IP1

Fast Approximation of the Stability Radius and the H_∞ Norm for Large-Scale Linear Dynamical Systems

The stability radius and the H_∞ norm are well-known quantities in the robust analysis of linear dynamical systems with output feedback. These two quantities, which are reciprocals of each other in the simplest interesting case, respectively measure how much system uncertainty can be tolerated without losing stability, and how much an input disturbance may be magnified in the output. The standard method for computing them, the Boyd-Balakrishnan-Bruinsma-Steinbuch algorithm from 1990, is globally and quadratically convergent, but its cubic cost per iteration makes it inapplicable to large-scale dynamical systems. We present a new class of efficient methods for approximating the stability radius and the H_∞ norm, based on iterative methods to find rightmost points of spectral value sets, which are generalizations of pseudospectra for modeling the linear fractional matrix transformations that arise naturally in analyzing output feedback. We also discuss a method for approximating the real structured stability radius, which offers additional challenges. Finally, we describe our new public-domain MATLAB toolbox for low-order controller synthesis, HIFOOS (H-infinity fixed-order optimization — sparse). This offers a possible alternative to popular model order reduction techniques by applying fixed-order controller design directly to large-scale dynamical systems. This is joint work with Nicola Guglielmi, Mert Gurbuzbalaban and Tim Mitchell. This speaker is supported in cooperation with the International Linear Algebra Society.

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IP2

Tuned Preconditioners for Inexact Two-Sided Inverse and Rayleigh Quotient Iteration

Computing both right and left eigenvectors of a generalised eigenvalue problem simultaneously is of interest in several important applications. We provide convergence results for inexact two-sided inverse and Rayleigh quotient iteration, which extend the previously established theory to the generalized non-Hermitian eigenproblem and inexact solves with a decreasing solve tolerance. Moreover, we consider the simultaneous solution of the forward and adjoint problem arising in two-sided methods and extend the successful tuning strategy for preconditioners to two-sided methods, creating a novel way of preconditioning two-sided algorithms. This is joint work with Patrick Kuerschner (MPI Magdeburg, Germany).

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IP3

Sketching-Based Matrix Computations for Large-Scale Data Analysis

Matrix computations lies at the core of a broad range of methods in data analysis and machine learning, and certain numerical linear algebra primitives (e.g. linear least-squares regression and principal component analysis) are widely and routinely used. Devising scalable algorithms that enable large scale computation of the aforementioned primitives is crucial for meeting the challenges of Big Data applications. Sketching, which reduces dimensionality through randomization, has recently emerged as a powerful technique for scaling-up these primitives in the presence of massive data, for an extensive class of applications. In this talk, we outline how sketching can be used to accelerate these core computations, and elaborate on the tradeoffs involved in their use. We will also demonstrate the utility of the presented algorithms for data analysis and machine learning applications

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IP4

Point-Spread Function Reconstruction in Ground-Based Astronomy

Because of atmospheric turbulence, images of objects in outer space acquired via ground-based telescopes are usually blurry. One way to estimate the blurring kernel or point spread function (PSF) is to make use of the aberration of wavefronts received at the telescope, i.e., the phase. However only the low-resolution wavefront gradients can be collected by wavefront sensors. In this talk, I will discuss how to use regularization methods to reconstruct high-resolution phase gradients and then use them to recover the phase and the PSF in high accuracy. I will also address related numerical linear algebra issues such as the estimation of the regularization parameter and the solution of the linear systems arising from the model.

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IP5

Accelerating Direct Linear Solvers with Hardware and Algorithmic Advances

Factorization-based algorithms often play a significant role in developing scalable solvers. The higher fidelity simulations and extreme-scale parallel machines present unique challenges for designing new parallel algorithms and software. In this talk, we first present some techniques to enhance sparse factorization algorihtms to exploit the newer heterogeneous node architectures, such as nodes with GPU accelerators or Intel Xeon Phi. Secondly, we present a new class of scalable factorization algorithms that have asymptotically lower complexity in both flops and storage, for which the acceleration power comes form exploiting low-rank submatrices and randomization.

