic methods. Results will be presented for both constant and variable coefficient elliptic problems, systems arising from both scalar and coupled system PDEs, as well as linear systems not arising from PDEs. The simplicity of the method will allow it to be easily incorporated into existing multigrid codes while providing a powerful tool for adaptively constructing smoothers tuned to the problem.

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# $\mathbf{CP8}$

# Halley and Newton Are One Step Apart

In this talk we onsider numerical solution of a nonlinear system of equations F(x) = 0 where the function is sufficiently smooth. While Newton's method which has second order rate of convergence method, is usually used for solving such systems, third order methods like Halley's method will in general use fewer iterations than a second order method to reach the same accuracy. However, the number of arithmetic operations per iteration is higher for third order methods than second order methods. We will show that for a large class of problems the ratio of the number of arithmetic operations of a third order method and Newton's method is constant per iteration using a direct method to solve the linear systems including the cost of computing the function and the derivatives. We also discuss replacing the direct method using an iterative method.

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## $\mathbf{CP8}$

On the Parameterized Uzawa Methods for Saddle

### Point Problems

Bai, Parlett and Wang recently proposed an efficient parameterized Uzawa method for solving the nonsingular saddle point problems (see Numer. Math. 102(2005)1-38). In this paper we investigates the W- norm convergence of the parameterized Uzawa methods for saddle point problems under the a suitable weighted norm of the iterative matrix. Based on the estimates of the weighted norm of the iterative matrix, an new inexact parameterized Uzawa methods for saddle point problems is presented.

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## CP9

### Implementing the Retraction Algorithm for Factoring Symmetric Banded Matrices

Problems arising when modeling structures subject to vibrations or in designing optical fibers wrapped around a spool give rise to eigenvalue problems and linear systems with symmetric, banded matrices. We present various variations of the retraction algorithm which factors a matrix into a product of matrices while preserving symmetry, the bandwidth, and element growth even when the original matrix is indefinite. The factorization may be used to solve a system or compute the inertia of a matrix. It is based on the algorithm of Bunch and Kaufman for symmetric nonbanded systems.

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## CP9

## Compact Fourier Analysis for Deriving Multigrid As Direct Solver

A Compact Fourier Analysis (CFA) for designing new efficient multigrid (MG) methods is considered. The principal idea of CFA is to model MG by means of generating functions and block symbols. We utilize the CFA for deriving MG as a direct solver and give necessary conditions that have to be fulfilled by the MG components for this purpose. General practical smoothers and transfer operators that lead to powerful MG algorithms are introduced.

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### CP9

# Diagonal Pivoting Methods for Solving Unsymmetric Tridiagonal Systems

This talk concerns the LBM<sup>T</sup> factorization of unsymmetric tridiagonal matrices, where L and M are unit lower triangular matrices and B is block diagonal with  $1 \times 1$  and  $2 \times 2$  blocks. In some applications, it is necessary to form this factorization without row or column interchanges while the tridiagonal matrix is formed. We propose methods for forming such a factorization that both exhibit bounded growth factors and are normwise backward stable.

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## $\mathbf{CP9}$

# Orthosymmetric Block Reflectors and Qr Factorizations

Reflectors and block reflectors are widely used tools in numerical linear algebra. Both types of reflectors are needed for the construction of non-Euclidean variants of the QR factorization, for example, in hyperbolic and symplectic scalar products. We shall present implementation details, perturbation and error analysis of the hyperbolic and the symplectic QR factorization.

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# **CP10**

# Solutions of Systems of Algebraic Equations from a Physical model of Induction Machine

This work deals with the study of a system of algebraic equations arising in the mathematical modeling of an electric machine. The machine considered may be an Induction machine, a synchronous machine, or a transformer. Our model is primarily based on a transformer. - The transformer may be used to transfer large amount of power, voltage, or current. In the present case we consider the machine windings for homogeneous or non-homogeneous medium with Dirichlet and Mixed Boundary conditions. We study time independent equations first, and later compare it with time dependent equations. Many cases of time dependent as well as time independent Maxwell's equations have been studied before. A comparison of exact solutions to numerical solutions is established for different layers of transformer windings under dissimilar structures. We further look for extra eddy currents produced and the loss of power therein. A Power-current or skin depth plot and Torque-skin depth plot will be done to find out how to control and minimize the power loss and increase amount of torque required to start the machine or stop the machine in minimum time by using transient analysis and classical Nyquist and Bode plots. An example is considered that depicts how equations and solutions behave differently in different media/materials with respect to power and torque control. The analysis is being done by using a combination of software tools, which include FEMLAB, Mat-Lab and Simulink, and SCILAB.

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# **CP10**

### Eigenvalue Localization for Matrices with Constant Row Or Column Sum

Motivated by some research on synchronization on networks of mobile agents, we are interested in finding a good eigenvalue localization for a square, real-valued, non symmetric matrix with the number k on the main diagonal and exactly k "-1" on off-diagonal places (in random position) in each row. According to Geršgorin theorem, all the eigenvalues of such a matrix are located within the circle with center in k and radius equak to k, but this localization is not good enough. We are interested in tighter localization of all eigenvalues, different from zero. More generalized resuts for matrices with constant row or column sum are obtained.

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# **CP10**

# A Hadamard Product Involving Inverse-Positive Matrices with Checkerboard Pattern

A nonsingular real matrix A is said to be inverse-positive if all the elements of its inverse are nonnegative. This class contains the M-matrices. The Hadamard product involving M-matrices has studied for several authors, Markham, Johnson, Neumann and other. Recently Chen in 2006 prove a conjeture concerning the Hadamard powers of inverse M-matrices. In this work we study the Hadamard product of certain classes of inverse-positive matrices. And we prove that for any pair A, B of triangular inverse-positive matrices with the checkerboard pattern, the Hadamard (entry-wise) product  $A \circ B^{-1}$  is again triangular inverse-positive matrices with the checkerboard pattern. Some interesting inequalities about of the minors of this class of matrices are presented in this work.

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## $\mathbf{CP10}$

# Spectral Inclusion Sets for Structured Matrices

We derive eigenvalue inclusion sets for centrohermitian, skew-centrohermitian, perhermitian, skew-perhermitian, and persymmetric matrices, that can be considered structured analogs of the Geršgorin sets. We also present the nonsingularity conditions associated with these spectral inclusion sets. In addition, we derive sets that can be considered the structured analogs of the Brauer sets. Our techniques are general enough to allow for other symmetries as well.

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# **CP11**

### Parallel Preconditioning for Block-Structured CFD Problems

At the Institute for Propulsion Technology of the German Aerospace Center (DLR), the parallel simulation system TRACE (Turbo-machinery Research Aerodynamic Computational Environment) has been developed specifically for the calculation of internal turbo-machinery flows. The finite volume approach with block-structured grids requires the parallel, iterative solution of large, sparse systems of linear equations. For convergence acceleration of the iteration, parallel preconditioners based on multi-level imcomplete factorizations have been investigated. Numerical and performance results of these methods will be presented for typical TRACE problems on parallel computer systems, including multi-core architectures.

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# **CP11**

## Extending Algorithm Based Fault Tolerance in Order to Support Error on the Fly

In a previous paper, we showed that Algorithm Based Fault Tolerance can be used to perform high performant and fault tolerant matrix-matrix multiplication. We extend these ideas to most of linear algebra operations. We believe our approach is systematic and simply relies on a ABFT BLAS. We will show result of a prototype ABFT LAPACK.

## Julien Langou

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# **CP11**

# On the use of Cholesky in the CholeskyQR algorithm

In practice, the CholeskyQR algorithm is the fastest known algorithm for the QR factorization of a tall and skinny ma-

trix. Unfortunately, this algorithm is unstable and, for illconditioned matrices, the resulting vectors do not form an orthonormal basis. Several variants have been proposed, all requiring the eigenvalue decomposition of the symmetric matrix  $A^T A$ . We propose shifted Cholesky to cure the problem of breakdown in Cholesky, and a subsequent reorthogonalization step.

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### **CP11**

# Resolution of Large Sparse Non-Hermitian Complex Linear Systems on a Nationwide Cluster of Clusters

To solve a large sparse non-Hermitian complex linear system Ax=b, we asynchronously compute in parallel the dominant eigenelements of A and a preconditioned restarted GMRES method on GRID5000, a Nationwide cluster of heterogeneous distributed clusters. We exploit the computed eigenvalues to accelerate the GMRES method using a LS method. This preconditioned method is known to not be mathematically correct when the matrix elements are complexes. Then, we propose a solution to use this method using the same storage space on each nodes that other classical GMRES methods. We propose numerical experimentations using several GRID5000 sites and we compare the obtained performance, time and iteration, with other methods for large matrices from industrial applications.

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# CP12

# Numerical Approaches for Nonlinear Ill-Posed Inverse Problems

Difficult nonlinear inverse problems arise in a variety of scientific applications, and iterative optimization algorithms are often used to efficiently compute solutions to largescale problems. In this work, we investigate Krylov-based solvers and appropriate preconditioners for linear systems that arise within nonlinear optimization schemes. Furthermore, regularization methods for nonlinear ill-posed problems are required for computing stable solution approximations. Applications from medical image processing are considered.

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# **CP12**

#### Calculating the Numerical Rank of Sparse Matrices

Algorithms for calculating the numerical rank of sparse matrices are compared. The algorithms include (1) rank calculation using Sylvester's inertia theorem, (2) calculating the rank using the sparse QR factorization spqr (http://www.cise.ufl.edu/research/sparse/SPQR/) and (3) post-processing the spqr results. The comparison will be based on matrices from the San Jose State University Singular Matrix Database (http://www.math.sjsu.edu/singular/matrices/).

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# $\mathbf{CP12}$

# Limited Approximation of Numerical Range of Normal Matrix

Let A be an  $n \times n$  normal matrix, whose numerical range NR[A] is a k-polygon. Adam and Maroulas (On compressions of normal matrices, Linear Algebra Appl., 341(2002), 403-418) established that if a unit vector  $v \in W \subseteq C^n$ , with dimW = k and the point  $v^*Av \in IntNR[A]$ , then NR[A] is circumscribed to  $NR[P^*AP]$ , where P is an  $n \times (k--1)$  isometry of  $\{span\{v\}\}_{W}^{\perp} \to C^n$ . In this paper, we investigate an internal approximation of NR[A] by an increasing sequence of  $NR[C_s]$  of compressed matrices  $C_s = R_s^*AR_s$ , with  $R_s^*R_s = I_{k+s--1}$ ,  $s = 1, 2, \cdots, n - k$  and additionally NR[A] is expressed as limit of numerical ranges of k-compressions of A.

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# CP12

# Accurate Solutions of Structured Linear Systems from Rank-Revealing Decompositions.

For many structured linear systems (among them, Cauchy and Vandermonde, either totally positive, or non totally positive) for which there are not accurate solvers, we show how to compute accurate solutions by using rank-revealing decompositions (RRD). In this way we take advantage of the great effort done in the last decades to compute accurately the SVD using RRD's. The algorithms used involve  $O(n^3)$  flops.

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# **CP13**

# Title of the Paper Here. Don't Use All Caps.

In this paper the positive realness problem in circuit and

control theory is studied. A numerical method is developed for verifying the positive realness of a given proper rational matrix H(s) for which  $H(s) + H^{T}(-s)$  may have purely imaginary zeros. The proposed method is only based on orthogonal transformations, it is structure-preserving and has a complexity which is cubic in the state dimension of H(s). Some examples are given to illustrate the performance of the proposed method.

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## **CP13**

# Dimension of Orbits of Singular Systems under Proportional and Derivative Feedback

We consider triples of matrices (E, A, B), representing singular linear time invariant systems in the form  $E\dot{x}(t) = Ax(t) + Bu(t)$ , with  $E, A \in M_{p \times n}(C)$  (not necessarily squares), and  $B \in M_{n \times m}(C)$ , under proportional and derivative feedback. After to obtain a canonical reduced form preserving the structure of the systems where the standard subsystem is maximal and using geometric techniques, we obtain the tangent and normal space to the orbits of equivalent triples. This description permit us to deduce the dimension of the orbits and analyze structural stability of the triples.

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## **CP13**

# Analyzing Controllability and Observability by Exploiting the Stratification of Matrix Pairs

The qualitative information about nearby linear timeinvariant (LTI) systems is revealed by the theory of stratification. Utilizing the software tool StratiGraph, we show how the stratification theory is used to analyze the controllability and observability characteristics. We demonstrate with two examples, a mechanical system consisting of a thin uniform platform supported at both ends by springs, and a linearized Boeing 747 model. For both examples, nearby uncontrollable systems are identified as subsets of the complete closure hierarchy for the associated system pencils. Some quantitative results are also reported.

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# **CP13**

# Exposing Structure Algorithms for a Nonsymmetric Algebraic Riccati Equation Arising in Transport Theory.

The nonsymmetric algebraic Riccati equation arising in transport theory is a special algebraic Riccati equation whose coefficient matrices having some special structures. By reformulating the Riccati equation, they were found that its arbitrary solution matrix is of a Cauchy-like form and the solution matrix can be computed from a vector form Riccati equation instead of the matrix form that. In this talk, we review some classical-type and Newton-type iterative methods for solving the vector form Riccati equation and present some work under investigation .

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# **CP13**

## A Parameter Free ADI-like Method for the Numerical Solution of Large Scale Lyapunov Equations

A parameter free ADI-like method is presented for constructing an approximate numerical solution to a large scale Lyapunov equation. The algorithm uses an approximate power method iteration to obtain a basis update and then constructs a re-weighting of this basis update to provide a factorization update that satisfies ADI-like convergence properties.

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# **CP13**

## Nonnegativity of the Group-Projectors Used to Obtain the Nonnegativity of Control Singular Systems

In POSTA06 we studied the nonnegativity of control singular systems via state-feedbacks by using a characterization of the nonnegativity of the group-projector of a square matrix E assuming the nonnegativity of the matrix E. In POSTA09 we will present a characterization of the nonnegativity of the group-projector, slightly simplified. In this work, we use this last characterization to improve the study mentioned at the beginning. This work has been partially supported by Grant DGI MTM2007-64477.

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## **CP14**

# A Note on the dqds Algorithm with Rutishauser's Shift

We are concerned with the behaviour of the dqds algorithm for computing sigular values, when incorporated with Rutishauser's shift. It is proved that in the iterative process Rutishauser's shift is selected finally and the dqds converges cubically. Furthermore the phenomenon is observed that once Rutishauser's shift is selected ever after it is selected. In this talk we will give an theoretical explanation for the phenomenon.

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# **CP14**

# Extraction Strategies for Nonsymmetric Eigenvalue Problems

We consider the extraction phase of subspace methods like the Jacobi-Davidson method for solving large eigenvalue problems. In the nonsymmetric case, known approaches do not satisfy any optimality property and, in practice, their behavior may be unsatisfactory, especially when searching for the eigenvalues with largest real part. In this talk, we shall review and compare existing methods, and also propose some new strategies providing enhanced robustness.

### Julien Callant

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# $\mathbf{CP14}$

# **On Singular Two-Parameter Eigenvalue Problem**

In the 1960s Atkinson introduced an abstract algebraic setting for multiparameter eigenvalue problems. He showed that a nonsingular multiparameter eigenvalue problem is equivalent to the associated system of generalized eigenvalue problems. We extend his result to singular twoparameter eigenvalue problems and show that under very mild conditions the finite regular eigenvalues of both problems agree. This enables one to solve such problems by computing the common regular eigenvalues of two singular generalized eigenvalue problems.

### Andrej Muhic

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# **CP14**

# **Tropical Scaling of Polynomial Eigenvalue Problem**

We introduce a general scaling technique, based on tropical algebra, to compute the eigenvalues of a matrix polynomial. We show that under nondegeneracy conditions, the orders of magnitude of the different eigenvalues are given by certain "tropical roots'. We use them to construct a scaling, and we show by experiments that this improves the accuracy of the computations, particularly when the data have various orders of magnitude.

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# **CP14**

## On MRRR-Type Algorithms for the Tridiagonal Symmetric Eigenproblem and the Bidiagonal SVD

The focus of our research is extending Dhillon & Parlett's algorithm MR<sup>3</sup> to compute accurate singular vectors for a bidiagonal matrix. Doing this without spoiling accuracy is a challenge. Among other aspects we had to evaluate how key parts of MR<sup>3</sup> could be varied to improve reliability and efficiency. As main theoretical contribution we regard our investigation of using block factorizations, allowing  $2 \times 2$ -pivots, in the representation tree. Numerical results will detail the effectiveness of our techniques.

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# CP14 Numerical Solutions of Generalized Eigenvalue

# Problems with Spectral Transformations

This talk concerns algorithms for solving generalized eigenvalue problems, with emphasis on efficient iterative solution of the sequence of linear systems that arise when inexact subspace iteration and implicitly restarted Arnoldi method are applied to detect interior eigenvalues. We provide new insights into the tuning of preconditioning proposed by Spence and his collaborators, and show that the cost of solving these linear systems can be further reduced by the combined use of several other strategies.

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# CP15

## An Algorithm for Constructing a Canonical Basis and the Jordan Normal Form of Arbitrary Linear Operators over Any Field.

It is well known that the Jordan normal form for a linear operator  $\mathcal{A}$  is defined and is constructed together with the corresponding basis in case when the basic field k is algebraically closed or, more generally, if the characteristic (equivalently, the minimal) polynomial of  $\mathcal{A}$  is decomposed into a product of linear polynomials. We define the (generalized) Jordan normal form (of the second kind) for a linear operator  $\mathcal{A}$  of a linear space L over an arbitrary field k and with an arbitrary characteristic polynomial. For such an operator we give an algorithm which is used to construct this form by finding a corresponding canonical basis. As application some other results are obtained, too.

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# CP15

## A General Subspace Structure Parameterization of a Pre-Compesator for a Non-Interacting Controller in Robotic Manipulation Systems and Mechanisms

This paper deals with a total general geometric approach to the study of robotics manipulators and general mechanisms dynamics. In particular a parametrization of a precompensator through structures of subspaces for a noninteracting controller is presented. Due to the technological development, robotics applications are growing in many industrial sectors and even in such applications as medical one (micro manipulation of internal tissues or laparoscopy). In such a framework some typical problems in robotics are mathematically formalized and analyzed. The outcomes are so general that it is possible to speak of structural properties in robotic manipulation and mechanisms. The problem of designing of force/motion controller is investigated. A generalized linear model is used and a careful analysis is made. The presented results consist of proposing a general geometric structure to the study of mechanisms. In particular, a Lemma and a Theorem are shown which offer a parametrization of a pre-compesator for a task-oriented choice of input subspaces. The existence of these input subspaces are a necessary condition for a structural noninteraction property.

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# CP15

# A Sinkhorn-Knopp Fixed Point Problem

We consider the fixed point problem  $\vec{x} = (A^T (A\vec{x})^{(-1)})^{(-1)}$  (where (-1) is the entry-wise inverse), which arises from the Sinkhorn-Knopp Algorithm for transforming a positive matrix into a unique doubly stochastic matrix. We discuss basic properties of solutions, including for non-positive and complex matrices, and we consider some special cases, including some interesting results involving patterned matrices. This work was performed in part by four undergraduates as part of an NSF-sponsored undergraduate research project.

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## CP15

# Some Properties of the K and (s+1) - Potent Matrices

The situations where a square matrix A coincides with any of its powers have been studied as well as another class of matrices which involves an permutation matrix. So, the concept of idempotency can be generalized. This concept is widely used in several applications. We introduce a new kind of matrices called K and (s+1)-potent matrices as an extension of both situations mentioned above. A study of these matrices is developed with some examples.

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# CP15

# On Efficient Numerical Approximation of the Scattering Amplitude

This talk presents results on efficient and numerically wellbehaved estimation of the scalar value  $c\Lambda x$ , where  $c\Lambda$  denotes the conjugate transpose of c and x solves the linear system Ax = b, A 2 CNN is a nonsingular complex matrix and b and c are complex vectors of length N. In other words, we wish to estimate the scattering amplitude cAA-1b. In our understanding, various approaches for numerical approximation of the scattering amplitude can be viewed as applications of the general mathematical concept of matching moments model reduction, formulated and used in applied mathematics by Vorobyev in his remarkable book [3]. Using the Vorobyev moment problem, matching moments properties of Krylov subspace methods can be described in a very natural and straightforward way, see [1]. This talk further develops the ideas from [1] into efficient estimates of  $c\Lambda A-1b$ , see [2]. We briefly outline

the matching moment property of the Lanczos, CG and Arnoldi methods, and specify techniques for estimation of cAA-1b with A non- Hermitian, including a new algorithm based on the BiCG method. We show its mathematical equivalence to the existing estimates which use a complex generalization of Gauss quadrature, and discuss its numerical properties. The proposed estimate will be compared with existing approaches using analytic arguments and numerical experiments on a practically important problem that arises from the computation of diffraction of light on media with periodic structure.

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# CP15

#### Jordan Forms For Two Matrices Which Commute

This article gives a method of obtaining the Jordan form of two commuting matrices R and A when R is diagonalizable. An nxn complex matrix R with the property that a positive power of R gives the identity is examined and examples are given to demonstrate the methods developed in the paper.

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## **CP16**

# Matching Figures with Sentences in Technical Abstracts

Figures are key content in technical literature, so the ability to quickly access images relevant to a sentence in a document's abstract would provide a valuable resource to scientists. We use two main ideas to realize this goal: a mixture language model, which can be viewed as a nonnegative matrix factorization, and a Markov model. We introduce a utility metric and report results of applying both models to 100 documents from the biomedical literature.

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# **CP16**

# Perturbation Theory for the LDU Factorization of Diagonally Dominant Matrices and Its Application to Accurate Computation of Singular Values

We present a new structured perturbation theory for the LDU factorization of diagonally dominant matrices that allows us to prove that the relative errors in the factors computed by using an algorithm developed by Q. Ye in 2008 are bounded by  $O(n^4\epsilon)$ , where *n* is the dimension of the matrix and  $\epsilon$  the machine precision. The previous error bounds proved for this algorithm were  $O(8^n\epsilon)$ , that are useless for matrices with dimension as small as n = 20 in double precision. This new error bound proves rigurously that the computed LDU factorization can be used to compute accurately the SVD of this type of matrices.

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## **CP16**

# PageRank As a Function of a Matrix Instead of a Scalar

The PageRank vector for a stochastic matrix is a rational function of a scalar parameter. Replacing the scalar with a matrix yields a PageRank function of a matrix parameter. The trivial relationship between the Markov chain and linear system for PageRank then disappears. We therefore investigate a few other analogies. These ideas are preliminary and one goal is to solicit feedback on other potential relationships. We show a few numerical examples.

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# **CP16**

## Models for Beta-Wishart Random Matrices

We present our recent progress on developing empirical models for Beta-Wishart random matrices. These models bridge the gap between the classical real, complex, and quaternion Wishart random matrices and provide a continuous treatment of the theory for any positive beta. This work generalizes the identity-covariance (Beta-Laguerre) models of Dumitriu and Edelman to arbitrary covariance.

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# CP16 A Simplified Newton's Method for a Rational Ma-

## trix Problem

Motivated by the classical Newton-Schulz method for finding the inverse of a nonsingular matrix, we develop a new inversion-free method for obtaining the minimal Hermitian positive semidefitive solution  $X_{-}$  of the matrix rational equation  $X + A^*X^{-1}A = I$ , where I is the identity matrix and A is a given matrix. This equation appears in many applied areas including control theory, dynamical programming, ladder networks, stochastic filtering and statistics. We present convergence results and discuss stability properties when the method starts from the available matrix  $AA^*$ . We also present numerical results to compare our proposal with some recently developed inversion-free techniques for solving the same rational matrix equation.

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# **CP16**

# Markov Chain Small-World Model with Asymmetric Transition Probabilities

Motivated by existing results concerning the case of symmetric transition probabilities, we study the effects of a varying degree of asymmetry in transition probabilities on the behavior of the Markov chain small-world model of D. Higham. Asymptotic results in this regard are developed following a matrix-theoretic approach. An interesting outcome is that the behavior of the model is strongly influenced by the intensity of asymmetry, which may find applications in real-world networks involving imbalanced interactions.

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### **CP17**

# A Numerical Method for Quadratic Constrained Maximization

The problem of maximizing a quadratic function subject to an ellipsoidal constraint is considered. The algorithm produces a nearly optimal solution in a finite number of iterations. In particular, the method can be used to solve the ill-conditioned problems in which the solution consists of two parts from two orthogonal subspaces. Without restrictive assumptions, the solution generated by the method satisfies the first and second order necessary conditions for a maximizer of the objective function. Numerical experiments clearly demonstrate that the method is successful.

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# **CP17**

## Joint Spectral Characteristics of Matrices: a Conic Programming Approach

The joint spectral radius and subradius are a research topic of growing impact in hybrid systems, combinatorics, numerical analysis, etc. We propose a new approach to compute them. To our knowledge this constitutes the first method to compute the joint spectral subradius. We show how previous results can be interpreted as particular cases of ours. We show the efficiency of our algorithms by applying them to several problems of combinatorics, number theory and discrete mathematics.

### Raphael Jungers

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# **CP17**

## Minimization of the Kohn-Sham Energy with a Localized, Projected Search Direction

With the constantly increasing power of computers, the realm of experimental chemistry is increasingly being brought into the field of computational mathematics. This work integrates non-linear programming methods with a projected search direction to directly minimize the Kohn-Sham energy. By ensuring that the search direction remains sparse, we guarantee that the computationallyintensive energy function is only evaluated at sparse iterates. Maintaing sparsity, while avoiding local minima, is a critical first-step in developing a fully linear-scaling algorithm to minimize the Kohn-Sham energy.

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# **CP17**

## Variable Projection Methods for Separable Nonlinear Least Squares Learning

We describe variable projection methods (VPM) for neuralnetwork learning. We explain why classical VPM may not work excellently, and describe how to modify VPM to include the second-order information of the residual Hessian matrix unlike the standard VPM that uses the Levenberg-Marquardt Hessian. The modification, supported by efficient stage-wise evaluation of the Hessian that requires essentially no more computation than for the Gauss-Newton Hessian, allows us to exploit the negative curvature if it exists.

## Eiji Mizutani

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### **CP17**

# Solving Large-Scale Eigenvalue Problems from Optimization

We describe parameterized eigenvalue problems arising in methods for large-scale trust-region subproblems and regularization. We present comparisons of matrix-free methods for solving the eigenproblems.

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# **CP17**

# Preconditioning for PDE-Constrained Optimization

Advances in algorithms and hardware have enabled more research on the optimization of functions with constraints given by partial differential equations. Problems of this type arise in a variety of applications and pose significant challenges to optimization algorithms and numerical methods. In this talk we present preconditioners for problems in a general setup and also when additional box constraints are introduced for the control. These constraints add an extra layer of complexity to the optimization method and the efficient solution of the linear system is very important. Block-diagonal preconditioners present one possibility to solve the arising saddle point problems efficiently. In addition, we discuss the use of block-triangular preconditioners that can be used in a non-standard inner product iterative method. We show that the drawbacks of this method can be easily overcome by choosing appropriate preconditioners for the blocks of the saddle point system. We present an eigenvalue analysis for the preconditioners and illustrate their competitiveness on some examples.

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# **CP18**

# Generalized Laplacians and First Transit Times for Directed Graphs

We extend results on average commute-times for undirected graphs to fully-connected directed graphs, corresponding to irreducible Markov chains. We show how the pseudo-inverse of an unsymmetrized generalized Laplacian matrix yields the first-transit times and commute times with formulas, almost matching the undirected graph case. The matrices are positive semi-definite, leading to a natural embedding in Euclidean space preserving commute times. These results are illustrated with an application to an analysis of ad-hoc asymmetric wireless networks.

### Daniel L. Boley

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# **CP18**

### Graph Laplacians and Logarithmic Forest Distances

A new family of distances for graph vertices is proposed. They are a kind of logarithmically transformed forest distances. They reduce to the shortest path distance and to the resistance distance at the extreme values of the family parameter. Additionally, they satisfy *bottleneck additivity*: d(i, j) + d(j, k) = d(i, k) if and only if every path from *i* to *k* contains *j*. The construction of the distances is based on the matrix forest theorem and the graph bottleneck inequality.

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# **CP18**

## Parallel Unsymmetric Nested Dissection Ordering for Sparse Direct Solvers

Fill-reducing ordering algorithms for unsymmetric problems are often inherently sequential (e.g., COLAMD). For large problems, a common approach is to apply nested dissection on the symmetrized matrix. The HUND algorithm, based on hypergraph partitioning, was recently proposed to overcome these drawbacks. We present the first parallel implementation of the HUND algorithm, soon available in the Zoltan toolkit. We show preliminary results for some application matrices.

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# **CP18**

# Multivariable Toeplitz Matrices

We are interested in formulas for inverse of positive definite *multivariable* Toeplitz matrices  $T = (t_{\mathbf{k}-1})_{\mathbf{k},\mathbf{l}\in\Lambda}$  with  $\Lambda \subset N^d$ . Attempts to provide a direct generalization of the Gohberg-Semencul formula have failed so far. In this paper we use a multivariable Gohberg-Semencul type expression which serves as an upper bound for the inverse.

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### **CP18**

# Structured Distance to Normality in the Banded Toeplitz Case

In this talk we are concerned with the structured and unstructured distances to normality of banded Toeplitz matrices in the Frobenius norm. We present formulas for the distance of banded Toeplitz matrices of suitable restricted bandwidth to the algebraic variety of similarly structured normal matrices. We then investigate the distance to generalized circularity, formulating a conjecture on the distance to the variety of normal matrices. The talk is based on joint work with Lothar Reichel.

## Silvia Noschese

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# **CP18**

## Factorization of Block Toeplitz Matrices. Applications to Wavelets and Functional Equations.

Block (or slanted) Toeplitz matrices have found a lot of applications in functional equations, wavelets theory, probability, combinatorics, etc. In the simplest case, 2-block Toeplitz matrices are  $N \times N$ -matrices  $(T_s)_{ij} = p_{2i-j+s-1}$ ,  $s = 0, 1, \text{ and } i, j \in \{1, \dots, N\}$  for a sequence of complex coefficients  $p_0, \ldots, p_N$ . We obtain a complete spectral factorization of those matrices depending on the sequence  $p_k$ , describe the structure of their kernels, root subspaces, and all common invariant subspaces. These results allow us to simplify a formula for the exponent of regularity of wavelets, to obtain a factorization theorem for refinable functions, and to characterize the manifold of smooth refinable functions. This also solves the problem of continuity of solutions of the refinement equations with respect to their coefficients and gives a criterion of convergence of the corresponding cascade algorithms and subdivision schemes.

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# MS1 Title Not Available at Time of Publication

Abstract not available at time of publication.

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# MS1

### Rational Approximation to Trigonometric Operators

We will discuss the approximation of trigonometric operator functions that arise in the numerical solution of wave equations by trigonometric integrators. It is well known that Krylov subspace methods for matrix functions without exponential decay show superlinear convergence behavior if the number of steps is larger than the norm of the operator. Thus, Krylov approximations may fail to converge for unbounded operators. In this talk, a rational Krylov subspace method is proposed which converges not only for finite element or finite difference approximations to differential operators but even for abstract, unbounded operators. In contrast to standard Krylov methods, the convergence will be independent of the norm of the operator and thus of its spatial discretization. We will discuss efficient implementations for finite element discretizations and illustrate our analysis with numerical experiments.

Volker Grimm

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# $\mathbf{MS1}$

# A New Scaling and Squaring Algorithm for the Matrix Exponential

The scaling and squaring method for the matrix exponential is based on the approximation  $e^A \approx (r_m (2^{-s}A))^{2^s}$ , where  $r_m(x)$  is the [m/m] Padé approximant to  $e^x$  and the integers m and s are to be chosen. Several authors have identified a weakness of existing scaling and squaring algorithms termed overscaling, in which a value of s much larger than necessary is chosen, causing a loss of accuracy in floating point arithmetic. Building on the scaling and squaring algorithm of Higham [SIAM J. Matrix Anal. Appl., 26 (4):1179–1193, 2005], which is used by MATLAB's expm, we derive a new algorithm that alleviates the overscaling problem.

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Awad H. Al-Mohy School of Mathematics The University of Manchester almohy@maths.manchester.ac.uk

# MS1

# Computing the Phi-function of a Matrix

The phi-functions are certain functions related to the exponential: the zeroth phi-function is the exponential itself and the first one is defined by  $\phi_1(x) = (e^x - 1)/x$ . They play an important role in exponential integrators. We present an algorithm to evaluate the action of  $\phi_k(A)$  on a vector. The key ingredients in the algorithm are a Krylov-subspace method to reduce the size of the matrix and a time-stepping method akin to the scaling-and-squaring method for matrix exponentials.

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### MS2

## Ritz Value Localization and Convergence of Non-Hermitian Eigensolvers

Rayleigh-Ritz eigenvalue estimates for Hermitian matrices obey the well-known interlacing property, which plays a crucial role in explaining convergence of the restarted Lanczos method with exact shifts. Much less is understood about Ritz values of non-Hermitian matrices, and consequently a satisfactory convergence theory for the restarted Arnoldi method has proved elusive. We shall describe recent progress on the localization of Ritz values, which provide sufficient (though strict) conditions for restarted Arnoldi convergence.

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### MS2

## Low Rank Tensor Approximation

We present a black-box type algorithm for the approximation of tensors in high dimension d. The algorithm determines adaptively the positions of entries of the tensor that have to be computed or read, and using these few entries it constructs a low rank tensor approximation. For efficiency reasons the positions are located on fibre-crosses. The minimization problem is solved by Newton's method which requires the Hessian. It can be evaluated in datasparse form in O(d).

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### MS2

## The Concept of Augmented Backward Stability for Some Iterative Algorithms, with Emphasis on the Lanczos Process

Jim Wilkinson developed the ideas of backward stable numerical algorithms. Some crucial algorithms are clearly not backward stable, but provide useful computed results. Several of these are based on orthogonality, but fail miserably to provide this orthogonality. However there exists a truly orthogonal higher dimensional matrix for each computed one. By using this fact, some of these algorithms are shown to give correct answers for "nearby' higher dimensional problems. We call this "augmented backward stability'.

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# MS2

## **Tensor Network Computations and Analysis**

A tensor network is a way to build high-order tensors through structured contractions of many low-order tensors. The manipulation of such objects can lead to sequences of QR factorizations and SVDs. Product versions of these well known matrix tools turn out to be important for numerical reasons.

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# MS3

### Algebraic Multigrid

In this talk, we will give an overview of the algebraic multigrid (AMG) method and some of the research issues associated with it. The talk will primarily serve as background and motivation for the other presentations in the minisymposium, filling in on topic areas that will not otherwise be covered. In particular, we will discuss in more detail developments in AMG theory and on coarsening techniques based on compatible relaxation.

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# MS3 Bootstrap AMG in Lattice QCD

Operators arising in lattice quantum-chromodynamics (LQCD) simulations pose various challenges to current solvers. For physically interesting configurations the performance of Krylov-subspace methods deteriorates quickly which fueled the search for preconditioners. Due to the nature of the background SU(n) gauge field classical algebraic multigrid (AMG) fails that task, but by introduction of adaptive techniques and generalization of AMG principles we were able to overcome some of the immanent challenges with our Bootstrap approach.

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# MS3

## Towards Nonsymmetric Adaptive Smoothed Aggregation for Systems of Pdes

Smoothed aggregation (SA) applied to nonsymmetric linear systems,  $A\mathbf{x} = \mathbf{b}$ , lacks a minimization principle in coarse-grid correction. Consider applying SA to symmetric positive definite (SPD) matrices,  $\sqrt{A^t A}$  or  $\sqrt{AA^t}$ , for which minimization principles exist. It is not computationally efficient to use either matrix directly in coarse-grid correction as they are typically full. The proposed approach efficiently approximates these corrections using SA adaptively to approximate right and left singular vectors of A. Linear systems arising from discretizations of nonsymmetric systems of PDEs are considered.

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## MS3

# Algebraic Multigrid for Massively Parallel Multi-Core Architectures

Algebraic multigrid has shown to be extremely efficient on distributed-memory architectures. However, the new generation of high-performance computers with an increasing number of nodes, which include multiple cores sharing the bus and several caches and an increased core-to-main memory performance gap, presents new challenges. Algorithms need to have good data locality, few synchronization conflicts, and increased small grain parallelism while at the same time improving scalability to deal effectively with millions of cores. This presentation discusses the design and implementation of algebraic multigrid on such architectures.

Ulrike Yang

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# Computing the Distance to Bounded Realness via the Solution of Structured Eigenvalue Problems

We study control systems  $\dot{x} = Ax + Bu$ , y = Cx + Duthat arise via discretization and model reduction in electric and magnetic field computation. While the original system is typically strictly passive (in simple words it does not generate energy) the approximate system often has lost its passivity. The system is then usually made passive by small perturbations to the system matrices. The computation of small or smallest perturbations that perform this task leads to the task of finding smallest perturbations of Hamiltonian matrices that move eigenvalues off the imaginary axis. We give explicit formulas for the minimal perturbations to move purely imaginary eigenvalues of different sign characteristics together and also to move multiple purely imaginary eigenvalues to specific values in the complex plane. We also present a numerical method to compute upper bounds for the minimal perturbations and discuss how to employ these ideas in the context of passivation.

#### Rafikul Alam

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# $\mathbf{MS4}$

## Structured Distance to Normality and Eigenvalue Sensitivity in the Banded Toeplitz Case

Matrix nearness problems have been the focus of much research in linear algebra. In particular, characterizations of the algebraic variety of normal matrices and distance measures to this variety have received considerable attention. Banded Toeplitz matrices arise in many applications in signal processing, time-series analysis, and numerical methods for the solution of partial differential equations. In this talk we first describe spectral properties of normal (2k + 1)-banded Toeplitz matrices of order n, with  $k \leq \lfloor n/2 \rfloor$ . We then present formulas for the distance of (2k+1)-banded Toeplitz matrices to the algebraic variety of structured normal matrices of same bandwidth. We focus on the perturbation analysis in connection with the distance to normality, devoting special attention to the sensitivity of the spectrum to structure-preserving perturbations in the tridiagonal Toeplitz case, and describing an interesting example involving a Jordan block. Finally, we report on an application regarding the determination of a set containing the field of values of a (2k + 1)-banded matrix. The talk is based on joint work with Lionello Pasquini and Lothar Reichel.

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## MS4

# Structured Quadratic Matrix Polynomials: Solvents and Inverse Problems

A monic Hermitian matrix polynomial  $Q(\lambda)$  of degree 2 can be factorized into a product of two linear matrix polynomials, say  $Q(\lambda) = (I\lambda - S)(I\lambda - A)$ . For the inverse problem of finding a quadratic matrix polynomial with given spectral data it is natural to prescribe a right divisor A and then determine compatible left divisors S. In applications,  $Q(\lambda)$ may be Hermitian, real symmetric, hyperbolic, elliptic, or have mixed real/non-real spectrum, and these structures add extra constraints to the inverse problem. These issues are explored in this talk.