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IP6

Variational Gram Functions: Convex Analysis and Optimization

We propose a class of convex penalty functions, called

"Variational Gram Functions", that can promote pairwise relations, such as orthogonality, among a set of vectors in a vector space. When used as regularizers in convex optimization problems, these functions of a Gram matrix find application in hierarchical classification, multitask learning, and estimation of vectors with disjoint supports, among other applications. We describe a general condition for convexity, which is then used to prove the convexity of a few known functions as well as new ones. We give a characterization of the associated subdifferential and the proximal operator, and discuss efficient optimization algorithms for loss-minimization problems regularized with these penalty functions. Numerical experiments on a hierarchical classification problem are presented, demonstrating the effectiveness of these penalties and the associated optimization algorithms in practice.

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IP7

Combinatorial Matrix Theory and Majorization

Majorization theory provides concepts for comparing mathematical objects according to "how spread out' their elements are. In particular, two n-vectors may be ordered by comparing the partial sums of the k largest components for $k \leq n$. This is a fruitful concept in many areas of mathematics and its applications, e.g., in matrix theory, combinatorics, probability theory, mathematical finance and physics. In this talk we discuss some combinatorial problems for classes of matrices where majorization plays a role. This includes $(0,1)$-matrices with line sum and pattern constraints, doubly stochastic matrices and Laplacian matrices of graphs. An extension of majorization to partially ordered sets is presented. We also discuss a problem motivated by mathematical finance which leads to interesting questions in qualitative matrix theory. This speaker is supported in cooperation with the International Linear Algebra Society.

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IP8

Numerical Solution of Eigenvalue Problems Arising in the Analysis of Disc Brake Squeal

We present adaptive numerical methods for the solution of parametric eigenvalue problems arsing from the discretization of partial differential equations modeling disc brake squeal. The eigenvectors are used for model reduction to achieve a low order model that can be used for optimization and control. The model reduction method is a variation of the proper orthogonal decomposition method. Several important challenges arise, some of which can be traced back to the finite element modeling stage. Compared to the current industrial standard our new approach is more accurate in vibration prediction and achieves a better reduction in model size. This comes at the price of an increased computational cost, but it still gives useful results when the traditional method fails to do so. We illustrate the results with several numerical experiments, some from real industrial models and indicate where improvements of the current black box industrial codes are advisable. We then also discuss the use of adaptive methods such as the adaptive finite element model and the algebraic multilevel substructering method for the discussed problem, and we point out the challenges and deficiencies in these approaches.

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IP9

Linear Algebra Computations for Parameterized Partial Differential Equations

The numerical solution of partial differential equations (PDEs) often entails the solution of large linear systems of equations. This compute-intensive task becomes more challenging when components of the problem such as coefficients of the PDE depend on parameters that are uncertain or variable. In this scenario, there there is a need to compute many solutions for a single simulation, and for accurate discretizations, costs may be prohibitive. We discuss new computational algorithms designed to improve efficiency in this setting, with emphasis on new algorithms to handle stochastic problems and new approaches for reduced-order models.

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IP10

Accurate Linear Algebra in Computational Methods for System and Control Theory

We discuss the importance of robust and accurate implementation of core numerical linear algebra procedures in computational methods for system and control theory. In particular, we stress the importance of error and perturbation analysis that identifies relevant condition numbers and guides computation with noisy data, and careful software implementation. The themes used as case studies include rational matrix valued least squares fitting (e.g. least squares fit to frequency response measurements of an LTI system), model order reduction issues (e.g. the Discrete Empirical Interpolation Method (DEIM)), accurate computation with structured matrices such as scaled Cauchy, Vandermonde and Hankel matrices.

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IP11

Low Rank Decompositions of Tensors and Matrices: Theory, Applications, Perspectives

Numerical data are frequently organized as d-dimensional matrices, also called tensors. However, only small values of d are allowed since the computer memory is limited. In the case of many dimensions, special representation formats are crucial, e.g. so called tensor decompositions. Recently, the known tensor decompositions have been considerably revisited and the two of them, previously used only in theoretical physics, are now recognized as the most adequate and useful tools for numerical analysis. These two are the Tensor-Train and Hierarchical-Tucker decompositions. Both are intrinsically related with low-rank matrices associated with a given tensor. We present these

decompositions and the role of low-rank matrices for the construction of efficient numerical algorithms.