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## MS4

#### Computing the Hamiltonian Schur Form by Blocks

We discuss block methods for computing the Hamiltonian Schur form of a Hamiltonian matrix. By placing each cluster of eigenvalues together in a block, we obtain a more robust algorithm. This is joint work with Christian Schroeder and Volker Mehrmann.

David S. Watkins Washington State University Department of Mathematics watkins@math.wsu.edu

### MS5

# High Performance Algorithms for Materials from Nanocrystals to Crystals

A challenging problem in materials physics is to develop algorithms that permit prediction of materials properties at disparate length scales. Most algorithms are specialized for a periodic system such as a crystal, or a localized system such as a nanocrystal. I will discuss new algorithms to handle both regimes. Our algorithms are based on implementing the Kohn-Sham problem in real space and solving the corresponding eigenvalue problem without explicit resort to standard diagonalization methods.

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# $\mathbf{MS5}$

## The Quantum Monte Carlo Method and Linear Algebra Problems

In the Quantum Monte Carlo method we must evaluate determinant ratios for successive matrices in a very long sequence. One approach is to solve a sequence of linear systems, another to solve generalized eigenvalue problems, and yet another to approximate the determinants or ratios directly estimating bilinear forms of matrix functions. We will give a brief overview and then focus on linear solvers, particularly on a multilevel preconditioner that can be updated very cheaply.

<u>Eric De Sturler</u> Virginia Tech sturler@vt.edu

### MS5

# Electronic Structure: Basic Theory and Practical Methods

Recent advances in quantitative theory of electronic properties of materials have occurred through the combination of new theoretical developments, clever algorithms, and increased computational power. This talk will focus on aspects of the basic theory, with emphasis upon the structure of the methods. In particular, I will describe current work to combine density functional theory with many-body methods in order to create robust methods to treat broad classes of materials.

## <u>Richard M. Martin</u> Department of Applied Physics Stanford University rmartin@uiuc.edu

### MS5

# On the Convergence of the Self Consistent Field Iteration for a Class of Nonlinear Eigenvalue Problems

Methods based on Density Functional Theory (DFT) require solving a nonlinear eigenvalue problem derived from the Schrodinger equation. At the heart of these codes, one typically finds a Self Consistent Field (SCF) iteration, which is the predominant method for solving this underlying nonlinear eigenvalue problem. Despite its popularity however, there are few convergence results available. I will discuss some new and interesting results showing the convergence behavior for the SCF iteration.

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# MS6

# CPU-GPU Hybrid Eigensolvers for Symmetric Eigenproblems

We examine the use of CPU-GPU hybrid systems to accelerate a few symmetric eigensolvers. We investigate the bisection and inverse iteration methods for tridiagonal matrices by performing redundant computation, optimizing for higher resource utilization and reduced memory traffic. We then examine a Lanczos method for a particular spectral partitioning problem, finding that using the Cullum-Willoughby test without reorthogonalization leads to a 180x speedup on a CPU-GPU system. Our approaches are generally applicable to hybrid systems with heterogeneous parallel processors.

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Kurt Keutzer EECS Department University of California, Berkeley keutzer@eecs.berkeley.edu

## MS6

### Parallel Distributed Reduction to Condensed Forms - Scheduling Sequences of Givens Rotations

Some algorithms for two-sided reduction of matrices and matrix pairs to condensed forms generate sequences of Givens rotations acting on rows or columns i and i + 1 for contiguous indices i. This raises some interesting scheduling problems when using 2D block-cyclic distribution of the matrices. We present static scheduling techniques based on partial wavefronts for both rectangular and triangular matrices. The techniques also apply to the application of accumulated Givens rotations using level 3 BLAS.

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# $\mathbf{MS6}$

## Iterative Refinement of Schur Decompositions for Mixed Precision Computation

Assume that the Schur or spectral decomposition of a matrix A is available at a considerably low machine precision but the application demands for higher accuracy. Examples for this setting of current interest include mixed single/double precision computations on Cell processors and GPUs as well as mixed double/quad precision on standard CPUs. In both cases, the operations performed in high precision are significantly more costly and should therefore be limited to the bare minimum. This talk will discuss refinement procedures for entire decompositions that allow us in many cases to have a highly accurate Schur decomposition. Particular attention will be paid to situations where some of the eigenvalues of A are highly ill-conditioned.

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Christian Schröder TU Berlin schroed@math.tu-berlin.de

## MS6

## A Novel Parallel QR Algorithm for Hybrid Distributed Memory HPC Systems

Key techniques used in our novel parallel QR algorithm include multi-window bulge chain chasing and distributed aggressive early deflation, which enable level 3 chasing operations and improved eigenvalue convergence. Mixed MPI-OpenMP coding techniques are utilized for DM platforms with multithreaded nodes, such as multicore processors. Application and test benchmarks confirm the superb performance of our parallel QR algorithm. In comparison with the existing ScaLAPACK code, the new parallel software is one to two orders of magnitude faster for sufficiently large problems.

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# $\mathbf{MS6}$

## Accelerating the Reduction to Upper Hessenberg Form through Hybrid GPU-based Computing

We present a Hessenberg reduction algorithm for hybrid multicore+GPU systems that gets 16x performance improvement over the current LAPACK algorithm running just on multicores (in double precision). This enormous acceleration is due to proper matching of algorithmic requirements to architectural strengths of the hybrid components. The reduction is an important linear algebra problem, especially with its relevance to eigenvalue solvers. The results are significant because Hessenberg reduction has not yet been accelerated on multicore architectures.

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## MS7

## **Computing Enclosures for the Matrix Square Root**

Given an approximation X to the square root of a matrix A, we present methods based on interval arithmetic which compute an entrywise enclosure for the 'true' square root. Our approach is based on a modification of Krawczyk's method which reduces the complexity from  $\mathcal{O}(\backslash)$  to  $\mathcal{O}(\backslash^{\ni})$ .

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Numerical results using the Matlab toolbox Intlab will be reported.

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# MS7

#### Green's Function Calculations in Nano Research

The non-equilibrium Green's function formalism provides a powerful conceptual and computational framework for treating quantum transport in nanodevices. The Green's function that we are interested in is a function of a biinfinite block tridiagonal Hermitian matrix, and only one special diagonal block of the Green's function is required in applications. Computing this special matrix has been a challenging problem for nano-scientists. In this talk we present a satisfactory solution to this problem.

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# MS7 Computing Matrix Means

The definition of geometric mean of two positive definite matrices is not straightforward. However, imposing some expected properties leads to the following matrix

$$A(A^{-1}B)^{1/2}$$

which is defined as the geometric mean of A and B and denoted by A#B. For more than two matrices the situation is more complicated. Filling a list of properties that a geometric mean should verify does not lead to a unique matrix. In fact, there is no complete agreement on the definition of the geometric mean of more than two matrices. We briefly survey some applications and problems related to the matrix geometric means and present some numerical methods to compute them.

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# MS7

## An Effective Matrix Geometric Mean Satisfying the Ando-Li-Mathias Properties

There are in literature several proposals to define a proper generalization of the geometric mean to  $k \ge 3$  positive definite matrices. Ando, Li and Mathias listed ten properties that a "good" mean should fulfill, and proposed a definition satisfying them, based on the limit of an iteration process. We propose another definition, as the limit of a cubically convergent iteration, having all the desired properties but much easier to compute.

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<u>Federico Poloni</u> Scuola Normale Superiore f.poloni@sns.it

# $\mathbf{MS8}$

## Missing Value Estimation Using Matrix Factorizations

Many predictive modeling tasks in data analysis may be posed as missing value estimation problems. Recently, such problems have sparked enormous interest in the context of recommender systems, specifically due to the Netflix million-dollar challenge problem. In this talk, I will survey and discuss methods for such missing value estimation problems that rely on low-rank matrix factorizations of incomplete data matrices.

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# $\mathbf{MS8}$

# Krylov Subspace-Based Techniques for Order Reduction of Large-Scale RCL Networks

The development of many of the most powerful algorithms in linear algebra was driven by the need to solve challenging problems arising in new application areas. In this talk, we describe how the need for order reduction of large-scale RCL networks arising in VLSI circuit simulation led to the development of Krylov subspace-based order-reduction of linear dynamical systems. In particular, we focus on recent advances in reduction techniques that preserve certain structures of RCL networks.

Roland W. Freund University of California, Davis Department of Mathematics freund@math.ucdavis.edu

# $\mathbf{MS8}$

## Polynomial Approximation Problems and Convergence of Krylov Subspace Methods

The convergence of Krylov subspace methods for solving linear algebraic systems or eigenvalue problems can be described or at least bounded by the value of certain polynomial approximation problems involving the given matrix. Unfortunately, such problems are notoriously difficult to analyze, particularly for nonnormal matrices. In this talk I will review some of the results in this area, and discuss recent work on the so-called Chebyshev polynomials of matrices.

Jörg Liesen Institute of Mathematics TU Berlin liesen@mail.math.tu-berlin.de

## MS8

# Do We Understand Gaussian Elimination?

Despite the enormous progress in improving efficiency of algorithms based on Gaussian elimination for solving large sparse systems of linear equations, there is still a strong need for analyzing and improvements of the resulting procedures, in particular, in the field of incomplete decompositions. This talk will review some results in this area and discuss the possibilities for further developments. A special attention will be given to the role of the matrix inverse which is implicitly present in the considered algorithms.

# Miroslav Tuma

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## $\mathbf{MS9}$

# A Week in the Life of an Industrial Linear Algebraist

We will present a survey of all of the linear algebra problems that we have been working on during our years at LSTC including - KKT systems for nonlinear solution for implicit mechanics - Block matrix methods including low rank approximations for subblocks for applications in electromagnetics and acoustics - Iterative methods for CFD and thermal mechanics - Consistent constraint explicit where we are applying the consistent constraint technology of implicit to the explicit formulation.

Cleve Ashcraft Livermore Software Technology Corporation cleve@lstc.com

Roger Grimes Livermore Software Technology Corporation grimes@lstc.com

# MS9

## The Role of Numerical Linear Algebra in Large-Scale Electromagnetic Modeling

We will present a survey of all of the linear algebra problems that we have been working on during our years at LSTC including KKT systems for nonlinear solution for implicit mechanics, block matrix methods including low rank approximations for subblocks for applications in electromagnetics and acoustics, iterative methods for CFD and thermal mechanics, and consistent constraint explicit where we are applying the consistent constraint technology of implicit to the explicit formulation.

Lie-Quan Lee SLAC National Accelerator Laboratory liequan@slac.stanford.edu

## MS9

### Role of Numerical Linear Algebra in DOE

The U.S. Department of Energy is the owner of one of the largest research enterprises in the United States. It has more than ten research laboratories scattered throughout the country. These laboratories are well known for their work in physical and biological sciences. Numerical linear algebra plays a crucial role in many of the scientific applications. In this talk the speaker will sample some of these applications and highlight the impact of numerical linear algebra.

Esmond G. Ng Lawrence Berkeley National Laboratory Lawrence Berkeley National Laboratory egng@lbl.gov

# MS9

#### Linear Algebra Meets the Long Tail

In this presentation we discuss large data problems for a marketplace like eBay. eBay is a Long tail market place where buyers and sellers come together to trade for, typically, one-of-a-kind items. Given this long tail nature of products for sale building applications like Search, Recommender systems and Classification solutions pose huge challenges. Data dimensions are represented by users, keywords, products, items, item properties, or categories. Most of these dimensions extend to tens to hundreds of millions. Matrices representing combinations of these dimensions tend to be sparse and are candidates for dimensionality reduction. Given the scale of the data these computations need to be highly parallelized. Other sets of problems include large volume text data short text (feedback comments) or long text (product description and product reviews). We will discuss the problem space and the challenges and also approaches to address these challenges.

<u>Neel Sundaresan</u> eBay Research Labs tba

## MS10

## Maximum Entropy Principle for Composition Vector Method in Phylogeny

The composition vector (CV) method is an alignment-free method for phylogeny. Since the phylogenetic signals in the biological data are often obscured by noise and bias, denoising is necessary when using the CV method. Recently a number of denoising formulas have been proposed and found to be successful in phylogenetic analysis of bacteria, viruses etc. By using the maximum entropy principle for denoising and utilizing the structure of the constraint matrix to simplify the optimization, we derive several new formulas. With these formulas, we obtain a phylogenetic tree which identifies correct relationships between different gerera of Archaea strains in family Halobacteriaceae by using the 16S rRNA dataset; and also a phylogenetic tree which correctly groups birds and reptiles together, and then Mammals and Amphibians successively by using the 18S rRNA dataset.

Raymond Chan The Chinese University of Hong Kong tba

# MS10

## Alternative Minimization Method with Automatic Selection of Regularization Parameter for Total Variation Image Restoration

Total variation (TV) based image restoration has been intensively studied recent years for its nice property of edge preservation. In this talk, we present an alternative minimization method with automatic selection of regularization parameter for TV based image restoration problem. Under the framework of alternative minimization method, we solve each sub-problem and update the regularization parameter iteratively. Experimental results show that the performance of the proposed method is quite promising.

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Michael K. Ng Department of Mathematics, Hong Kong Baptist University mng@math.hkbu.edu.hk

## **MS10**

# A Fast Algorithm for Updating and Tracking the Dominant Kernel Principal Components

Many important kernel methods in the machine learning area, i.e., kernel Principal Component Analysis, feature approximation, denoising, compression, prediction require the computation of the dominant set of eigenvectors of the symmetrical kernel Gram matrix. Recently, an algorithm for tracking the dominant kernel eigenspace has been proposed. In this talk, a new algorithm to incrementally compute the dominant kernel eigenbasis, allowing to track the kernel eigenspace dynamically, will be presented. This approach exploits the properties of some structured matrices, like arrowhead, Cauchy and Householder ones.

<u>Nicola Mastronardi</u> Istituto per le Applicazioni del Calcolo National Research Council of Italy, Bari N.Mastronardi@ba.iac.cnr.it

## **MS10**

# Tensor Decomposition Methods in Hyperspectral Data Analysis

Nonnegativity constraints on solutions, or approximate solutions, to numerical problems are pervasive throughout computational science and engineering [?]. An important research area in hyperspectral image data analysis is to use nonnegativity constraints to identify materials present in the object or scene being imaged and to quantify their abundance in the mixture. Since spectral unmixing is an ill-posed inverse problem, the use of prior information and regularization constraints are essential tools. In this work, we develop analysis methods based on nonnegative matrix and tensor decompositions that focus on the following goals: material identification, material abundance estimation, data compression, segmentation, and compressed sensing. Applications include satellite and debris tracking and analysis for space activities [?].

<u>Bob Plemmons</u> Wake Forest University Dept. Mathematics, Box 7388 plemmons@wfu.edu

### MS11

# Full Multigrid and Least Squares for Incompressible Resistive Magnetohydrodynamics

Magnetohydrodynamics (MHD) is a fluid theory that describes Plasma Physics by treating the plasma as a fluid of charged particles. Hence, the equations that describe the plasma form a nonlinear system that couples Navier-Stokes with Maxwells equations. This talk develops a nestediteration-Newton-FOSLS-AMG approach to solve this type of system. Most of the work is done on the coarse grid, including most of the linearizations. We show that at most one Newton step and a few V-cycles are all that is needed on the finest grid. Here, we describe how the FOSLS method can be applied to incompressible resistive MHD and how it can be used to solve these MHD problems efficiently in a full multigrid approach. An algorithm is developed which uses the a posterior error estimates of the FOSLS formulation to determine how well the system is being solved and what needs to be done to get the most accuracy per computational cost. In addition, various aspects of the algorithm are analyzed, including a timestepping analysis to confirm stability of the numerical scheme as well as the benefits of an efficiency based adaptive mesh refinement method. A 3D steady state and a reduced 2D time-dependent test problem are studied. The latter equations can simulate a large aspect-ratio tokamak. The goal is to resolve as much physics from the test problems with the least amount of computational work. This talk shows that this is achieved in a few dozen work units. (A work unit equals one fine grid residual evaluation.)

James H. Adler University of Colorado at Boulder james.adler@colorado.edu

# MS11 Algebraic Multigrid for Linear Elasticity

We are interested in the efficient solution of large systems of PDEs arising from elasticity applications. We propose extending the AMG interpolation operator to exactly interpolate the rotational rigid body modes by adding additional degrees of freedom at each node. Our approach is an unknown-based approach that builds upon any existing AMG interpolation strategy and requires nodal coarsening. The approach fits easily into the AMG framework and does not require any matrix inversions. We demonstrate the effectiveness on 2D and 3D elasticity problems.

## Allison H. Baker

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Tzanio V. Kolev, Ulrike Meier Yang Center for Applied Scientific Computing Lawrence Livermore National Laboratory tzanio@llnl.gov, umyang@llnl.gov

# MS11

## AMG for Definite and Semi-definite Maxwell Problems

Recently, there has been a significant interest in auxiliaryspace methods for linear systems arising in electromagnetic diffusion simulations. Based on a novel stable decomposition of the Nedelec finite element space due to Hiptmair and Xu, we implemented a scalable solver for second order (semi-)definite Maxwell problems, utilizing internal AMG V-cycles for scalar and vector Poisson-like matrices. In this talk we present the linear algebra theory, numerical performance, and discuss some recent developments in the algorithm. in its implementation.

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# MS11

### Local Fourier Analysis for Systems of PDEs

For many systems of PDEs, multigrid methods are amongst the most efficient techniques for solving the resulting matrix systems. This efficiency results from achieving appropriate complementarity in the smoothing and coarse-grid correction processes. In this talk, we discuss recent work in local Fourier analysis of multigrid methods for systems of PDEs, including staggered discretizations and overlapping multiplicative smoothers. The resulting tools are demonstrated for the Stokes, curl-curl, and grad-div systems.

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Kees Oosterlee Delft University of Technology c.w.oosterlee@cwi.nl

# MS12

## The Use of Sylvester Equation Solvers for the Computation of Eigenvalues of Integral Operators

Sylvester equations are important in mathematical models of many areas of applied mathematics, such as control theory, stochastic dynamic general equilibrium models, etc. Here we consider its application to the computation of spectral elements of integral operators when there are eigenvalues of multiplicity greater than 1. In this case, a method for the computation of eigenpairs of Fredholm integral operators in a Banach space, which combines defect correction with power iteration method, requiring the solution of an intermediate Sylvester equation, will be used. Different solvers for Sylvester equations will be compared.

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Paulo B. VASCONCELOS Fac. Economia Univ. Porto CMUP - Centro Matemática Univ. Porto pjv@fep.up.pt

### MS12

# Triple dqds Algorithm: Eigenvalues of Real Unsymmetric Tridiagonals

The progressive quotient difference algorithm with shifts (qds) was presented by Rutishauser as early as 1954. It is equivalent to the shifted LR algorithm written in a special notation for tridiagonal matrices. The much more recent differential qds (dqds) is a sophisticated variant of qds. We will present the 3dqds algorithm which performes implicitly three dqds steps and such that real arithmetic is maintained in the presence of complex eigenvalues. We will show some interesting numerical experiments.

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# $\mathbf{MS12}$

### A Framework for Analyzing Nonlinear Eigenproblems and Parametrized Linear Systems

Associated with an  $n \times n$  matrix polynomial of degree  $\ell$ ,  $P(\lambda) = \sum_{j=0}^{\ell} \lambda^j A_j$ , are the eigenvalue problem  $P(\lambda)x = 0$ and the linear system problem  $P(\omega)x = b$ , where in the latter case x is to be computed for many values of the parameter  $\omega$ . Both problems can be solved by conversion to an equivalent problem  $L(\lambda)z = 0$  or  $L(\omega)z = c$  that is linear in the parameter  $\lambda$  or  $\omega$ . This linearization process has received much attention in recent years for the eigenvalue problem, but it is less well understood for the linear system problem. We develop a framework in which more general versions of both problems can be analyzed, based on onesided factorizations connecting a general nonlinear matrix function  $N(\lambda)$  to a simpler function  $M(\lambda)$ , typically a polynomial of degree 1 or 2. Our analysis relates the solutions of the original and linearized problems and in the linear system case indicates how to choose c and recover x from z. For the eigenvalue problem this framework includes many special cases studied in the literature, including the vector spaces of pencils  $\mathbf{L}_1(P)$  and  $\mathbf{L}_2(P)$  recently introduced by Mackey, Mackey, Mehl, and Mehrmann and a class of rational problems. We use the framework to investigate the conditioning and stability of the parametrized linear system  $P(\omega)x = b$  and thereby study the effect of scaling, both of the original polynomial and of the pencil L. Our results identify situations in which scaling can potentially greatly improve the conditioning and stability and our numerical results show that dramatic improvements can be achieved in practice.