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IP12

Constrained Low Rank Approximations for Scalable Data Analytics

Constrained low rank approximations have been widely utilized in large-scale data analytics where the applications reach far beyond the classical areas of scientific computing. We discuss some fundamental properties of nonnegative matrix factorization (NMF) and introduce some of its variants for clustering, topic discovery in text analysis, and community detection in social network analysis. In particular, we show how a simple rank 2 NMF combined with a divide-and-conquer framework results in a simple yet significantly more effective and scalable method for topic discovery. This simple approach can be further generalized for graph clustering and community detection. Substantial experimental results illustrate significant improvements both in computational time as well as quality of solutions obtained.

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SP1

SIAG/Linear Algebra Prize Lecture - Localizing Nonlinear Eigenvalues: Theory and Applications

Vibrations are everywhere, and so are the eigenvalues that describe them. Physical models that include involve damping, delay, or radiation often lead to nonlinear eigenvalue problems, in which we seek complex values for which an (analytic) matrix-valued function is singular. In this talk, we show how to generalize eigenvalue localization results, such as Gershgorin's theorem, Bauer-Fike, and pseudospectral theorems, to the nonlinear case. We demonstrate the usefulness of our results on examples from delay differential equations and quantum resonances.

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CP1

An Augmented Hybrid Method for Large Scale Inverse Problems

In this work we use the weighted-GCV hybrid method of Chung/Nagy/Oleary for solving ill-posed inverse problems. This method restricts the solution to a Krylov subspace and then uses regularization techniques on the projected problem in order to stop the typical semiconvergence behavior of iterative methods. Difficulties arise for large problems where we are required to store the full Krylov space. We have developed a technique to compress the space using harmonic Ritz vectors. Computational examples are provided.

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CP1

On a Nonlinear Inverse Problem in Electromagnetic Sounding

Electromagnetic induction measurements are often used for non-destructive investigation of certain soil properties, which are affected by the electromagnetic features of the subsurface layers. Starting from electromagnetic data collected by a ground conductivity meter, we propose a regularized inversion method based on a low-rank approximation of the Jacobian of the nonlinear model. The method depends upon a relaxation parameter and a regularization parameter, both chosen by automatic procedures. The performance of the method is investigated by numerical experiments both on synthetic and experimental data sets.

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CP1

Localized-Deim: An Overlapping Cluster Framework with Application in Model Reduction for Nonlinear Inversion

A numerically efficient application of parametric model reduction critically depends on affine parametrization of the full-order state-space quantities so that the online projection step does not depend on the dimension of full model. Discrete Empirical Interpolation Method (DEIM) is commonly used to construct such affine approximations. In this talk, we propose overlapping clustering methods to improve the approximation power of local DEIM and investigate efficient implementations of the underlying greedy selection procedure. A nonlinear parametric inversion example arising in diffuse optical tomography is used to illustrate the approach.

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CP1

Matrix Affine Transformation Algorithm for Rank-Reducing Image Data Informatics Process

Matrix affine transformation T=QR+C is used in a way of maximizing informatics content in orthogonal QR process. Sample matrices were taken from images of quadrant pixel-shift patches across evenly spaced 128x128 grid points. Our

proposed algorithm cures the ill-posedness in the matrix inversion. By retrieving a specific rank-one pattern from a correction matrix C, we can enrich the principal QR factorization. We tested the optimal matrix-rank-reducing process particularly with the SVD analysis.

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CP1

Efficiencies in Global Basis Approximation for Model Order Reduction in Diffuse Optical Tomography

We consider the nonlinear inverse problem of reconstructing parametric images of optical properties from diffuse optical tomographic data. Recent work shows MOR techniques have promise in mitigating the computational bottleneck associated with solving for the parameters. In this talk, we give an algorithm for efficiently computing the approximate global basis needed in MOR by utilizing a new interpretation of the transfer function and by capitalizing on Krylov recycling in a novel way.