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# $\mathbf{MS12}$

# Newton-like Methods for Schur and Gauss Triangular Forms

Ill conditioned eigenproblems may lead to poor numerical approximations of eigenvalues, for example when the data matrix is far from being a normal one or of eigenvectors, for example when the data matrix has close eigenvalues. However, these numerical approximations may serve as initial points of iterative schemes which are able to refine them up to a desired precision. The goal of this paper is to show how the classical Newton-Kantorovich method for differentiable nonlinear problems and its Fixed Slope variant can be adapted in real arithmetic to refine eigenelements of a square complex matrix. Numerical evidence is provided with famous matrices of the Gallery collection. We propose a nonlinear formulation of Schur and Gauss triangularizations in such a way that Newton-like methods can be used to refine the initial approximations to these upper triangular forms.

#### Alain LARGILLIER

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### **MS13**

# On the Early History of Matrix Iterations: The Italian Contribution

In this talk I will review some early work on iterative methods for solving linear systems by Italian mathematicians during the 1930s, with particular attention to the contributions of Lamberto Cesari (1910–1990) and Gianfranco Cimmino (1908–1989). I will also provide some background information on Italian applied mathematics and especially on Mauro Picone's *Istituto Nazionale per le Applicazioni del Calcolo*, where most of this early numerical work took place. Finally, I will illustrate the influence of Cimmino's work on modern and current research.

### <u>Michele Benzi</u>

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# MS13

# Cayley, Sylvester, and Early Matrix Theory

Last year marked the 150th anniversary of "A Memoir on the Theory of Matrices' by Arthur Cayley (1821–1895) the first paper on matrix algebra. The subject was developed by Cayley and his colleague James Joseph Sylvester (1814–1897), who coined the term "matrix', along with many others, in particular the Berlin school of Weiertrass, Kronecker, and Frobenius. I will give an overview of these early developments, leading up the time when matrices became an accepted tool in applied mathematics.

Nicholas J. Higham University of Manchester School of Mathematics higham@ma.man.ac.uk

### MS13

# Hermann Grassmann and the Foundations of Linear Algebra

Hermann Grassmann (1809-1877), one of the mathematical geniuses of the 19th century, laid the foundations of Linear Algebra with his "Calculus of Extension" of 1844. Being notoriously difficult to read and far ahead of its time, Grassmann's work was accepted only gradually by other mathematicians. On the occasion of Grassmann's 200th birthday, I will discuss his main mathematical achievements as well as some of the influences that led to his creation of Linear Algebra.

Jörg Liesen Insitute of Mathematics TU Berlin liesen@math.tu-berlin.de

# MS13

## Kron(A,B): A Product of the Times

A quick study of Zehfuss (1858) and subsequent developments suggests that the Kronecker product (KP) should really be referred to as the "Zehfuss product." But never mind, we will fast forward to the 1960s and later and trace how this all-important matrix operation has worked its way into mainstream numerical linear algebra. Connections to fast transforms, PDE discretization, high-dimensional modeling, and tensor computations will be stressed. Using history as a guide, we will argue that KP-based problemsolving will become increasing prominent as N approaches infinity.

<u>Charles Van Loan</u> Cornell University Department of Computer Science cv@cs.cornell.edu

# MS14

## Lyapunov Equations, Energy Functionals, and Model Order Reduction

We give an overview on the use of algebraic Gramians in the context of model order reduction (MOR). Particularly, we emphasize their relation to energy functionals, Lyapunov(-type) equations, and balancing transformations. New results on using these concepts for balanced truncation MOR methods for stochastic and bilinear systems will be presented. Using Carleman linearization together with balanced truncation for bilinear systems, nonlinear reduced-order models for nonlinear systems can be computed. Numerical examples illustrate our results.

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Tobias Damm TU Kaiserslautern Germany damm@mathematik.uni-kl.de

# MS14

### Model Reduction in Computational Flight Testing

Brute-force use of usual CFD-methods for numerical simulation in the context of flight testing is not feasible due to large numbers of different simulation settings and high simulation cost per setting. Models of reduced order for the calculation of stationary and instationary aerodynamical data of the airplane are desired, which are applicable for a wide range of flight envelopes. We will report on first steps towards the use of model reduction methods in this context.

<u>Heike Fassbender</u> TU Braunschweig, Germany Institut Computational Mathematics h.fassbender@tu-bs.de

## MS14

# Discrete Empirical Interpolation for Nonlinear Model Reduction

A dimension reduction method called Discrete Empirical Interpolation (DEIM) is proposed and shown to dramatically reduce the computational complexity of the Proper Orthogonal Decomposition (POD) method for constructing reduced-order models for unsteady and/or parametrized nonlinear partial differential equations (PDE). DEIM is a modification of POD that reduces the complexity as well as the dimension of general nonlinear systems of ordinary differential equations. In particular it applies to nonlinear ODE arising from discretization of PDE.

Danny C. Sorensen, Saifon Chaturantabut Rice University sorensen@rice.edu, sc3@rice.edu

# MS14

### Approaches to Nonlinear Model Order Reduction

In the design of electrical circuits, simulation has always been a crucial factor, e.g., for circuit and system level verification and for capturing parasitic effects. Shrinking structure sizes and increasing packing densities require refined models, causing very high dimensional linear and nonlinear dynamical systems to be treated numerically. Measures have to be taken to enable simulation in adequate time. Model order reduction for linear and nonlinear problems is one, industry is interested in. We give an overview of techniques and present questions and approaches from semiconductor industry.

<u>Michael Striebel</u>

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Joost Rommes NXP Semiconductors, The Netherlands joost.rommes@nxp.com

#### **MS15**

# Nonlinear Eigenvalue Problems in Accelerator Cavity Modeling

Computational design and optimization of accelerator cavities involves solving large-scale numerical eigenvalue problems. The electromagnetic power loss due to external coupling in the cavities leads to nonlinear terms which depend on the eigenvalues. Due to the complexity of cavity geometries, the problem size of the systems is often very large. We will present the formulation and algorithms we employed to solve those large-scale nonlinear eigenvalue problems from accelerator cavity modeling.

# Lie-Quan Lee

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# $\mathbf{MS15}$

# The Computation of Purely Imaginary Eigenvalues with Application to the Detection of Hopf Bifurcations in Large Scale Problems

The computation of purely imaginary eigenvalues with application to the detection of Hopf Bifurcations in large scale problems The determination of Hopf bifurcations of a dynamical system is often a challenging problem. The goal is to compute the system parameter values for which the system has purely imaginary eigenvalues. In this talk, we present a method that computes these parameter values without computing the imaginary eigenvalues themselves. The method is based on residual inverse iteration for a problem of squared dimension.

Karl Meerbergen K. U. Leuven karl.meerbergen@cs.kuleuven.be

# MS15

## On the Stationary Schrödinger Equation Describing Electronic States of Quantum Dots in a Magnetic Field

In this work we derive a pair/quadruple of nonlinear eigenvalue problems corresponding to the one–band effective Hamiltonian governing the electronic states of a quantum dot in a homogenous magnetic field. Exploiting the minmax characterization of its eigenvalues we devise an efficient iterative projection methods simultaneously handling the pair/quadruple of nonlinear problems and thereby saving about 25%/40-50% of the computation time comparing to the Nonlinear Arnoldi method applied to each of the problems separately.

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Marta M. Betcke Univ of Manchester School of Mathematics m.betcke@maths.manchester.ac.uk

### MS15

# A Parallel Additive Schwarz Preconditioned Jacobi-Davidson Algorithm for Polynomial Eigenvalue Problems in Quantum Dot Simulation

Abstract not available at time of publication.

Weichung Wang National Taiwan University Department of Mathematics wwang@math.ntu.edu.tw

# MS16

### Eigenvalue Problems in Sensing and Imaging

Nonuniqueness arises from typical sensing and imaging problems, and can be resolved by seeking sparse solution to underdetermined linear (integral) equations, usually with a Fourier kernel. We connect the task of sparse solution to the design of Gaussian quadratures and to a class of eigenvalue problems with their computational issues. Courant Institute, NYU USA yuchen@cims.nyu.edu

## MS16

### Minimizing Communication in Linear Algebra

A lower bound on communication (words of data moved) needed to perform dense matrix multiplication is known to be Omega(f/sqrt(M)) where f is the number of multiplications  $(n^3)$  and M is the fast memory size. We extend this result to all direct methods of linear algebra (BLAS, LU, QR, eig, svd, etc), to sequential or parallel algorithms, and to dense or sparse matrices. We show large speedups over algorithms in LAPACK and ScaLAPACK.

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Oded Schwartz Technische Universitat Berlin odedsc@math.tu-berlin.de

### **MS16**

# Structured Matrix Computations: Recent Advances and Future Work

Fast algorithms for structured matrices, such as the Toeplitz matrices and Cauchy matrices, have a long and rich history. Recent advances have made many of such algorithms both fast and numerically stable. In addition, structured matrix techniques have been successfully used to solve new classes of problems that are not structured in the classical sense. In this talk, we discuss some recent advances and interesting open questions in structured matrix computations.

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# MS16

### Minimum Sobolev Norm Schemes

Minimum Sobolev Norm (MSN) schemes are a higher order mesh-free discretization schemes that suppress the Runge Phenomenon. The main idea is to find interpolatory polynomials of order >> N-the number of nodes, with minimum Sobolev Norm. The infinite order case of the interpolation operator, produces a Golumb Wienberger kernel, that has FMM structure. We present the ideas behind the MSN scheme, results from convergence, and fastalgorithms for their evaluation.

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# MS16

# **Fast Inversion of Integral Operators**

The talk will describe a scheme for rapidly constructing an approximate inverse to the dense matrices arising from the discretization of 1D integral operators and boundary integral operators in the plane. The scheme is easily derived via hierarchical application of the Woodbury formula for matrix inversion. Its computational cost typically scales linearly with problem size, with a small constant of proportionality. The use of randomized sampling to facilitate the compression of matrices will be discussed.

<u>Gunnar Martinsson</u> Dept. of Applied Mathematics U. of Colorado, Boulder martinss@colorado.edu

# MS17

## The Extended Krylov Subspace Method and Orthogonal Laurent Polynomials

An orthogonal basis for the extended Krylov subspace  $K^{\ell,m}(A) = \operatorname{span}\{A^{-\ell+1}v, \ldots, A^{-1}v, v, Av, \ldots, A^{m-1}v\}$  can be generated using short recursion formulas. These formulas are derived using properties of Laurent polynomials. The derivation is presented for the general case when  $m = k\ell$  where k is a positive non-zero integer. The method is applied to the approximation of matrix functions of the form f(A)v.

Carl Jagels Hanover College jagels@hanover.edu

## MS17

## A Newton-Smith-Block Arnoldi Method for Large Scale Algebraic Riccati Equations

In this talk, we present a Newton-Block Arnoldi method for solving large continuous algebraic Riccati equations. Such problems appear in control theory, model reduction, circuit simulation and others. At each step of the Newton process, we solve a large Lyapunov matrix equation with a low rank right hand side. These equations are solved by using the block Arnoldi process associated with a preconditioner based on the Alternating Direction Implicit (ADI) iteration method. We give some theoretical results and report numerical tests to show the effectiveness of the proposed approach.

## Khalid Jbilou

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# MS17

# A New Implementation of the Block GMRES Method

The Block GMRES is a block Krylov solver for solving non symmetric systems with multiple right hand side. This method is classically implemented by first applying the Arnoldi iteration as a block orthogonalization process to create a basis of the block Krylov space and then solving a block least squares problems, which is equivalent to solving several least squares problems but with the same Hessenberg matrix. These laters are solved by using a block updating procedure for the QR decomposition of the Hessenberg matrix based on Givens rotations. A more effective alternative was given in which uses the Householder reflectors.

In this paper we will propose a new and a simple implementation of the block least squares problem. Our approach is based on a genralization of Ayachour's method, given for the GMRES with a single right hand side. Finally we will give some numerical experiments to illustrate the performance of the new implementation.

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Lothar Reichel Kent State University reichel@math.kent.edu

# **MS17**

#### On a Structure-preserving Arnoldi-like Method

In this talk, an Arnoldi-like method is presented. The method preserves the structures of Hamiltonian or skew-Hamiltonian matrices. Different variants are also introduced. The obtained structure-preserving methods are needed for reducing the size of large and sparse Hamiltonian or skew-Hamiltonian matrices. Numerical experiments are given.

Ahmed Salam

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## **MS18**

### **Recent Developments on the Inertias of Patterns**

A number of techniques have been introduced in the literature to show a specific pattern is inertially arbitrary. We will focus on the problem of finding sets of inertias that a pattern can attain. To do this, we describe the inertias realizable by certain sets of polynomials, the effect the inertia of a matrix has on its characteristic polynomial, and provide sufficient conditions for reducible patterns to be inertially arbitrary.

<u>Michael Cavers</u> Dept of Mathematics and Statistics University of Regina cavers2m@math.uregina.ca

# **MS18**

### **On Nilpotence Indices of Sign Patterns**

We provide classes of n by n sign patterns of nilpotence indices at least 3, if they are potentially nilpotent. Furthermore it is shown that if a full sign pattern  $\mathcal{A}$  of order n has nilpotence index k with  $2 \leq k \leq n - 1$ , then sign pattern  $\mathcal{A}$  has nilpotent realizations of nilpotence indices  $k, k + 1, \ldots, n$ .

In-Jae Kim Minnesota State University, Mankato in-jae.kim@mnsu.edu MS18

# Allow Problems Concerning Spectral Properties of Sign Patterns

A sign pattern has entries in  $\{+, -, 0\}$ . For a given property  $\mathcal{P}$ , a sign pattern  $\mathcal{S}$  allows  $\mathcal{P}$  if there exists at least one real matrix with the sign pattern of  $\mathcal{S}$  that has property  $\mathcal{P}$ . The following problems are surveyed: sign patterns that allow all possible spectra (spectrally arbitrary); sign patterns that allow all inertias (inertially arbitrary); and sign patterns that allow nilpotency (potentially nilpotent patterns). Proof techniques, constructions and examples will be discussed, and open problems identified.

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# **MS18**

# Potentially Nilpotent Zero-Nonzero Patterns over Finite Fields

The idea of exploring spectrally arbitrary patterns was initially related to inverse eigenvalue and eigenvalue completion problems. For various patterns, one seemingly critical step for determining whether a pattern is spectrally arbitrary is to determine if the pattern is potentially nilpotent (PN). We introduce an investigation into which zerononzero patterns are PN over finite fields. Tools from algebraic geometry and commutative algebra are developed. We classify irreducible PN patterns of order three over  $Z_p$ .

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# MS19

# Quantum Monte Carlo Methods: The Use of Linear Solvers and Evaluating Determinant Ratios

Quantum Monte Carlo is one of the most accurate methods to calculate physical properties of large systems. Simulations are currently done on a number of electrons N between 100 and 1000. These calculations involve evaluating a series of determinants of  $N \times N$  matrices that change (slowly) throughout the simulation. Asymptotically this evaluation costs  $O(N^3)$  and is one of the dominating practical bottlenecks in simulating larger systems. In addition, functions of these determinants such as gradients and laplacians must be calculated. We will discuss the nature of this problem and explore a series of techniques that are designed to decrease the asymptotic cost of these evaluations in system of physical interest.

Bryan Clark

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# MS19

# Computing the Matrix Sign Function in the Overlap Fermion Model of QCD

At non-zero chemical potential, the overlap Dirac operator is obtained as the sign function of a non-hermitian matrix. We consider techniques to compute the action of the sign function on a vector, including the deflation of small eigenvalues. One approach uses rational functions and a multishift version of deflated FOM, the other is based on the Arnoldi-Lanczos recurrence with a new idea to evaluate the matrix function on the projected system.

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# **MS19**

# Title Not Available at Time of Publication

Abstract not available at time of publication.

<u>Scott Maclachian</u> Tufts University Scott.MacLachlan@tufts.edu

## **MS19**

# Large-scale Eigenvalue Solvers in Computational Materials

Eigenvalue problems continue to be a largely unavoidable bottleneck in materials science applications. We discuss current state of the art eigenmethods and revisit Lanczos type algorithms which have fallen out of favor because they cannot utilize multiple initial guesses and preconditioning. We show that our recent eigCG technique that finds Lanczos quality eigenpairs without keeping the whole Lanczos basis can be used by itself or together with other methods such as Jacobi-Davidson in PRIMME to improve eigenvalue convergence.

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## MS20

## PMOR, an Interpolation Approach

Recently, the Loewner matrix pencil framework to system identification from measured data has been developed. In this talk we will propose an extension to this framework which includes systems depending on parameters. This amounts to treating the transfer function of the system as a rational function in several complex or real variables. Reduction of the order of the underlying system follows naturally, as in the single parameter case.

# Athanasios C. Antoulas

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# $\mathcal{H}_{\in}$ -Optimal Interpolation for Model Reduction of Parameterized Systems

We consider interpolatory model reduction of parameterized linear dynamical systems executed in such a way that the parametric dependence of the original system is reproduced in the reduced order model. Interpolation is guaranteed both respect to selected complex frequencies and selected parameter value choices. We develop optimal parameter selection strategies that will produce  $\mathcal{H}_{\in}$ -optimal reduced order systems that also minimize a least squares error measure taken over the parameter range.

## Christopher A. Beattie

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## MS20

# Interpolation Based Optimal Model Reduction for LTI-Systems

The input-output behaviour of a linear time invariant (LTI) system can be characterized by the transfer function H(s) of the system, a  $p \times m$  dimensional rational matrix function, where m is the number of inputs and p the number of outputs of the system. To compute reduced order models for a large-scale LTI system we may project the state space such that the transfer functions of the reduce order systems are rational tangential Hermite interpolations of the original transfer function. The interpolation data can be chosen in such a way that first order necessary conditions for an optimal approximation in the  $H_{2,\alpha}$ -, or  $h_{2,\alpha}$ -norm are satisfied, where  $\alpha$  is a bound for the poles of the systems. Properties as well as the computation of such reduced order models are presented and relations to balanced truncation methods are discussed.

#### Angelika Bunse-Gerstner, Dorota Kubalinska

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# MS21

# Large Scale Non-linear Eigenvalue Optimization in Electronic Structure Calculations

We will discuss very large scale non-linear eigenvalue problems that arise in Density Functional Theory calculations. In particular, we are interested in simulations that involve many thousands of atoms and we will illustrate the challenges that arise in extreme scale-out of such problems. We will illustrate the success of powerful non-linear optimization methods and show their scalability to thousands of processors.

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### MS21

## Subspace Accelerated Inexact Newton Method for Solving the Kohn-Sham Equations in Large Scale Condensed Matter Applications.

Discretizing the Kohn-Sham equations of Density Functional Theory by Finite Differences methods leads to large sparse matrix eigenvalue problems. To calculate the eigenvectors associated to the lowest eigenvalues we propose a Subspace Accelerated Inexact Newton (SAIN) method combined with a multigrid preconditioner. This efficient iterative solver takes into account the non-linear character of the Hamiltonian operator and avoids solving a series of surrogate linearized problems. The method is illustrated with examples of real applications with hundreds of eigenvectors.

<u>Jean-Luc Fattebert</u> Lawrence Livermore National Lab. fattebert1@llnl.gov

# **MS21**

#### **Nonlinear Subspace Iteration**

To compute the electronic structure of materials, the Density Functional Theory (DFT) technique converts the original *n*-particle problem into an effective one-electron system, resulting in a coupled one-electron Schrödinger equation and a Poisson equation. This coupling is nonlinear and rather complex. A recently proposed method [Y. Zhou et al., Phys. Rev. E. 74, pp.066704 (2006)] to solve this problem is to resort to a nonlinear variant of subspace iteration. The usual (linear) subspace iteration [Bauer, 1960] builds a basis of the subspace associated with the p largest eigenvalues of a matrix by a kind of polynomial iteration (filtering) on an initial basis. Convergence is usually enhanced by using Chebyshev acceleration. The nonlinear form of this approach consists of only updating the Hamiltonian matrix at each restart. We will illustrate this approach and show techniques to enhance its robustness by using Homotopy.

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## MS21

# Solving Nonlinear Eigenvalue Problems in Electronic Structure Calculations

One of the key tasks in electronic structure calculation is to solve a nonlinear eigenvalue in which the matrix Hamiltonian depends on the eigenvectors to be computed. This problem can be solved either as a system of nonlinear equations or as a constrained nonlinear optimization problem. We will examine the numerical algorithms used in both approaches and compare their convergence properties. We will also discuss the use of Broyden updates and trust region techniques in these algorithms.

## Chao Yang

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#### MS22

## Use of Semi-Separable Approximate Factorization and Direction-Preserving for Constructing Effective Preconsitioners

For a symmetric positive definite matrix A of size n-byn, we developed a fast and backward stable algorithm to approximate A by a symmetric positive-definite semiseparable Cholesky factorization, accurate to any prescribed tolerance. Our algorithm ensures that the Schur complements during the Cholesky factorization all remain positive definite after approximation. In addition, it preserves the product, AZ, for a given matrix Z of size n-by-d, where  $d \ll n$ . We present numerical results to demonstrate the effectiveness of the preconditioners, and discuss applications in large-scale computations.

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Panayot Vassilevski Lawrence Livermore National Laboratory vassilevski1@llnl.gov

## MS22

# On the Schur Complements of the Discretized Laplacian

We show that the Schur complements of the matrix obtained by finite difference discretization of the Laplacian on the unit square with Dirichlet and Neumann boundary conditions exhibit off-diagonal blocks with low rank. This is also true of the finite difference matrix in three dimensions under suitable reordering of the grid. This in turn implies that fast direct solvers could be used to efficiently solve these problems.

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Patrick DeWilde TU Delft, Netherlands p.dewilde@ewi.tudelft.nl

# MS22

# Robust and Efficient Factorization and Preconditioning for Sparse Matrices

We present a robust approximate factorization and preconditioning method for sparse matrices such as those arising from the discretization of some PDEs. Sparse matrix techinques are combined with structured factorizations of dense matrices. Structural compressions of dense matrix blocks lead to high efficiency. Robustness enhancement is automatically integrated into the factorization without extra cost. The factor can work as an effective preconditioner without strict structural requirement. The cost and storage for such a factorization are roughly linear in the matrix size. The efficiency, robustness, and effectiveness are discussed and demonstrated with examples such as Helmholtz, linear elasticity, and Maxwell equations. Numerical experiments show that this preconditioner is also relatively insensitive to frequencies or wave numbers.

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Ming Gu University of California, Berkeley Mathematics Department mgu@math.berkeley.edu

# MS22

## **Butterfly Algorithm and its Applications**

We describe the Butterfly algorithm, which is a general approach for the rapid evaluation of oscillatory interactions. We also discuss two applications: sparse Fourier transform and discrete Fourier integral operators. In each case, the butterfly algorithm is combined with special interpolation tools to achieve optimal computational complexity.

## Lexing Ying

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## MS23

# FORTRAN 77 Implementations of Superfast Solvers

We will describe the current status of FORTRAN 77 implementations of superfast algorithms for solving positive definite Toeplitz systems of equations. The algorithms include the original  $O(n \log^2 n)$  method described in [SIMAX 9(1988):61–76] as well as the  $O(n \log^3 n)$  procedure of Stewart [SIMAX 25(2003):669–693], which has improved stability properties.

Greg Ammar Northen Illinois University ammar@math.niu.edu

## MS23

# An Implicit Multishift QR-algorithm for Symmetric Plus Low Rank Matrices

We present an efficient computation of all the eigenvalues of the Hessenberg form of a hermitian matrix perturbed by a possibly non-symmetric low-rank correction. We propose a representation based on Givens transformations that allows to perform steps of the implicit multishift QR algorithm using  $\mathcal{O}(\backslash)$  operations per iteration. A deflation technique is proposed as well. The representation by means of Givens rotations, makes the algorithm numerically stable as confirmed by the extensive numerical tests.

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Raf Vandebril Katholieke Universiteit Leuven Department of Computer Science raf.vandebril@cs.kuleuven.be

# MS23

# Tikhonov's Method

We consider the solution of linear discrete ill-posed problems with the aid of Tikhonov regularization. The regularized problem is said to be in standard form if the regularization operator is the identity. Tikhonov regularization problems in standard form are easier to solve than regularization problems in general form. We discuss the construction of structured square regularization operators that allow easy transformation of the regularized problem to standard form. This talk presents joint work with Qiang Ye.

Lothar Reichel Kent State University reichel@math.kent.edu

## MS23

# On Tridiagonal Matrices Unitarily Equivalent to Normal Matrices

In this talk the unitary equivalence transformation of normal matrices to tridiagonal form is studied. It is wellknown that any matrix is unitarily equivalent to a tridiagonal matrix. In case of a normal matrix the resulting tridiagonal inherits a strong relation between its superand subdiagonal elements. The corresponding elements of the super- and subdiagonal will have the same absolute value. In this talk some basic facts about a unitary equivalence transformation of an arbitrary matrix to tridiagonal form are firstly studied. Both an iterative manner based on Krylov sequences as a direct manner via Householder transformations are deduced. This equivalence transformation is then reconsidered for the normal case and equality of the absolute value between the super- and subdiagonals is proved. Self-adjointness of the resulting tridiagonal matrix with regard to a specific scalar product will be proved. Flexibility in the reduction will then be exploited and properties when applying the reduction on symmetric, skew-symmetric, Hermitian, skew-Hermitian and unitary matrices and their relations with, e.g., complex-symmetric and pseudo-symmetric matrices are presented. It will be shown that the reduction can then be used to compute the singular value decomposition of normal matrices making use of the Takagi factorization. Finally some extra properties of the reduction as well as an efficient method for computing a unitary complex symmetric decomposition of a normal matrix are given.

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# MS24

### The Minimum Rank Problem for Planar Graphs

The minimum rank problem for a given simple, undirected graph G is to determine the minimum rank (or maximum nullity ) over all symmetric matrices whose off-diagonal nonzero pattern corresponds to G. Two graph parameters, the path cover number and zero forcing number, have played an important role in the determination of the maximum nullity for trees, unicyclic graphs, outerplanar graphs, and rectangular grids. This talk will survey several known results and report on recent progress.

Wayne Barrett Brigham Young University wayne@math.byu.edu

# MS24

# Acyclic and Unicyclic Graphs Whose Minimum Skew Rank is Equal to the Minimum Skew Rank of a Diametrical Path

The minimum skew rank of a simple graph G over the field of real numbers is the smallest possible rank among all skew-symmetric real matrices whose (i, j)-entry (for  $i \neq j$ ) is nonzero whenever  $\{i, j\}$  is an edge in G and is zero otherwise. In this paper we give necessary and sufficient conditions for a connected acyclic graph to have minimum skew rank equal to the minimum skew rank of a diametrical path. We also characterize connected unicyclic graphs with this property.

<u>Luz M. DeAlba</u> Drake University Department of Mathematics luz.dealba@DRAKE.EDU

# MS24

# Minimum Rank Problems

A graph (directed or undirected, simple or allowing loops) can be used to describe a pattern of nonzero entries of a matrix (over the real numbers, or more generally over a field). A minimum rank problem is a problem of determining the minimum of the ranks of the matrices described by a graph, perhaps requiring additional matrix properties such as symmetry or positive semidefiniteness. This talk will survey recent developments in minimum rank problems and applications, and serve as an introduction to the mini-symposium.

Leslie Hogben Iowa State University lhogben@iastate.edu

## MS24

# **Diagonal Rank and Skew Symmetric Matrices**

A beautiful result of Fiedler's is that if A is an  $n \times n$  symmetric matrix such that the rank of D + A is at least n - 1 for each diagonal matrix D, then A is permutationally similar to an irreducible, tridiagonal matrix. In this talk, we discuss the analogous problem for skew-symmetric matrices.

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## MS25

## Application of the IDR Theorem to Stationary Iterative Methods and their Performance Evaluation

The appearance of IDR(s) methods based on the IDR Theorem strongly influenced some researchers in Krylov subspace (KS) methods. Like some KS methods, classical stationary iterative (SI) methods, e.g, Gauss-Seidel and SOR, may be seen in a new light too. This change of view builds on the relation between the conventional residual recursion  $r_{k+1} = Br_k$  of the SI method and the recursion  $r_{k+1} = B(r_k + \gamma_k(r_k - r_{k-1}))$  of the IDR(s) method. Here B is the iteration matrix, and  $\gamma_k$  is a scalar.

Seiji Fujino Computing and Communications Center Kyushu University fujino@cc.kyushu-u.ac.jp

# MS25 IDR — A Brief Introduction

The Induced Dimension Reduction (IDR) method introduced first by Sonneveld in 1979 has been reconsidered and generalized by Sonneveld and van Gijzen recently. While the original IDR became the forerunner of Bi-CGSTAB, the new IDR(s) is related to the ML(k)BiCGSTAB method of Yeung and Chan and to the nonsymmetric band Lanczos algorithm. It proved amazingly effective and offers some flexibility. This talk intends to give a brief overview of these approaches and their connections.

Martin H. Gutknecht Seminar for Applied Mathematics ETH Zurich mhg@math.ethz.ch

## MS25

# ML(n)BiCGStab: Reformulation, Analysis and Implementation

With the help of index functions, we rederive the ML(n)BiCGStab algorithm in a more systematic way. There are n ways to define the ML(n)BiCGStab residual vector. Each different definition will lead to a different ML(n)BiCGStab algorithm. We demonstrate this by deriving a second algorithm which requires less storage. We also analyze the breakdown situations. Implementation issues are also addressed. We discuss the choices of the parameters in ML(n)BiCGStab and their effects on the performance.

Man-Chung Yeung University of Wyoming myeung@uwyo.edu

## MS25

## An IDR-variant that Efficiently Exploits Biorthogonality Relations

The IDR theorem provides a way to construct a sequence of nested subspaces, of which the smallest subspace is zero dimensional. IDR-based algorithms construct residuals that are in these nested subspaces. The translation from theorem to algorithm is not unique. In the talk we will present a variant of IDR(s) that imposes bi-orthogonalization conditions on the iteration vectors. The resulting algorithm is accurate and efficient.

Martin B. van Gijzen, Peter Sonneveld Delft Inst. of Appl. Mathematics Delft University of Technology m.b.vangijzen@tudelft.nl, p.sonneveld@tudelft.nl

## MS26

## Linear Algebra and Stochastic Finite Element Computations

Stochastic Finite Element methods for solving partial differential equations with random data have become an established technique for uncertainty quantification (UQ). Its implementation involves a number of challenging linear algebra tasks, among these the solution of very large linear systems of equations, long sequences of closely related linear and nonlinear systems of equations and large dense eigenvalue problems. This talk will lead into the minisymposium by describing the basic UQ problem setting, introducing the key discretization techniques and also present some of our own recent work in addressing these tasks.

## <u>Oliver G. Ernst</u>

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# MS26

## Parallelization and Preconditioning of Iterative Solvers for Linear SFEM Systems

We develop iterative solvers for the solution of linear systems stemming from a stochastic Galerkin projection of stochastic partial differential equations. We demonstrate the parallelism potential of these solvers and implement them with the Trilinos high performance computing environment. We show how these algorithms can mitigate the curse of dimensionality while being very efficient and attuned to high performance resources. These solvers are variations on solvers previously developed by one of the authors which have been adapted to current computational resources.

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## MS26

# Iterative Solvers for Stochastic Galerkin Finite Element Discretizations

A linear stochastic partial differential equation can be converted by the stochastic Galerkin method into a high dimensional algebraic system. Such system, characterized by a tensor product structure, can be solved efficiently by a multigrid solver. This yields a convergence rate independent of the discretization parameters. Non-optimal methods, based on block splitting approaches or on a hierarchy in stochastic space, may require however less computing time. A comparison of several solvers will be presented.

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### MS26

Iterative Solvers in Stochastic Galerkin Finite Element Computations: Preconditioners and MultiThe discretization of linear stochastic partial differential equations (SPDEs) by means of the stochastic Galerkin finite element method [1] results in general in a very large and coupled but structured linear system of equations. Our task is the design of efficient iterative solvers for these Galerkin equations. The stochastic diffusion equation serves as our model problem. For the primal formulation of this SPDE we review the recently proposed Kronecker product preconditioner [2] for the Galerkin matrix which - in contrast to the popular mean-based preconditioner - makes use of the entire information contained in the Galerkin matrix. Furthermore, we extend the idea of Kronecker product preconditioning to the discretized mixed formulation of the stochastic diffusion equation and present numerical results of test problems where the stochastic diffusion coefficient is a lognormal random field. Finally we report on our attempts to utilize multilevel techniques for the Galerkin equations. In contrast to previous works, where many researchers have applied multilevel methods exclusively to the deterministic finite element spaces, we focus on multilevel decompositions for the stochastic variational space and combined deterministic/stochastic multilevel approaches for the global Galerkin system.

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## MS27

## Adaptive Least Squares Algebraic Multigrid for Complex-valued Systems

We present an algebraic multilevel method for solving HPD linear systems. The proposed approach adaptively computes a set of testfunctions and then uses them in a least squares fit to define interpolation. In this way, the algorithm iteratively improves the multilevel hierarchy to better approximate the lowest modes of the MG relaxation (solver) until suitable performance is achieved. We test the proposed approach for a variety of applications in both the Classical AMG and Smoothed Aggregation settings, showing promising results.

James Brannick Department of Mathematics Pennsylvania State University brannick@psu.edu

# MS27

### Smoothed Aggregation Multigrid on Multicore Architectures

Multicore computer architectures present new challenges to linear solvers, including algebraic multigrid multigrid. The advent of many cores has effectively increased the imbalance between node compute power and off-node communication throughput. We report our experiences using nonstandard smoothed aggregation multigrid on multicore architectures to address the computation/communication imbalance. We consider multigrid variants with domain decomposition smoothing, where domains are allowed to cover more than one core in a compute node and present parallel numerical results.

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## **MS27**

## Smoothed Aggregation AMG Solvers for Least-Squares Finite Element Systems

Least-squares finite element methods are an attractive class of methods for the numerical solution of certain div-curl systems. We consider a discretization where we approximate  $H(curl, \Omega) \cup H(div, \Omega)$  conformally with respect to the divergence operator (e.g. using face elements) and use a discrete approximation of the curl operator. We derive a multigrid method from the previous work of Bochev, Hu, Siefert, Tuminaro, Xu and Zhu (2007), using specialized prolongators to transform the system into a nodal Laplace-like problem.

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Kara Peterson Sandia National Laboratories kjpeter@sandia.gov

# **MS27**

## A Generalization of Energy Minimization Ideas to Algebraic Multigrid for Nonsymmetric Systems

We consider the generalization of energy minimization algebraic multigrid concepts to nonsymmetric systems. A new method is proposed where construction of prolongation (and restriction) is based on a few iterations of GM-RES. These iterations essentially minimize the sum of the  $A^T A$  norm of the grid transfer basis functions. This minimization occurs within some Krylov space while satisfying a set of constraints. Numerical comparison are given on a set of highly convective nonsymmetric problems.

Ray S. Tuminaro Sandia National Laboratories Computational Mathematics and Algorithms rstumin@sandia.gov

# MS28

## Teaching Introductory Linear Algebra Incorporating MATLAB

The first wave of technology supporting mathematics instruction surged during the 90s. We took the opportunity to offer a laboratory experience to accompany our general introductory linear algebra course. A fundamental objective was to support linear algebra concepts with graphics for visualization, design experiments to engage students on a variety of levels, and explore connections. A discussion of tactics, examples, student reactions, changes encountered, and challenges involved with the current second wave of technologies that are emerging will be included.

David Hill Temple University dhill001@temple.edu

# MS28

# A Second Course in Linear Algebra for Science and Engineering

This talk will describe a second course in linear algebra that has evolved over the past ten years. The course is aimed at students in engineering and in the physical and computer sciences. Main new topics: (1) geometry in vector spaces, (2) matrix games and linear programming, and (3) finitestate Markov chains. Enrollment has grown over the past five years and now ranges around 200 students annually.

David Lay University of Maryland lay@math.umd.edu

# MS28

# When MATLAB Gives "Wrong" Answers; How to Get Students in Numerical Linear Algebra Classes Excited About Finite-precision Computations

One of the main differences between teaching the standard linear algebra course and a course in numerical linear algebra is that in the latter course all computations are done using finite precision arithmetic. One way to illustrate the importance of this difference is to look at examples where computational software packages such as MATLAB appear to be giving wrong answers. In this talk we examine four or five such scenarios. In each case we look at examples and explain how and why MATLAB arrives at its answers. In our final example we examine a MATLAB program that clearly produces an impossible answer. In this case, when the author of the program tried to debug it by printing out intermediate results, the value of the computed solution changed. What is going on? Is MATLAB exhibiting some sort of Heisenberg effect? All will be explained at the talk.

<u>Steven J. Leon</u> University of Massachusetts Dartmouth leonste@gmail.com

# MS28

# Key Points in a Linear Algebra Course

I will discuss my experience in teaching and writing about linear algebra. I will focus on three points in the course, one at the start and one at the heart and one at the very end (often barely reached):

1. I now give an early lecture to point the way – matrix multiplication and words like independence are introduced by specific examples. I believe we learn language this way, by hearing words, making mistakes, and eventually getting them right.

2. The "Four Fundamental Subspaces" give a structure to the subject. Students catch on to the big picture – dimensions and orthogonality.

3. A highlight at the end is the SVD. How to introduce this idea? It depends on A(A'A) = (AA')A. It involves positive definiteness. And it gives perfect bases for the four subspaces.

Gil Strang MIT gs@math.mit.edu

## **MS29**

# Interpolation with Semi-separable Matrices: the Ratio-of-Polynomials Case

An interesting problem connected to semi-separable matrices and operators is the issue of interpolation. Given a general (upper) matrix or operator, one may wish to find reduced approximate representations for it of the semiseparable type. This issue leads to all sort of generalizations of classical interpolation problems, with very similar approximation properties. An interesting case is when the representation is of the type 'ratio of generalized polynomials'. In the generalized case the polynomials are series of shifted diagonals, their ratio are essentially ratios of (nonuniformly) banded matrices. The theory provides for a generalization to matrices of the classical Löwner interpolation theory as originally developed by Antoulas, Ball, Kang and Willems, has interesting connections with control theory and is also computationally attractive.