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CP1

Robust Multi-Instance Regression

Multi-instance regression consists in building a regression model that maps sets of instances (bags) to real-valued outputs. The Primary-Instance Regression (PIR) method assumes that there is some primary instance (unknown during training) which is responsible for the real valued label and that the rest of the items in the bag are noisy observations of the primary instance. To immunize the primary instance selection to noise, we propose an hyperplane fitting procedure which exploits the algebraic equivalence between regularization (technique to prevent overfitting) and robustness (technique to immunize against set-induced uncertainty) and finds regularizers without requiring cross validation.

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CP2

Iterative Refinement for Symmetric Eigenvalue Decomposition and Singular Value Decomposition

An efficient iterative refinement algorithm is proposed for symmetric eigenvalue problems. The algorithm is simple, and it mainly consists of matrix multiplications. It constructs an arbitrarily accurate eigenvalue decomposition, up to the limit of computational precision. Using similar techniques, an iterative refinement algorithm for the singular value decomposition is also derived. Since the proposed algorithms are based on Newton's method, they converge quadratically. Numerical results demonstrate the excellent performance of the proposed algorithm.

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CP2

Some Inverse Numerical Range Problems

We generalize the inverse field of values problem to the q-numerical range and the rank-k numerical range of a matrix. We propose an algorithm for solving the inverse q-numerical range problem. Our algorithms exploits the convexity of the q-numerical range. Approximating the boundary of the q-numerical requires constructing approximation of the Davis-Weilandt shell of a matrix. We note some connections to computing pseudospectra. For the rank-k numerical range, we have found a particular generalized eigenvalue problem whose solution facilitates constructing subspaces for generating points in the rank-k numerical range of a matrix, and also addresses the question of covering numbers for points in the rank-k numerical range. The results in this work could have applications in computing eigenvalues as well as quantum computing.

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CP2

An Algorithm for Finding a 2-Similarity Transformation from a Numerical Contraction to a Con-

traction

Any matrix A with numerical radius at most 1 can be written as $A = STS^{-1}$, where $\|T\| \leq 1$ and $\|S\| \cdot \|S^{-1}\| \leq 2$. However, no explicit algorithm was given for producing such a similarity transformation. In this paper, we give a method for constructing such similarity transformations. As a side benefit, the algorithm indicates if the numerical radius of A is greater than than some given number and so can be used to determine if the numerical radius is greater than a given value.

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CP2

The Markovian Joint Spectral Radius: What It Is and How to Compute It Efficiently

Given a finite set of matrices $\mathcal{F} = \{A_i\}_{i=1}^N$, with $A_i \in \mathbb{C}^{d \times d}$, the Joint Spectral Radius (JSR) of $\mathcal{F}$ is given by the generalization of the Gelfand's formula for the spectral radius of a matrix. In recent works it has been proved that the JSR can be computed exactly, under suitable and general conditions, using polytope norms. In some cases, however, not all the products are allowed, because the matrices in $\mathcal{F}$ are multiplied each other following some Markovian law. Recently Kozyakin showed in [1] that it is still possibile to compute Joint Spectral Radius in the Markovian case as the classical JSR of a significantly higher dimensional set of matrices $\widehat{\mathcal{F}} = \left\{\widehat{A}_i\right\}_{i=1}^N$, with $\widehat{A}_i \in \mathbb{C}^{Nd \times Nd}$. This implies that the exact evaluation of the Markovian JSR can be achieved in general using a polytope norm in $\mathbb{C}^{Nd}$, which is a challenge task if N is large. In this talk we address the question whether it is possible to reduce the computational complexity for the calculation of the Markovian JSR showing that it is possible to transform the problem into the evaluation of N polytope norms in $\mathbb{C}^d$. This approach is strictly related with the idea of multinorms introduced by Jungers and Philippe for discrete–time linear constrained switching systems [2]. As an illustrative application we shall consider the zero–stability of variable stepsize 3–step BDF formulas.

[1] V. Kozyakin. The Berger–Wang formula for the Markovian joint spectral radius. Linear Algebra and its Applications. 448 (2014), 315–328. [2] M. Philippe and R. Jungers. Converse Lyapunov theorems for discrete-time linear switching systems with regular switching sequences. (2014) arXiv preprint arXiv:1410.7197.

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CP2

Two-Level Orthogonal Arnoldi Method for Large Rational Eigenvalue Problems

We propose a two-level orthogonal Arnoldi method for solving large rational eigenvalue problems (REP), which exploits the structure of the Krylov subspace of a Frobenius-like linearization of the REP. We develop such method by using a different representation of the Krylov vectors, which is much more memory efficient than standard Arnoldi applied on the linearization. In addition, we present numerical examples that show that the accuracy of the new method is comparable to standard Arnoldi.

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CP2

A Communication-Avoiding Arnoldi-Type of the Complex Moment-Based Eigensolver

For solving interior eigenvalue problems, complex moment-based eigensolvers have been actively studied because of their high parallel efficiency. Recently, we proposed the Arnoldi-type complex moment-based eigensolver named the block SS–Arnoldi method. In this talk, we propose an improvement of the block SS–Arnoldi method using a communication-avoiding Arnoldi process (s-step Arnoldi process). We evaluate the performance of the proposed method and compare with other complex moment-based eigensolvers.

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CP3

Block-Smoothers in Multigrid Methods for Structured Matrices

Usually in multigrid methods for structured matrices, like Toeplitz matrices or circulant matrices, as well as in geometric multigrid methods point-smoothers are used. Analysis for structured matrices mostly focusses on simple methods like Richardson, smoothers like multicolor-SOR are not considered. In this talk we assess general block-smoothers, where small blocks are inverted instead of single unknowns. The presented analysis fits in the established analysis framework and results in better converging multigrid methods.

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CP3

Multigrid Preconditioners for Boundary Control of

Elliptic-Constrained Optimal Control Problems

Our goal is to design and analyze efficient multigrid preconditioners for solving boundary control problems for linear-quadratic elliptic-constrained optimal control problems. We have considered Dirichlet and Neumann boundary conditions. Thus far, we have numerically obtained an optimal order preconditioner for the Hessian of the reduced Neumann boundary control problem and suboptimal order preconditioner for the Hessian of the reduced Dirichlet boundary control problem. Currently we are analyzing the behavior of the preconditioner in theory.

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CP3
A Multigrid Solver for the Tight-Binding Hamiltonian of Graphene

Since the Nobel prize has been awarded in 2010 for the isolation of graphene, research on this miraculous 2-dimensional material has flourished. In order to calculate the electronic properties of graphene structures a tight-binding approach can be used. The resulting discrete eigenvalue problem leads to linear systems of equations that are maximally indefinite and possess a Dirac pseudo-spin structure. In this talk we present a spin-preserving geometric multigrid approach for these linear systems and show its scalability with respect to several geometric parameters.

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CP3
Adaptive Algebraic Multigrid for Lattice QCD

In this talk, we present a multigrid approach for systems of linear equations involving the Wilson Dirac operator arising from lattice QCD. It combines components that have already been used separately in lattice QCD, namely the domain decomposition method "Schwarz Alternating Procedure" as a smoother and the aggregation based interpolation. We give results from a series of numerical tests from our parallel MPI-C Code with system sizes of up to 200,000,000 unknowns.

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CP3
Multigrid for Tensor-Structured Problems

We consider linear systems with tensor-structured matrices

$$A = \sum \bigotimes E_j^t.$$

These problems are found in Markov chains or high-dimensional PDEs. Due to this format, the dimension of A grows rapidly. The structure has to be exploited for solving these systems efficiently. To use multigrid for these models we build a method which keeps the structure intact to guarantee computational savings on all grids. We present how to adapt the AMG framework to this setting using tensor truncation.

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CP3
Multigrid Preconditioning for the Overlap Operator in Lattice QCD

One of the most important operators in lattice QCD is given by the Overlap Dirac Operator. Due to bad conditioning solving linear systems with this operator can become rather challenging when approaching physically relevant parameters and lattice spacings. In this talk we present and analyze a novel preconditioning technique that yields significant speedups. Furthermore we take a closer look at the matrix sign function and its evaluation as part of the Overlap Dirac Operator.

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CP4

Devide-and-conquer Method for Symmetric-definite Generalized Eigenvalue Problems of Banded Matrices on Manycore Systems

We have recently proposed a divide-and-conquer method for banded symmetric-definite generalized eigenvalue problems based on the method for tridiagonal ones (Elsner, 1997). The method requires less FLOPs than the conventional methods (e.g. DSBGVD in LAPACK) when the band is narrow and has high parallelism. In this presentation, we describe the implementation of the proposed method for manycore systems and demonstrate the efficiency of our solver.