# Patrick Dewilde

Institute for Advanced Study of TUM tba

### **MS29**

## Structured Matrix Methods for the Construction of Interpolatory Subdivision Masks

In this talk we present a general approach for the construction of interpolatory subdivision masks based on polynomials and structured matrix computations. This is a joint work with Costanza Conti from the University of Florence and Lucia Romani from the University of Milano-Bicocca.

Luca Gemignani Univeristy of Pisa (Italy) Department of Mathematics gemignan@dm.unipi.it

# MS29

# Efficient Computations with Tensor Structured Matrices

In this talk we present a new method for basic matrix operations with multilevel tensor structured matrices, It is based on a special low-parametric and stable representation for tensors and keeps the complexity linear in the number of levels. Some of these results are presented in the following papers:

I.V.Oseledets and E.E.Tyrtyshnikov, Breaking the curse od dimensionality, or how to use SVD in many dimensions, Research Report 09-03, Kowloon Tong, Hong Kong: ICM HKBU, 2009 (www.math.hkbu.edu.hk/ICM/pdf/09-03.pdf). I.V.Oseledets,

D.V.Savostyanov, and E.E.Tyrtyshnikov, Linear algebra for tensor problems, Research Report 08-02, Kowloon Tong, Hong Kong: ICM HKBU, 2008 (www.math.hkbu.edu.hk/ICM/pdf/08-02.pdf).

#### Eugene Tyrtyshnikov

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## MS29

### Multivariable Orthogonal Polynomials and Struc-

## tured Matrix Computations

The recurrence coefficients of polynomials in one variable with respect to a discrete inner product can be computed by solving a structured inverse eigenvalue problem. In this talk we will investigate how this inverse eigenvalue problem is modified in case of multivariable orthogonal polynomials. We will also indicate how this inverse eigenvalue problem can be solved only using orthogonal similarity transformations. Some numerical experiments will show the validity of this approach.

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# MS30

## Low-rank Matrix Recovery From Noisy Observations Using Nuclear Norm Minimization

The field of Compressed Sensing has demonstrated that sparse signals can be recovered robustly from incomplete sets of measurements. It is natural to ask what other objects or structures might also be recovered from incomplete, limited, and noisy measurements. It has been shown recently that a similar framework can be developed for recovering low-rank matrices from limited observations, by minimizing the nuclear norm of the matrix. In this talk, we extend this framework to include cases where the observations are noisy and the matrix is not perfectly low-rank, and provide bounds on the recovery error for several classes of measurements. Furthermore, we discuss conditions under which the matrix recovered from noisy measurements will have the correct rank and singular spaces.

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# MS30

## Nuclear Norm Minimization for the Maximum Clique and Biclique Problems

We consider the problems of finding a maximum clique in a graph and finding a maximum-edge biclique in a bipartite graph. Both problems are NP-hard. We write both problems as matrix-rank minimization and then relax them using the nuclear norm. This technique, which may be regarded as a generalization of compressive sensing, has recently been shown to be an effective way to solve rank optimization problems. In the special cases that the input graph has a planted clique or biclique (i.e., a single large clique or biclique plus diversionary edges), our algorithm successfully provides an exact solution to the original instance. For each problem, we provide two analyses of when our algorithm succeeds. In the first analysis, the diversionary edges are placed by an adversary. In the second, they are placed at random. In the case of random edges for the planted clique problem, we obtain the same bound as Alon, Krivelevich and Sudakov as well as Feige and Krauthgamer, but we use di erent techniques.

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# MS30

# Explicit Sensor Network Localization using Semidefinite Programming and Clique Reductions

The sensor network localization (SNL) problem in embedding dimension r, consists of locating the positions of ad hoc wireless sensors, given only the distances between sensors that are within radio range and the positions of a subset of the sensors (called anchors). There are advantages for formulating this problem as a Euclidean distance matrix completion (EDMC) problem, and ignoring the distinction between anchors and sensors. Current solution techniques relax this problem to a weighted, nearest, (positive) semidefinite programming, SDP, completion problem, by using the linear mapping between EDMs and SDP matrices. The relaxation consists in ignoring the rank r for the SDP matrices. The resulting SDP is solved using primaldual interior point solvers, yielding an expensive and inexact solution. Moreover, the relaxation is ill-conditioned in two ways. First, it is implicitly highly degenerate in the sense that the feasible set is restricted to a low dimensional face of the SDP cone. This means that the Slater constraint qualification fails. Second, nonuniqueness of the optimal solution results in large sensitivity to small perturbations in the data. The degeneracy in the SDP arises from cliques in the graph of the SNL problem. These cliques implicitly restrict the dimension of the face containing the feasible SDP matrices. In this paper, we take advantage of the absence of the Slater constraint qualification and derive a technique for the SNL problem, with exact data, that explicitly solves the corresponding rank restricted SDP problem. No SDP solvers are used. We are able to efficiently solve this NP-hard problem with high probability, by finding a representation of the minimal face of the SDP cone that contains the SDP matrix representation of the EDM. The main work of our algorithm consists in repeatedly finding the intersection of subspaces that represent the faces of the SDP cone that correspond to cliques of the SNL problem.

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# MS30

# Fast and Near–Optimal Matrix Completion via Randomized Basis Pursuit

Motivated by the philosophy and phenomenal success of compressed sensing, the problem of reconstructing a matrix from a sampling of its entries has attracted much attention recently. Such a problem can be viewed as an information-theoretic variant of the well-studied matrix completion problem, and the main objective is to design an *efficient* algorithm that can reconstruct a matrix by inspecting only a *small* number of its entries. Although this is an impossible task in general, it has heen recently shown that under a so-called *incoherence* assumption, a rank r  $n \times n$  matrix can be reconstructed using semidefinite pro-

gramming (SDP) after one inspects  $O(nr \log^6 n)$  of its entries. In this paper we propose an alternative approach that is much more efficient and can reconstruct a larger class of matrices by inspecting a significantly smaller number of the entries. Specifically, we first introduce a class of so-called *stable* matrices and show that it includes all those that satisfy the incoherence assumption. Then, we propose a randomized basis pursuit (RBP) algorithm and show that it can reconstruct a stable rank  $r n \times n$  matrix after inspecting  $O(nr \log n)$  of its entries. Our sampling bound is only a logarithmic factor away from the information-theoretic limit and is essentially optimal. Moreover, the runtime of the RBP algorithm is bounded by  $O(nr^2 \log n + n^2 r)$ , which compares very favorably with the  $\Omega(n^4r^2\log^{12}n)$  runtime of the SDP-based algorithm. Perhaps more importantly, our algorithm will provide an *exact* reconstruction of the input matrix in polynomial time. By contrast, the SDPbased algorithm can only provide an *approximate* one in polynomial time.

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#### MS31 BiCGStab2 and GPBiCG

# **BiCGStab2** and **GPBiCG** Variants of the IDR(s) Method

The

hybrid BiCG methods such as BiCGSTAB, BiCGStab2, GPBiCG, and BiCGstab $(\ell)$  are well-known efficient solvers for linear system with nonsymmetric matrices. Recently, IDR(s) has been proposed, and it has been reported to be more effective than the hybrid BiCG methods. Moreover, IDR(s) variants incorporating BiCGstab $(\ell)$  strategies have been designed, which converge even faster than the original IDR(s) method. Here, we propose IDR(s) variants incorporating strategies of BiCGStab2 and GPBiCG.

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### MS31

# Exploiting $BiCGstab(\ell)$ Strategies to Induce Dimension Reduction

IDR(s) and  $BiCGstab(\ell)$  are among the most efficient iterative methods for solving nonsymmetric linear systems of equations. Here, we derive a new method called IDRstab combining the strengths of IDR(s) and  $BiCGstab(\ell)$ . To derive IDRstab we extend previous work, where we considered Bi-CGSTAB as an IDR method. We analyze the structure of IDR in detail and introduce the new concept of a Sonneveld space. Numerical experiments show that IDRstab can outperform both IDR(s) and  $BiCGstab(\ell)$ .

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# MS31

#### On the Convergence Behaviour of IDR(s)

During the development of the prototype IDR(s) method [Sonneveld and van Gijzen, SIAM J. Sci. Comput. **31**, 1035-1062 (2008)], several "intelligent" choices for the s auxiliary vectors were tried, with poor results. Only a random choice for these vectors appears to be suitable. In numerical experiments the convergence plots show, for increasing s, a kind of "convergence" to full GMRES. A statistical explanation of this behaviour will be given in relation to the random choice of the auxiliary vectors.

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## **MS31**

### Eigenvalue Perspectives of the IDR Family

We investigate the natural correspondence between Krylov methods for the approximate solution of linear systems of equations and the approximation of eigenvalues tailored to the IDR family. This is work in progress.

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## MS32

### Model Reduction of Switched Dynamical Systems

A hybrid dynamical system is a system described by both differential equations (continuous flows) and difference equations (discrete transitions). It has the benefit of allowing more flexible modeling of dynamic phenomena, including physical systems with impact such as the bouncing ball, switched systems such as the thermostat, and even the internet congestion as examples. Hybrid dynamical systems pose a challenge since almost all reduction methods cannot be directly applied. Here we show some recent developments in the area of model reduction of switched dynamical systems.

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## MS32

## A Structure-Preserving Method for Positive Realness Problem

In this talk the positive realness problem in circuit and control theory is studied. A numerical method is developed for verifying the positive realness of a given proper rational matrix H(s) for which  $H(s) + H^{T}(-s)$  may have purely imaginary zeros. The proposed method is only based on orthogonal transformations, it is structure-preserving and has a complexity which is cubic in the state dimension of H(s). Some examples are given to illustrate the performance of the proposed method.

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# MS32

# Thick-Restart Krylov Subspace Techniques for Order Reduction of Large-Scale Linear Dynamical Systems

In recent years, Krylov subspace techniques have proven to be powerful tools for order reduction of large-scale linear dynamical systems. The most widely-used algorithms employ explicit projection of the data matrices of the dynamical systems, using orthogonal bases of the Krylov subspaces. For truly large-scale systems, the generation and storage of such bases becomes prohibitive. In this talk, we explore the use of thick-restart Krylov subspace techniques to reduce the computational costs of explicit projection.

Roland W. Freund

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# MS32

## AMLS for an Unsymmetric Eigenproblem Governing Free Vibrations of Fluid-Solid Structures

Automated Multi-Level Substructuring (AMLS) has been developed to reduce the computational demands of frequency response analysis and is very efficient for huge symmetric and definite eigenvalue problems. This contribution is concerned with an adapted version of AMLS for an unsymmetric eigenvalue problem governing free vibrations of fluid solid structures. Although we take advantage of an equivalent Hermitian eigenproblem of doubled dimension our method needs essentially the same computational work as the original AMLS algorithm.

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### **MS33**

#### Scalable Tensor Factorizations with Missing Data

Handling missing data is a major challenge in many disciplines. Missing data problem has been addressed in the context of matrix factorizations and these approaches have been extended to tensor factorizations. We are interested in fitting tensor models, in particular, the CANDE-COMP/PARAFAC (CP) model to data with missing entries. We propose the use of a gradient-based optimization algorithm (CP-WOPT) in order to have methods scalable to large tensors. Using numerical experiments we show that the algorithm we propose is accurate and faster than an alternative technique based on nonlinear least squares approach.

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## MS33

### Scalable Implicit Tensor Approximation

We describe some algorithms for producing a best multilinear rank r approximation of a symmetric tensor, useful for working with higher moments and cumulants of a large p-dimensional random vector. Since the approximated dway tensor has  $p^d$  entries, for large p it is critical never to explicitly represent the entire tensor. Working implicitly and approximately where appropriate, this approach enables the use of higher order factor models on large-scale data.

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### MS33

## Decomposing a Third-Order Tensor in Rank-(L,L,1) Terms by Means of Simultaneous Matrix Diagonalization

The decompositions of a third-order tensor in block components are new multilinear algebra tools, that generalize the Parallel Factor (PARAFAC) decomposition. We focus on one of these recently introduced decompositions, the Block-Component-Decomposition in rank-(L,L,1) terms, referred to as BCD-(L,L,1). In previous work, we have proposed an Alternating Least Squares (ALS) algorithm for the computation of the BCD-(L,L,1) and a sufficient bound for which uniqueness of this decomposition is guaranteed. In this talk, we show that the BCD-(L,L,1) can be equivalently reformulated as a problem of Simultaneous Diagonalization (SD) of a set of matrices. This reformulation has two major advantages. First, the resulting SD-based algorithm reveals to be more accurate and less sensitive to ill-conditioned data than the standard ALS algorithm. Second, the SD-based reformulation of the BCD-(L,L,1) involves itself a new sufficient uniqueness bound. The latter bound is more relaxed than the one previously derived, in the sense that the number of rank-(L,L,1) terms that can be extracted from the tensor is significantly greater, under a few conditions on the dimensions.

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# MS33

## On the Convergence of Lower Rank Approximations to Super-symmetric Tensors

We consider a type of rank-r approximation to supersymmetric tensors of even order (of size  $N \times N \times \cdots \times N$ ), in which a set of r orthonormal basis vectors and an  $r \times r \times \cdots \times r$  core tensor are sought (with r < N) to minimize a Froebenius norm discrepancy. The problem is equivalent to finding basis vectors which optimally compress a super-symmetric tensor into one of smaller dimensions via a standard multi-linear transformation. We propose an iterative algorithm that may be understood as a symmetrized version of alternating least squares, with an important distinction: whereas alternating least squares can only be shown to converge to a stationary point (which may be a minimum or saddle point of the approximation). the symmetric variant under study is shown to converge monotonically to a minimum of the approximation problem. The proof exploits inequalities induced by convexity of a related functional, and extends our earlier results for the rank-one super-symmetric approximation problem to the rank-r case.

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## MS34

## An Algebraic Multilevel Approach for Large Scale 3D Helmholtz Equations in Heterogenous Media

An algebraic multilevel preconditioner is presented for the Helmholtz equation in heterogeneous media. It is based on a multi-level block ILU that preserves the underlying complex symmetry. The preconditioner uses an algebraic coarsening strategy based on controlling  $||L^{-1}||$  for numerical stability. In combination with shifting and correcting the systems, a relatively robust preconditioner is contructed. Our numerical results demonstrate the efficiency of the preconditioner, even in the high-frequency regime. This is joint work with Marcus Grote and Olaf Schenk from the University of Basel and the ZUniversity of Castellon.

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## MS34

## Parallel Algebraic Hybrid Linear Solver for Frequency Domain Acoustic Wave Modeling

In this talk, we will present a parallel algebraic nonoverlapping domain decomposition methods for the solution of the Helmholtz equations involved in frequencydomain full-waveform inversion. The preconditioning approach is based on the shift Laplacian technique. The numerical behaviour and the parallel performance of the linear solver will be investigated on large 2D and 3D models.

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#### MS34

## An AMG Preconditioner Based on Damped Operators for Time-harmonic Wave Equations

An algebraic multigrid approximation of the inverse of an physically damped operator is used as a preconditioner for time-harmonic scattering problems in fluids and solids. The AMG uses a graph based coarsening and an underrelaxed Jacobi smoother. Numerical experiments demonstrate the behavior of the method in complicated domains. The number of GMRES iterations grows roughly linearly with respect to the frequency. This approach leads to an efficient solution procedure for low and medium frequency problems.

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### **MS34**

## Spectral Analysis of the Helmholtz Operator Preconditioned with a Shifted Laplacian

We present a comprehensive spectral analysis of the Helmholtz operator preconditioned with a shifted Laplacian. By combining the results of this analysis with an upper bound on the GMRES-residual norm we are able to provide an optimal value for the shift, and to explain the mesh-depency of the convergence of GMRES preconditioned with a shifted Laplacian. We will illustrate our results with a seismic test problem.

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## MS35

## Structures and Dimension of Linearizations of Singular Matrix Polynomials

Recently, the authors have found strong linearizations

which are valid for both regular and singular square matrix polynomials and that allow us to recover the whole eigenstructure of the polynomial. Nonetheless, the problem of finding structured linearizations of structured singular matrix polynomials remains open. In this talk, we study this problem for T-palindromic polynomials. In particular, we show how to construct T-palindromic linearizations of Tpalindromic polynomials with odd degree. In the case of even degree we provide necessary and sufficient conditions for the existence of T-palindromic linearizations, most of which have lower dimension than the usual one.

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### MS35

# Invariant Pairs for Polynomial and Nonlinear Eigenvalue Problems

We consider matrix eigenvalue problems that are polynomial or genuinely nonlinear in the eigenvalue parameter. One of the most fundamental differences to the linear case is that distinct eigenvalues may have linearly dependent eigenvectors or even share the same eigenvector. This can be a severe hindrance in the development of general numerical schemes for computing several eigenvalues of a polynomial or nonlinear eigenvalue problem, either simultaneously or subsequently. The purpose of this talk is to show that the concept of invariant pairs offers a way of representing eigenvalues and eigenvectors that is insensitive to this phenomenon. We will demonstrate the use of this concept with a number of numerical examples. This is partly joint work with Timo Betcke, University of Reading.

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### MS35

# **Diagonalizing Quadratic Matrix Polynomials**

A quadratic eigenvalue problem  $(M\lambda^2 + D\lambda + K)x = 0$ with M nonsingular is said to be diagonalizable if its linearization

$$\left[\begin{array}{cc} D & M \\ M & 0 \end{array}\right]\lambda + \left[\begin{array}{cc} -K & 0 \\ 0 & M \end{array}\right]$$

is diagonalizable by equivalence or congruence transformations, as appropriate. We characterize all admissible canonical forms. Also, we identify isomorphisms between the sets of transformations and subsets of the centralizer of the Jordan form. This is a report on collaborative work with Ion Zaballa.

### MS35

# Smith Forms of Structured Matrix Polynomials

A much-used computational approach to polynomial eigenproblems starts with a linearization of the underlying matrix polynomial P, such as the companion form, and then applies a general-purpose method like the QZ algorithm to this linearization. But when P is structured, it can be advantageous to use a linearization with the "same' structure as P, if one can be found. In this talk we discuss the scope of this structured linearization strategy for the classes of "alternating' and "palindromic' matrix polynomials, using the Smith form as the central tool.

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# MS36

# Fast and Accurate Computations with Some Classes of Quasiseparable Matrices

In the last decade many algorithms have been developed to perform fast computations with quasiseparable matrices by working with the quasiseparable generators. In general, the accuracy and stability of these algorithms is not guaranteed. We present in this talk some subsets of quasiseparable matrices that allow us to perform both fast and accurate computations if a proper parametrization is used. These subsets include totally nonnegative quasiseparable matrices and zero diagonal symmetric and skew-symmetric quasiseparable matrices.

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### **MS36**

A Survey of Some Recent Results for Quasisepara-

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### ble Matrices and their Applications

Abstract not available at time of publication.

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# MS36

# Wavelet Matrices as Green's Matrices with New Factorizations

Olshevsky and Zhlobich have identified a special class of five-diagonal matrices with a remarkable factorization. These matrices are 2 by 2 block bidiagonal. They are products of 2 by 2 block diagonal matrices in which the blocks of the second factor are shifted by a row and column. We identify these factors in the case of the famous Daubechies-4 wavelet filters. These are block Toeplitz and the new factorization shows how easily they could be made timevarying (and finite length) without losing their orthogonality.

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### MS36

# A Quasiseparable Matrices Approach to CMV and Fiedler Matrices

Several new classes of structured matrices have appeared recently in the scientific literature. Among them there are so-called CMV and Fiedler matrices which are found to be related to polynomials orthogonal on the unit circle and Horner polynomials respectively. Both matrices are five diagonal and have a similar structure, although they have appeared under completely different circumstances. We establish a link between these matrices by showing that they both belong to the wider class of twisted Hessenberg-Order-One quasiseparable matrices. We also obtain a general description of five-diagonal matrices in terms of recurrence relations satisfied by polynomials they are related to.