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CP4

Performance Analysis of the Householder Back-transformation with Asynchronous Collective Communication

Recently, communication avoiding and communication hiding technologies are focused on to accelerate the performance on parallel supercomputer systems. For dense eigenvalue computation, especially Householder back-transformation of eigenvectors, we observed asynchronous collective communication is applicable and some special performance characteristics and deviations via actual numerical experiences, specifically, the peak performance is unevenly distributed. We are going to build a performance model and analyze its response when we change some performance parameters defined in the performance model.

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CP4

Dynamic Parallelization for the Reduction of a Banded Matrix to Tridiagonal Form

In the talk a new dynamic parallelization for the reduction of a band matrix to tridiagonal form is considered. We present some details of implemented optimizations: dynamic parallelization of eigenvectors computations, speculative computations in QR, dynamic parallelization of the reduction of banded matrix to tridiagonal form and how these techniques are combined for achieving high performance.

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CP4

Performance of the Block Jacobi-Davidson Method for the Solution of Large Eigenvalue Problems on Modern Clusters

We investigate a block Jacobi-Davidson method for computing a few exterior eigenpairs of a large sparse matrix. The block method typically requires more matrix-vector and vector-vector operations than the standard algorithm. However, this is more than compensated by the performance gains through better data reusage on modern CPUs, which we demonstrate by detailed performance engineering and numerical experiments. The key ingredients to achieving high performance consist in both kernel optimizations and a careful design of the algorithm that allows using blocked operations in most parts of the computation. We show the performance gains of the block algorithm with our hybrid parallel implementation for a variety of matrices on up to 5 120 CPU cores. A new development we discuss in this context is a highly accurate and efficient block orthogonalization scheme that exploits modern hardware features and mixed precision arithmetic.

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CP4

Performance Comparison of Feast and Primme in Computing Many Eigenvalues in Hermitian Problems

Contour integration methods like FEAST are successfully used to partially solve large eigenproblems arising in Density Functional Theory. These methods are scalable and can show better performance than restarted Krylov solvers in computing many eigenpairs in the interior of the spectrum. Recently we have used polynomial filters with Generalized Davidson (GD) with similar success under limited

memory. In this talk, we compare FEAST with the GD available in PRIMME, solving Hermitian problems from different applications.

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CP4

The Implicit Hari-Zimmermann Algorithm for the Generalized Svd

We developed the implicit Hari–Zimmermann method for computation of the generalized singular values of matrix pairs, where one of the matrices is of full column rank. The method is backward stable, and, if the matrices permit, computes the generalized singular values with small relative errors. Moreover, it is easy to parallelize. Unlike the triangular routine `DTGSJA` from Lapack, the Hari–Zimmermann method needs no preprocessing to make both matrices triangular. Even when the matrices are preprocessed to a triangular form, the sequential pointwise Hari–Zimmermann method is, for matrices of a moderate size, significantly faster than `DTGSJA`. A significant speedup is obtained by blocking of the algorithm, to exploit the efficiency of BLAS-3 operations.

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CP5

Heuristics for Optimizing the Communicability of Digraphs

In this talk we investigate how to modify the edges of a directed network in order to tune its overall broadcasting/receiving capacity. We introduce broadcasting and receiving measures (related to the network's "hubs" and "authorities", respectively) in terms of the entries of appropriate functions of the matrices AA^T and A^TA, respectively, where A is the adjacency matrix of the network. The larger these measures, the better the network is at propagating information along its edges. We also investigate the effect of edge addition, deletion, and rewiring on the overall broadcasting/receiving capacity of a network. In particular, we show how to add edges so as to increase these quantities as much as possible, and how to delete edges so as to decrease them as little as possible.

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CP5

Generalizing Spectral Graph Partitioning to Sparse Tensors

Spectral graph partitioning is a method for clustering data organized as undirected graphs. The method is based on the computation of eigenvectors of the graph Laplacian. In many areas one wants to cluster data from a sequence of graphs. Such data can be organized as large sparse tensors. We present a spectral method for tensor partitioning based on the computation of a best multilinear rank aproximation of the tensor. A few applications are briefly discussed.

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CP5

Graph Partitioning with Spectral Blends

Spectral partitioning uses eigenvectors and eigenvalues to partition graphs. We show that blends of eigenvectors have better pointwise error bounds than the eigenvectors for graphs with small spectral gaps. We use a model problem, the Ring of Cliques, to demonstrate the utility of spectral blends for graph partitioning. This analysis provides a convergence criterion in terms of conductance and the Cheeger inequality.

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CP5

On the Relation Between Modularity and Adjacency Graph Partitioning Methods

Modularity clustering is a popular method in partitioning graphs. In this talk we will present the relation between the leading eigenvector $\mathbf{b}$ of a modularity matrix and the eigenvectors $\mathbf{u}_i$ of its corresponding adjacency matrix. This relation allows us to approximate the vector $\mathbf{b}$ with some of the $\mathbf{u}_i$. The equivalence between normalized versions of modularity clustering and adjacency clustering will also be demonstrated.

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CP5

Detecting Highly Cyclic Structure with Complex Eigenpairs

Highly 3- and 4-cyclic subgraph topologies are detectable via calculation of eigenvectors associated with certain complex eigenvalues of Markov propagators. We characterize this phenomenon theoretically to understand the capabilities and limitations for utilizing eigenvectors in this venture. We provide algorithms for approximating these eigenvectors and give numerical results, both for software that utilizes complex arithmetic and software that is limited to real arithmetic. Additionally, we discuss the application of these techniques to motif detection.

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CP5

Orthogonal Representations, Projective Rank, and Fractional Minimum Positive Semidefinite Rank: Connections and New Directions

This paper introduces r-fold orthogonal representations of graphs and formalizes the understanding of projective rank as fractional orthogonal rank. Fractional minimum positive semidefinite rank is defined and it is shown that the projective rank of any graph equals the fractional minimum positive semidefinite rank of its complement. An r-fold version of the traditional definition of minimum positive semidefinite rank of a graph using Hermitian matrices that fit the graph is also presented.

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CP6

Inverse Eigenvalue Problems for Totally Nonnegative Matrices in Terms of Discrete Integrable Systems

Several discrete integrable systems play key roles in matrix eigenvalue algorithms such as the qd algorithm for symmetric tridiagonal matrices and the dhToda algorithm for Hessenberg TN matrices whose minors are all nonnegative. In this talk, we consider inverse eigenvalue problems for TN matrices including symmetric tridiagonal matrices from the viewpoint of discrete integrable systems associated with matrix eigenvalue algorithms. Moreover, we propose a finite-step construction of TN matrices with prescribed eigenvalues.

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CP6

A Kinetic Ising Model and the Spectra of Some Jacobi Matrices

One-dimensional statistical physics models play a fundamental role in understanding the dynamics of complex systems in a variety of fields, from chemistry and physics, to social sciences, biology, and nanoscience. Due to their simplicity, they are amenable to exact solutions that can lead to generalizations in higher dimensions. In 1963, R. Glauber solved exactly a one-dimensional spin model, known in literature as the kinetic Ising chain, KISC, that led to many applications and two-temperature generalizations. In this talk we consider a case of temperature distributions, extracting information regarding the physical properties of the system from the spectrum analysis of matrix certain Jacobi matrix. We also analyze the eigenvalues of some perturbed Jacobi matrices. The results contain as particular cases the known spectra of several classes of tridiagonal matrices studied recently. This is a join work with S. Kouachi, D.A. Mazilu, and I. Mazilu.

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CP6

The Molecular Eigen-Problem and Applications

Referring to the classical eigenproblem of a matrix as the

atomic eigenproblem, we extend this notion to a *molecular eigenproblem*: Consider the module of matrices $\mathcal{M} = \mathbb{C}^{n\times m}$ with $n \geq m$, over the noncommutative matrix ring $\mathcal{R} = \mathbb{C}^{m\times m}$. The *m-molecular eigen-problem* is the problem of determining $\Lambda \in \mathbb{C}^{m\times m}$ and $X \in \mathbb{C}^{n\times m}$ such that $AX = X\Lambda$. Existence conditions and characterizations of its solution are given. If (X, Λ) is an *m-molecular eigenpair* of A, then so is (XR, Λ), for all $R \in C(\Lambda)$, the *centralizer* of the set of molecular eigenvalues. This freedom may be exploited to define a canonical molecular eigenvector. We apply this generalized formalism to solve matrix-ODE's, and give a lattice theoretic representation of the structure of the solution sets.