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# **MS37**

## Modified, Regularized Total Least Norm Approach to Signal Restoration

Total Least Norm (TLN) is a common choice for modeling blind deconvolution problems. In this talk, we present a modified, regularized TLN model for signal deblurring problems where both the blurring operator and the blurred signal contain noise. We introduce an alternating method that uses this model to obtain better restoration not only of the signal, but also of the blurring operator.

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### MS37

#### Non-smooth Solutions to Least Squares Problems

In an attempt to overcome the ill-posedness or illconditioning of inverse problems, regularization methods are implemented by introducing assumptions on the solution. Common regularization methods include total variation, L-curve, Generalized Cross Validation (GCV), and the discrepancy principle. It is generally accepted that all of these approaches except total variation unnecessarily smooth solutions, mainly because the regularization operator is in an  $L^2$  norm. Alternatively, statistical approaches to ill-posed problems typically involve specifying a priori information about the parameters in the form of Bayesian inference. These approaches can be more accurate than typical regularization methods because the regularization term is weighted with a matrix rather than a constant. The drawback is that the matrix weight requires information that is typically not available or is expensive to calculate. Ø The  $\chi^2$  method developed by the author and colleagues can be viewed as a regularization method that uses statistical information to find matrices to weight the regularization term. We will demonstrate that unique and simple  $L^2$  solutions found by this method do not unecessarily smooth solutions when the regularization term is accurately weighted with a diagonal matrix.

<u>Jodi Mead</u>

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# **MS37**

## Using Confidence Ellipsoids to Choose the Regularization Parameter for Ill-Posed Problems

Confidence ellipsoids for discretized ill-posed problems are elongated in directions corresponding to small singular values. Intersecting a confidence ellipsoid with another ellipsoid guaranteed to contain the solution gives better localization of that solution with the same confidence level. We present a regularization method with a one-to-one correspondence between values of the regularization parameter and convex combinations of the two ellipsoids. The parameter value is optimized by minimizing the size of the convex combination.

#### Bert W. Rust

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## **MS37**

### Regularization in Polynomial Approximations, Resolution of the Runge Phenomenon

The polynomial interpolation based on a uniform grid yields the well-known Runge phenomenon. The maximum point-wise error is unbounded for functions with complex roots in the Runge zone. In this work, we first investigate the Runge phenomenon with finite precision operations. Then a truncation method based on the truncated singular value decomposition is proposed to resolve the Runge phenomenon. The method consists of two stages: In the first stage a statistical filtering matrix is applied to the interpolation matrix as preconditioner. In the second stage a pseudo inverse of the interpolation matrix is formed using a truncated singular value decomposition. We investigate the structure of the singular vectors and singular values and determine a truncation point based on the oscillatory behavior of the signular vectors and decay behavior of the singular values. We then show with numerical examples that exponential decay of the approximation error can be achieved if an appropriate smoothness parameter that depends on the interpolated function is chosen.

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### MS38

## Block Preconditioners for Generalized Saddle-Point Matrices

Abstract not available at time of publication.

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# MS38

### A Geometric View of Krylov Subspace Methods on Singular Systems

We show why one can apply CG to consistent systems  $A\boldsymbol{x} = \boldsymbol{b}$  where A is symmetric and positive semi-definite, by decomposing CG into the  $\mathcal{R}(A)$  and  $\mathcal{N}(A)$  components, which shows that the method is essentially equivalent to CG applied to a positive diagonal system in  $\mathcal{R}(A)$ . Next, we analyze GMRES for systems where A is nonsymmetric and singular by decomposing GMRES into the  $\mathcal{R}(A)$  and  $\mathcal{R}(A)^{\perp}$  components, providing a geometric interpretation of the convergence conditions given by Brown and Walker.

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# MS38

## On Restrictively Preconditioned HSS Iteration Methods for Non-Hermitian Positive-Definite Linear Systems

A restrictively preconditioned Hermitian/skew-Hermitian splitting (RPHSS) iteration method is presented for the solution of the non-Hermitian and positive-definite system of linear equations. Theoretical analyses on the convergence condition for RPHSS method , the optimal parameters and the choice of preconditioners are given. From practical point of view, the implementation and convergence of the inexact RPHSS method are also discussed in detail. Finally, a number of numerical experiments are used to show that RPHSS method is efficient and comparable to standard HSS iteration method.

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#### **MS38**

# On Parameterized Uzawa Methods for Saddle-Point Problems

Abstract not available at time of publication.

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# MS39

## **Coupled Tensor and Matrix Factorizations**

Matrix and tensor factorizations have proved to be powerful tools in data analysis. There are limited, though, to data that can be represented as a single object. We propose to consider problems where the data has multiple aspects, represented by multiple matrices and tensors with shared modes. Our goal is to analyze these data simultaneously via coupled decompositions. Specifically, we propose all-atonce optimization techniques, which are more effective in our experiments than alternating methods. In this talk, we describe the problem, present several examples, and show computational results.

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### **MS39**

# A Fast and Efficient Algorithm for Low-rank Approximation of a Matrix and Generalization to Tensor

Abstract not available at time of publication.

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# MS39 Commuting Birth-and-Death Processes

## We use methods from combinatorics and algebraic statistics to study analogues of birth-and-death processes that have as their state space a finite subset of the mdimensional lattice and for which the m matrices that record the transition probabilities in each of the lattice directions commute pairwise. One reason such processes are of interest is that the transition matrix is straightforward

to diagonalize, and hence it is easy to compute n step transition probabilities. The set of commuting birth-and-death processes decomposes as a union of toric varieties, with the main component being the closure of all processes whose nearest neighbor transition probabilities are positive. We exhibit an explicit monomial parametrization for this main component, and we explore the boundary components using primary decomposition.

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## MS39

# Finitely Generated Cumulants: Developments and Applications

This continues work on algebraic aspects of cumulants developed in Pistone and Wynn (1999, Statistica Sinica) and (2000, J. Symb. Comp). The definition of the finitely generated cumulant (FGC) property is that, in the univariate or multivariate case, if K(s) is the cumulant generating function for a distribution then the vector of first partial derivatives with respect to s, namely K', and the matrix of second order (partial) derivatives, K', satisfy an implicit polynomial equation f(K',K') = 0. This generalizes the Morris class, in which K' is a quadratic function of K'. The FGC property is a way of introducing polynomial algebra, and symbolic methods, into continuous distribution theory and a surprisingly large class of distributions satisfy the FGC property. Applications include the asymptotic theory of maximum likelihood, saddle-point approximations, multivariate dependency for non-Gaussian random variables, mixture models and information geometry.

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## MS40

## A Key for the Choice of the Subspaces in Restarted Krylov Methods

The restarted Krylov subspace methods allow computing some eigenpairs of large sparse matrices. The size of the subspace in these methods is chosen empirically. A poor choice of this size could lead to the non-convergence of the methods. We propose a technique, based on the projection of the problem on several subspaces instead of a single one, to remedy to this problem. Our approach is validated by its application on IRA method.

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## MS40

# A Numerical Method Based on the Residue Theorem for Computing Eigenvalues in Multiply Connected Region

In this talk, we consider the solution of eigenvalues in a finite and multiply connected region. Such problems arise in the application of photonic crystal waveguides and there is a strong need for the fast solution of the problems. For solving the problems efficiently, we extend the Sakurai-Sugiura method which has been proposed for simply connected region. We also analyze the error of the computed eigenvalues.

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# MS40

# Efficient Subspace Alignment Technique for the Self-Consistent Field Iterations

The subspace alignment is a crucial preprocessing step for the self-consistent field iteration to solve nonlinear eigenvalue problems arising from electronic structure calculations. Its computational kernel involves the matrix polar decomposition. The popular scaled Newton method requires explicit matrix inversion, which is dominated by communication in distributed and multi-core computing. In this talk, we present a new polar decomposition algorithm based on the QR-decomposition (without pivoting) and a communication optimal implementation of the subspace alignment.

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### MS40

## A Hierarchical Parallel Method for Solving Nonlinear Eigenvalue Problems

In this talk, we present a parallel method for finding eigenvalues in a given domain and corresponding eigenvectors of nonlinear eigenvalue problems. In our method, the original problem is converted to a smaller generalized eigenvalue problem, which is obtained numerically by solving a set of linear equations. These linear equations are independent and can be solved in parallel.

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## MS41

# Fast Algorithms for Approximating the Pseudospectral Abscissa and Radius

The  $\epsilon$ -pseudospectral abscissa and radius of an  $n \times n$  matrix are respectively the maximum real part and the maximal modulus of points in its  $\epsilon$ -pseudospectrum. Existing techniques compute these quantities accurately but the cost is multiple SVDs of order n. We present a novel approach based on computing only the spectral abscissa or radius or a sequence of matrices, generating a monotonic sequence of lower bounds which, in many but not all cases, converges to the pseudospectral abscissa or radius.

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# MS41

## Structured Pseudospectra of Hamiltonian Matrices

We consider the variation of the spectrum of Hamiltonian matrices under Hamiltonian perturbations. The first part of the talk deals with the associated structured pseudospectra. We show how to compute these sets and give some examples. In the second part we discuss the robustness of linear stability. In particular we determine the smallest norm of a perturbation that makes the perturbed Hamiltonian matrix unstable.

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## MS41

### Multiple Eigenvalues with Prespecified Multiplicities and Pseudospectra

Suppose z is a point in the complex plane where two components of the epsln-pseudospectrum of A coalesce. Alam and Bora deduced the existence of matrices within epslnneighborhood of A with z as a multiple eigenvalue. Therefore smallest epsln such that two components of the epslnpseudospectrum coalesce is the distance to the nearest matrix with a multiple eigenvalue. Here we establish the connection between the pseudospectra and nearest matrices with eigenvalues with prespecified algebraic multiplicity.

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## MS41

## Characterization and Construction of the Nearest Defective Matrix via Coalescence of Pseudospectra

Let w(A) be the distance from A to the set of defective matrices. and let c(A) be the supremum of all  $\epsilon$  for which the pseudospectrum of A has n distinct components. It is known that  $w(A) \ge c(A)$ , with equality holding for the 2-norm. We show that w(A) = c(A) for the Frobenius norm too, and that the minimal distance is attained by a defective matrix in all cases. The results depend on the geometry of the pseudospectrum near points where coalescence of the components occurs.

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## MS42

# Hessenberg Quasiseparable Matrices and Polynomials

The classification of tridiagonal matrices in terms of polynomials orthogonal on a real interval, as well as the classification of unitary Hessenberg matrices in terms of Szegö polynomials (orthogonal on the unit circle) are well–known results, and form the basis for many fast algorithms involving these classes. In this talk, we give complete classifications of matrices having Hessenberg–quasiseparable structure in terms of the polynomials related in the same way as the above examples. Several subclasses are also classified, including Hessenberg–semiseparable matrices, and the motivating special cases of tridiagonal and unitary Hessenberg matrices.

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## MS42

## Characteristic Polynomials, Eigenvalues and Eigenspaces of Quasiseparable of Order One Matrices

We discuss spectral properties of quasiseparable of order one matrices. This class of matrices contains at least three well-known classes: diagonal plus semiseparable matrices, tridiagonal matrices, unitary Hessenberg matrices. We derive different recurrence relations for characteristic polynomials of principal leading submatrices of a quasiseparable matrix. Some basic algorithms to compute eigenvalues are presented. We obtain conditions when an eigenvalue of a quasiseparable matrix is simple. For the case of a multiple eigenvalue the structure of the corresponding eigenspace is described. Illustrative examples are presented.

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# MS42

## A Fast Euclidean Algorithm for Quasiseparable Polynomials via Non-casual Factorizations

We have elaborated that there exist a one to one correspondence of Classical Euclid algorithm with GKO, HO and OS algorithms when we express the Euclid algorithm in one way of the matrix form. It is noticeable that Bezoutian plays a major role in here by preserving different displacement structures according to the above three algorithms. All these result drive us to design a fast Euclid algorithm for polynomial represent in general bases and the result can be specialized for cases of Quasiseparable, Orthogonal and Szego polynomials.

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# MS42

# Parameterization and Stability of Methods for Quasiseparable Matrices

For the standard parameterization of a quasiseparable matrix, a small perturbation of the parameters ( i.e. small structured error) do not correspond to a small perturbation of the matrix (i.e. small normwise error). As a consequence, when working with a quasiseparable matrix, some additional stability assumption on the parameters is required to guarantee normwise backward stability. This talk describes alternate parameterizations based on plane rotations for which small structured error implies small normwise error.

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## MS43

## A More Efficient Version of the Lucas-Kanade Template Tracking Algorithm Using the Ulv Decomposition

Template tracking refers to the problem of tracking an object through a video sequence using a template. The template is the image of the tracked object, usually extracted from the first frame. The aspect of template tracking that we are interested in, is the problem of updating the template. Template updates are necessary, especially in long video sequences, because the appearance of the object changes significantly and the initial template is soon obsolete. In this work we suggest improvements, in a computational sense, to the template update algorithm proposed by Matthew et. al (The Template Update Problem). The update strategy proposed in Matthew et. al. requires computation of the principal components of the augmented image matrix at every iteration, since the PCs correspond to the left singular vectors of image matrix, we suggest using URV updates as an alternative to computing PCs *ab initio* at every iteration.

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## MS43

# Analysis of Model Uncertainty Using Optimization Iterates

Throughout the course of an optimization run, multiple points are generated and evaluated. In this talk, we will describe how this data can be used to evaluate parameter sensitivities and uncertainties while providing additional insight into the model. We will also describe how the optimization iterate set can be supplemented to provide more statistically significant results and how these results might be computed during the course of the optimization to improve the search results.

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## MS43

## Multisplitting for Regularized Least Squares: A Multiple Right Hand Side Problem for Image Restoration and Reconstruction

Least squares problems are one of the most often used numerical formulations n engineering. Many such problems lead to ill-posed systems of equations for which a solution may be found by introducing regularization. Here we extend the use of multisplitting least squares, as originally introduced by Renaut (1998) for well-posed least squares problems, to Tikhonov regularized large scale least squares problems. Regularization at both the global and subproblem level is considered, hence providing a means for multiple parameter regularization of large scale problems. We find out that in solving the local splitting, each local problem turn out to be a linear system with multiple right hand sides with updates. Utilizing the characteristics of the problem itself enables us to apply more efficient algorithm to obtain the solution. Basic convergence results follow immediately from the original formulation. Numerical validation is presented for some simple one dimensional signal restoration simulations.

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# MS43

# Accelerating the EM Algorithm

The EM algorithm is widely used for numerically approximating maximum-likelihood estimates in the context of missing information. This talk will focus on the EM algorithm applied to estimating unknown parameters in a (finite) mixture density, i.e., a probability density function (PDF) associated with a statistical population that is a mixture of subpopulations, using "unlabeled" observations on the mixture. In the particular case when the subpopulation PDFs are from common parametric families, the EM algorithm becomes a fixed-point iteration that has a number of appealing properties. However, the convergence of the iterates is only linear and may be unacceptably slow if the subpopulations in the mixture are not "well-separated" in a certain sense. In this talk, we will review the EM algorithm for mixture densities, discuss a certain method for accelerating convergence of the iterates, and report on numerical experiments.

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## MS44

# Development and History of Sparse Direct Methods

Direct methods for the solution of large sparse systems were used by the linear programming community from the 1950s but it was not until the 1960s that they were applied to a wider range of applications including the solution of stiff ODEs and power systems. We sketch these early origins and highlight the key points in the development of sparse direct techniques and software. We also examine the history of the direct v iterative debate and its current resolution.

<u>Iain Duff</u>

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# MS44

# Some History of Conjugate Gradients and Other Krylov Subspace Methods

In the late 1940's and early 1950's, newly available computing machines generated intense interest in solving "large' systems of linear equations. Among the algorithms developed were several related methods, all of which generated bases for Krylov subspaces and used the bases to minimize or orthogonally project a measure of error. The best known of these algorithms is conjugate gradients. We discuss the origins of these algorithms, emphasizing research themes that continue to have central importance.

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## MS44

#### Antecedents of the LR and QR Algorithms

The seminal idea in LR and QR is the reversal of factors to form a new matrix. In 1882 Darboux introduced a transform that takes a 2nd order linear operator (ODE) and writes it as the composition of two 1st order linear operators PQ and forms a new 2nd order operator QP as the desired transform. If you discretize properly you get an instance of the basic LR transform applied to a tridiagonal matrix. In the 20th century a few physicists (Weyl,Schroedinger, Infeld) applied the transform to obtain eigenfunctions for operators that occur in applications. In that work the transform was applied a small number of times, the goal was not to find eigenvalues, and shifts, though present, were incidental and not a tool to accelerate convergence.

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### MS44

## The Dual Flow Between Linear Algebra and Optimization

Optimization and linear algebra have been closely connected for more than 60 years, ever since Courant's 1943 introduction of the quadratic penalty function and Dantzig's 1947 creation of the simplex method for linear programming. A multitude of linear algebraic subproblems appear in optimization methods, which often impose special structure on the associated matrices. This talk will highlight a selection of symmetrically productive ties between linear algebra and optimization, ranging from classical to ultramodern.

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# MS45

## **Regularizing Iterations for ODF Reconstruction**

We use regularizing iterations to reconstruct local crystallographic orientations from X-ray diffraction measurements, and we demonstrate that right preconditioning is necessary to provide satisfactory reconstructions. Our right preconditioner is not a traditional one that accelerates convergence; its purpose is to modify the smoothness properties of the reconstruction. We also show that a new stopping criterion, based on the information available in the residual vector, provides a robust choice of the number of iterations.

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# MS45

# A Generalized Hybrid Regularization Approach for Partial Fourier MRI Reconstruction

Accelerated MR imaging techniques require regularization to ensure robust solutions which must be computed efficiently in a manner consistent with the speed of data acquisition. One difficulty is the efficient determination of one or more regularization parameters. We develop a generalization of the LSQR-Hybrid approach for the partial-Fourier reconstruction problem that allows us to efficiently select two parameters via information generated during various runs of the LSQR-Hybrid algorithm. Phantom and in-vivo results will be presented.

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# MS45

# Golub-Kahan Hybrid Regularization in Image Processing

Ill-posed problems arise in many image processing applications, including microscopy, medicine and astronomy. Iterative methods are typically recommended for these large scale problems, but they can be difficult to use in practice. Lanczos based hybrid methods have been proposed to slow the introduction of noise in the iterates. In this talk we discuss the behavior of Lanczos based hybrid methods for large scale problems in image processing.

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## MS45

# Golub-Kahan Iterative Bidiagonalization and Revealing Noise in the Data

Consider an ill-posed problem with a noisy right-hand side (observation vector), where the size of the (white) noise is unknown. We show how the information from the Golub-Kahan iterative bidiagonalization can be used for revealing the unknown level of the noise. Such information can be useful in construction of stopping criteria in solving large ill-posed problems.

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## MS46

## Randomized Algorithms in Linear Algebra: From Approximating the Singular Value Decomposition to Solving Regression Problems

The introduction of randomization in the design and analysis of algorithms for matrix computations (such as matrix multiplication, least-squares regression, the Singular Value Decomposition (SVD), etc.) over the last decade provided a new paradigm and a complementary perspective to traditional numerical linear algebra approaches. These novel approaches were motivated by technological developments in many areas of scientific research that permit the automatic generation of large data sets, which are often modeled as matrices. In this talk we will outline how such approaches can be used to approximate problems ranging from matrix multiplication and the Singular Value Decomposition (SVD) of matrices to approximately solving least-squares problems and systems of linear equations.

## Petros Drineas

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### MS46

# Fast Factorization Of Low-Rank Matrices via Randomized Sampling

The talk will describe a set of techniques based on randomized sampling that dramatically accelerate several key matrix computations, including many needed for solving partial differential equations and for extracting information from large data-sets (such as those arising from genomics, the link structure of the World Wide Web, etc). The algorithms are applicable to any matrix that can in principle be approximated by a low-rank matrix, are as accurate as deterministic methods, and are for practical purposes 100% reliable (the risk of "failure" can easily be rendered less than e.g. 1e - 12). Several numerical examples will be presented in which the randomized methods are applied to solve problems arising in potential theory, acoustic scattering, image processing, and other application areas.

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# MS46

## The Design and Analysis of Randomized Algorithms for High-dimensional Data: New Insights from Multilinear Algebra and Statistics

In recent years, the spectral analysis of appropriately defined kernels has emerged as a principled way to extract the low-dimensional structure often prevalent in highdimensional data. From selecting so-called landmark training examples in supervised machine learning, to solving large least-squares problems from classical statistics, randomized algorithms provide an appealing means of dimensionality reduction, helping to overcome the computational limitations currently faced by practitioners with massive datasets. In this talk we describe how new insights from multilinear algebra and statistics can be brought to bear on the design and analysis of such algorithms, in order to provide intuitive insight as well as concise formalisms. We discuss in particular the role of determinants and compound matrices as it arises in a variety of recent settings of interest to the theoretical computer science community, and illustrate the practical implications of our results by way of example applications drawn from signal and image processing. (Joint work with Mohamed-Ali Belabbas and other SISL members.)

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# MS47

# Tournaments, Landau's Theorem, Rado's Theorem, and Partial Tournaments

Landau's classical theorem gives necessary and sufficient conditions for the existence of a tournament with a prescribed score sequence. The theorem has been strengthened to give the existence of a tournament with special properties. Rado's theorem gives necessary and sufficient conditions for the existence of an independent transversal of a family of subsets of a set on which a matroid is defined. Rado's theorem can be used to give a nice proof of Landau's theorem, indeed to give conditions for a partial tournament to be completed to a tournament with a prescribed score sequence. In this talk, we shall discuss these topics.

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# MS47 Hadamard Diagonalizable Graphs

The general question of interest is to characterize the undirected graphs G such that the Laplacian matrix associated with G can be diagonalized by some Hadamard matrix. During this presentation, I will survey many interesting and fundamental properties about these graphs along with a partial characterization of the cographs that can be diagonalized by a Hadamard matrix.

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# MS47

# Near Threshold Graphs

A conjecture of Grone and Merris states that for any graph G, its Laplacian spectrum,  $\Lambda(G)$ , is majorized by its conjugate degree sequence,  $D^*(G)$ . That conjecture prompts an investigation of the relationship between  $\Lambda(G)$  and  $D^*(G)$ , and Merris has characterized the graphs G for which the multisets  $\Lambda(G)$  and  $D^*(G)$  are equal. In this talk, we provide a constructive characterization of the graphs G for which  $\Lambda(G)$  and  $D^*(G)$  share all but two elements.

Steve Kirkland

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# **MS47**

## Scrambling Index of Primitive Matrices

The scrambling index of a primitive matrix A is the smallest positive integer k such that  $A^k(A^t)^k = J$ , where  $A^t$  denotes the transpose of A and J denotes all-ones matrix. We prove two upper bounds on the scrambling index of primitive matrices. The first bound is in terms of Boolean rank, and the second bound is in terms of the diameter and girth of the adjacency matrix of A.

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# MS48

# Fixed Points Theorems for Nonnegative Tensors and Newton Methods

We discuss two theorems for nonnegative nonsymmetric tensors. First, the existence of a unique positive singular value and the corresponding singular vectors. Second, the rescaling of nonnegative tensors to balanced tensors, i.e. the tensor version of Sinkhorn's diagonal scaling to doubly stochastic matrices. In both cases the values of these solutions can be found efficiently by using the fix point theorem. We then discuss the Newton method to speed up the computations for these fixed points.

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### MS48

# Trust-region Method for the Best Multilinear Rank Approximation of Tensors

We work on reliable and efficient algorithms for the best low multilinear rank approximation of higher-order tensors. This approximation is used for dimensionality reduction and signal subspace estimation. In this talk, we express it as the solution of a minimization problem on a quotient manifold. Applying the Riemannian trust-region scheme with the truncated conjugate gradient method for the trust-region subproblems, superlinear convergence is achieved. We comment on the advantages of the algorithm, discuss the issue of local optima and show some applications.

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## MS48

### Multi-multilinear Methods: Computing with Sums of Products of Sums of Products

Representing a multivariate function as a sum of products of one-variable functions bypasses the curse of dimensionality. However, for the wavefunction of a quantummechanical system consisting of K non-interacting subsystems, one can show that the number of terms needed grows exponentially in K. A representation with sums of products of sums of products can handle this case, and potentially provide a size-consistent representation for general systems.

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# MS48

## Effective Ranks of Tensors and New Decompositions in Higher Dimensions

Decompositions and approximations of d-dimensional tensors are crucial either in structure recovery problems and merely for a compact representation of tensors. However, the well-known decompositions have serious drawbacks: the Tucker decompositions suffer from exponential dependence on the dimensionality d while fixed-rank canonical approximations are not stable. In this talk we present new decompositions that are stable and have the same number of representation parameters as canonical decompositions for the same tensor. Moreover, the new format possesses nice stability properties of the SVD (as opposed to the canonical format) and is convenient for basic operations with tensors (see: I.V.Oseledets and E.E.Tyrtyshnikov, Breaking the curse od dimensionality, or how to use SVD in many dimensions, Research Report 09-03, Kowloon Tong, Hong Kong: ICM HKBU, 2009 (www.math.hkbu.edu.hk/ICM/pdf/09-03.pdf). Last not the least, the new decomposition provides a useful method (comparable and even superior to wavelets) for compression of low-dimensional data.

## Eugene Tyrtyshnikov

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# **MS49**

Numerical Computation with Semiseparable Matrices: Distributed Algorithms for Quantum Transport with Atomistic Basis Sets (with Ragu Balakrishnan)

Two of the most demanding computational problems in quantum transport analysis involve mathematical operations with semiseparable matrices. First, we consider determining the diagonal of a semiseparable matrix that is the inverse of a block-tridiagonal matrix. The second operation corresponds to computing matrix products involving semiseparable matrices. We present a parallel inversion algorithm for block-tridiagonal matrices as well as distributed approaches for computing matrix products based upon an underlying compact representation for the semiseparable matrices.

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## MS49

### Semiseparable Matrices and Fast Transforms for Orthogonal Polynomials and Associated Functions

A new connection between classical orthogonal polynomials or the corresponding associated functions and semiseparable matrices will be developed. It will be shown how this can be exploited to obtain fast FFT-like algorithms for these functions. The results will be demonstrated with two recent methods to compute discrete Fourier transforms on the sphere  $\mathbf{S}^2$  and on the rotation group SO(3).

#### Jens Keiner

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## **MS49**

## **Hierarchical Matrix Preconditioners**

Hierarchical ( $\mathcal{H}$ -) matrices provide a powerful technique to compute and store approximations to dense matrices in a data-sparse format. The basic idea is the appoximation of matrix data in hierarchically structured subblocks by low rank representations. The usual matrix operations can be computed approximately with almost linear complexity. We use such an h-arithmetic to set up preconditioners for the iterative solution of sparse linear systems as they arise in the finite element discretization of PDEs.

<u>Sabine Le Borne</u> Tennessee Technological University Department of Mathematics SLeborne@tntech.edu

## MS49

# Root-finding, Structured Matrices and Additive Preprocessing

The classical problem of polynomial root-finding was recently attacked highly successfully based on effective algorithms for approximation of eigenvalues of rank structured matrices. We advance this approach with some techniques that employ the displacement structure of the associated matrices and their additive preprocessing.

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## MS50

# Hybrid Techniques in the Solution of Large Scale Problems

The most challenging problems for numerical linear algebra arguably arise from the discretization of partial differential equations from three-dimensional modelling. Often these problems are intractable to either direct methods (because of fill-in) and direct methods (because of non-convergence). In this talk we will review some recent work by researchers at CERFACS and ENSEEIHT on the combined use of direct and iterative methods for solving very large linear systems of equations arising in three-dimensional modelling.

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# MS50

# The Impact of Adaptive Solver Libraries on Future Many-cores

Solving linear systems takes many forms. Matrix properties (numerical and physical) and computational properties (program and architecture) affect performance delivered. The number of combinations is huge and growing over time. Adaptive libraries are essential to provide rational paths through this thicket no individual can grasp the optimization issues. A parameter-space exhaustively-trained selection system can make fast run-time selections for users. We describe an adaptive Spike-Pardiso (PSpike) combination poly-algorithm providing excellent performance compared to other direct and iterative solvers.

David Kuck Intel Parallel and Distributed Solutions Division david.kuck@intel.com

# $\mathbf{MS50}$

# On the PSPIKE Parallel Sparse Linear System Solver

The availability of large-scale computing platforms comprised of thousands of multicore processors motivates the need for highly scalable sparse linear system solvers for symmetric indefinite matrices. The solvers must optimize parallel performance, processor performance, as well as memory requirements, while being robust across broad classes of applications. We will present a new parallel solver that combines the desirable characteristics of direct methods (robustness) and iterative solvers (computational cost), while alleviating their drawbacks (memory requirements, lack of robustness).

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#### MS51

# A Parallel Version of GPBiCR Method Suitable for Distributed Parallel Computing

Abstract not available at time of publication.

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# MS51

# Structure Exploited Algorithms for Nonsymmetric Algebraic Riccati Equation Arising in Transport Theory

The nonsymmetric algebraic Riccati equation arising in transport theory is a special algebraic Riccati equation whose coefficient matrices having some special structures. By reformulating the Riccati equation, they were found that its arbitrary solution matrix is of a Cauchy-like form and the solution matrix can be computed from a vector form Riccati equation instead of the matrix form that. In this talk, we review some classical-type and Newton-type iterative methods for solving the vector form Riccati equation and present some work under investigation .

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## MS51

# On Hybrid Preconditioning Methods for Large Sparse Saddle-Point Problems

Based on the block triangular product approximation to an energy matrix, a class of hybrid preconditioning methods is designed for accelerating the MINRES method for solving the saddle point problems. The quasi-optimal values for the parameters involved in the new preconditioners are estimated, so that the numerical conditioning and the spectral property of the saddle-point matrix of the linear system can be substantially improved. Several practical hybrid preconditioners and the corresponding preconditioning iterative methods are constructed and studied, too.

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# MS51

# A Symmetric Homotopy and Hybrid Method for Solving Mixed Trigonometric Polynomial Systems

Abstract not available at time of publication.

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## MS52

## Subset Selection: Deterministic vs. Randomized

Subset selection methods try identify those columns of a matrix that are "most" linearly independent. Many deterministic subset selection methods are based on a QR decomposition with column pivoting. In contrast, randomized methods consist of two stages, where the first stage samples a smaller set of columns according to a probability distribution, and the second stage performs subset selection on these columns. We analyze and compare the performance of deterministic and randomized methods for subset selection.

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## MS52

## Randomized Algorithms for Matrices and Large-Scale Data Applications

Randomization can be a powerful resource in the design of algorithms for linear algebra problems. Although much of this work has roots in convex analysis and theoretical computer science, and thus has relied on techniques very different than those traditionally used in numerical linear algebra, recent research has begun to "bridge the gap" between the numerical linear algebra and theoretical computer science perspectives on these matrix problems. This has led to practical numerical implementations of algorithms for very traditional matrix problems arising in scientific computing and numerical linear algebra, and it has led to novel algorithms for new matrix problems arising in large-scale scientific and Internet data applications. Several examples of this paradigm will be described.

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## MS52

## A Near-optimal Performance Analysis for Randomized Matrix Approximation

Simple randomized algorithms are exceptionally efficient at identifying the numerical range of a matrix, which is a basic building block for constructing approximations of large matrices. This talk describes a unified analysis of the most common algorithms. The argument decouples the linear algebra from the probability, which permits the application of powerful results from random matrix theory. The new methods lead to sharper and more transparent conclusions than previous analyses.

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## MS53

## Stochastic Binormalization of Symmetric Matrices

A symmetric matrix A is binormalized if the norm of each row (and column) is the same. Many matrices can be binormalized by symmetric diagonal scaling, and the resulting matrix frequently has a smaller condition number. In 2004, Livne and Golub introduced an algorithm to find such a diagonal scaling matrix D. The algorithm must access the elements of A individually. We first answer three open questions from their paper concerning the existence and uniqueness of a binormalizing D. Then we introduce a stochastic algorithm to find D while accessing A only through matrix-vector products. Finally, we introduce a limited-memory quasi-Newton method that incorporates stochastic binormalization.

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## MS53

# Linear Algebra Issues in SQP Methods for Nonlinear Optimization

We consider some linear algebraic issues associated with the formulation and analysis of sequential quadratic programming (SQP) methods for large-scale nonlinearly constrained optimization. Recent developments in methods for mixed-integer nonlinear programming and optimization subject to differential equation constraints has led to a heightened interest in methods that may be "hot started" from a good approximate solution. In this context we focus on SQP methods that are best able to use "black-box" linear algebra software. Such methods provide an effective way of exploiting recent advances in linear algebra software for multicore and GPU-based computer architectures.

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## MS53

# An Active-set Convex QP Solver Based on Regularized KKT Systems

Implementations of the simplex method depend on "basis repair' to steer around near-singular basis matrices, and KKT-based QP solvers must deal with near-singular KKT systems. However, few sparse-matrix packages have the required rank-revealing features. For convex QP, we explore the idea of avoiding singular KKT systems by applying primal and dual regularization to the QP problem. A simplified single-phase active-set algorithm can then be developed. Warm starts are straightforward from any given active set, and the range of applicable KKT solvers expands. QPBLUR is a prototype QP solver that makes use of the block-LU KKT updates in QPBLU (Hanh Huynh's PhD dissertation, 2008) but employs regularization and the simplified active-set algorithm. The aim is to provide a new QP subproblem solver for SNOPT for problems with many degrees of freedom. Numerical results confirm the robustness of the single-phase regularized QP approach.

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# MS53

## Linear Algebra Computations in Sparse Optimization

"Sparse optimization" is a term often used to describe optimization problem in which we seek an approximate solution that is sparse, in the sense of having relatively few nonzeros in the vector of unknowns. The iterative optimization methods proposed for these problems make use of many tools from numerical linear algebra, including methods for linear equations, least squares, and singular value decompositions. This talk considers several sparse optimization problems of current interest, including compressed sensing and matrix completion, and outlines several algorithms for each problem. The role of linear algebra methods in these algorithms is highlighted, and the talk considers whether alternative techniques may be more effective.

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# $\mathbf{MS54}$

### **Randomized Preprocessing in Tensor Problems**

We develop and analyze the techniques of randomized preprocessing and show both theoretically and experimentally that it facilitates some most fundamental computations in numerical linear algebra such as the solution of general and structured linear systems of equations and matrix eigensolving. In the case of structured inputs the computational improvement is dramatic. The approach seems to be also promising for multi-linear algebraic computations.

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# $\mathbf{MS54}$

## Quasi-Newton-Grassamann and Krylov-type Methods for Tensors Approximation

In this talk we will describe two different methods for computing low multilinear rank approximations of a given tensor. The underlying structure of the tensor approximation problem involves a product of Grassmann manifolds, on which the related objective function is defined on. The first method, explicitly utilizing this fact, is a quasi-Newton algorithm that operates on product of Grassmann manifolds. The quasi-Newton methods are based on BFGS and limited memory BFGS updates. We will give a general description of the algorithms and discuss optimality of the BFGS update on Grassmannians. In the second method, for tensor approximation, we will generalize Krylov methods to tensors. For large and sparse matrix problems Krylov based methods are, in many cases, the only practically useful methods. As sparse tensors occur frequently in information sciences, tensor-Krylov based methods will enable the computation of low rank Tucker models of huge tensors.

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# $\mathbf{MS54}$

## Krylov Subspace Methods for Linear Systems with Kronecker Product Structure

The numerical solution of linear systems with certain Kronecker product structures is considered. Such structures arise, for example, from the finite element discretization of a linear PDE on a d-dimensional hypercube. A standard Krylov subspace method applied to such a linear system suffers from the curse of dimensionality and has a computational cost that grows exponentially with d. The key to breaking the curse is to note that the solution can often be very well approximated by a vector of low tensor rank. We propose and analyse a new class of methods, so called tensor Krylov subspace methods, which exploit this fact and attain a computational cost that grows linearly with d.

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# MS54

### P-factor Analysis for Nonlinear Tensor Mappings

This work presents the main concept and results of the p-regularity theory (also known as p-factor tensor analysis of nonlinear mappings). This approach is based on the construction of a tensor type operator (p-factor operator). The main result of this theory gives a detailed description of the structure of the zero set of an irregular nonlinear mapping F(x). Applications include a new numerical p-factor method for solving essentially nonlinear problems and p-order optimality conditions for nonlinear optimization problems.

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## MS55

## Preconditioners for 3D Modeling Problems Based on Generalized Schur Interpolation

We consider 3D modeling problems that lead to hierarchically multibanded matrices. As prototype example we use the matrix obtained for the Poisson equation on a regular 3D grid with a 27 point stencil. Using lexicographic ordering the matrix obtained is block tridiagonal, whereby each sub-block is again block tridiagonal and each subsub-block is a tridiagonal matrix. In the past no good preconditioner for such (often occurring) matrices has been determined, to the best of our knowledge. We propose a new method based on hierarchical Schur complementation, whereby each Schur complement is approximated by a low complexity representation, this time using an original Schur matrix interpolation method.

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### MS55

# Communication Complexity for Parallel and Sequential Eigenvalue/Singular Value Algorithms

The flops complexity of an algorithm does not always determine how fast the algorithm will run in practice; communication costs associated to algorithms can make a world of difference. Roughly speaking, one must take into account all movement of data between fast memory, where actual computations occur, and slow memory, where the data is stored for later access. Ideally, desirable algorithms minimize all three following key components: flops, bandwidth (proportional to the total number of data words moved), and *latency* (proportional to the total number of messages passed to and from layers of memory). Recently, there has been a lot of work on finding  $O(n^3)$  algorithms which achieve optimal communication costs (see the work of Demmel, Grigori, Hoemmen, and Langou, and also that of Ballard, Demmel, Holtz, and Schwartz). This talk will give a communication-optimizing algorithm (in the big-Oh sense) for computing eigenvalue, generalized eigenvalue, and singular value decompositions. The algorithm is based on an earlier algorithm by Bai, Demmel, and Gu, and it achieves communication optimality by using a randomized rankrevealing decomposition introduced by Demmel, Dumitriu, and Holtz. In addition to being  $O(n^3)$  and big-Oh optimal, this algorithm has the benefit that, with high probability, it is stable. This is joint work with Grey Ballard and James Demmel.

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## $\mathbf{MS55}$

# A Fast Implicit Qr Eigenvalue Algorithm for a Class of Structured Matrices

The talk presents a fast adaptation of the implicit QR eigenvalue algorithm for certain classes of rank structured matrices including companion matrices. This is a joint work with D. Bini, P. Boito, Y. Eidelman and I. Gohberg.

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# $\mathbf{MS55}$

## Signal Flow Graph Approach to Inversion of Quasiseparable Vandermonde Matrices

We use the language of signal flow graph representation of digital filter structures to solve three purely mathematical problems, including fast inversion of certain polynomialVandermonde matrices, deriving an analogue of the Horner and Clenshaw rules for polynomial evaluation in a (H,m)quasiseparable basis, and computation of eigenvectors of (H,m) quasiseparable classes of matrices. While algebraic derivations are possible, using elementary operations (specifically, flow reversal) on signal flow graphs provides a unified derivation, and reveals connections with systems theory.

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