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CP6

Spectral Properties of the Boundary Value Problems for the Discrete Beam Equation

In this talk, we will consider the boundary-value problem for the fourth-order discrete beam equation

$$\Delta^4 y_i + b_{i+2} y_{i+2} = \lambda a_{i+2} y_{i+2}, \quad -1 \leq i \leq n-2,$$

$$\Delta^2 y_{-1} = \Delta^3 y_{-1} = \Delta^2 y_{n-1} = \Delta^3 y_{n-1} = 0,$$

which is a discrete analogy to the following boundary-value problem for the fourth-order linear beam equation:

$$y^{(4)}(t)+b(t)y(t) = \lambda a(t)y(t), \quad y'(0) = y'(0) = y'(1) = y'(1) = 0.$$

For the ordinary differential equation boundary-value problem, the monotonicity of the smallest positive eigenvalue was studied in the literature. The special structure of the matrices associated with the discrete problem allows us to analyze the spectral properties of the problem and to establish the monotonicity of all eigenvalues of the discrete problem as the sequences $\{a_i\}_{i=1}^n$ and $\{b_i\}_{i=1}^n$ change.

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CP6

Matrix Nearness Problems for General Lyapunov-Type Stability Domains

In many applications asymptotic instability of the mathematical (dynamical) system leads to the loss of the structural integrity of the real physical system due to the amplification of the perturbations in the initial conditions. However, in some cases, although dynamical system is asymptotically stable, the corresponding physical system can loose its structural integrity due to transitional instability (due to too large amplitude or too high frequency) typical for dynamics governed by nonnormal matrices. To consider such applications, we review general Lyapunov-type domains and formulate two matrix nearness problems - the distance to delocalization and distance to localization to generalize the distance to instability and the distance to stability, in both, discrete and continuous sense. Then, we present numerical algorithms for their solution. Finally, present computations some medium size and large sparse matrices arising in different scientific and industrial applications.

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CP6

A Multigrid Krylov Method for Eigenvalue Problems

We propose a new multigrid Krylov method for eigenvalue problems of differential operators. Arnoldi methods are used on multiple grids. Approximate eigenvectors from a coarse grid can be improved on a fine grid. We compare the new method with other approaches, and we also give analysis of the convergence. This multigrid Arnoldi method is more robust than standard multigrid and has potential for dramatic improvement compared to regular Arnoldi.

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CP7

Block-Asynchronous Jacobi Iterations with Overlapping Domains

Block-asynchronous Jacobi is an iteration method where a locally synchronous iteration is embedded in an asynchronous global iteration. The unknowns are partitioned into small subsets, and while the components within the same subset are iterated in Jacobi fashion, no update order in-between the subsets is enforced. The values of the non-local entries remain constant during the local iterations, which can result in slow inter-subset information propagation and slow convergence. Interpreting of the subsets as subdomains allows to transfer the concept of domain overlap typically enhancing the information propagation to block-asynchronous solvers. In this talk we explore the impact of overlapping domains to convergence and performance of block-asynchronous Jacobi iterations, and present results obtained by running this solver class on state-of-the-art HPC systems.

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CP7

Performance Evaluation of the Choleskyqr2 Algorithm

Cholesky QR computes the QR factorization through the Cholesky factorization. It has excellent suitability for HPC but is rarely practical due to its numerical instability. Recently, we have pointed out that an algorithm that repeats Cholesky QR twice, which we call CholeskyQR2, has much improved stability. In this talk, we present the performance results of CholeskyQR2 and show its practicality. We also discuss its application to the block Gram-Schmidt orthogonalization and the block Householder QR algorithm.

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CP7

High Performance Resolution of Dense Linear Systems Using Compression Techniques and Application to 3D Electromagnetics Problems

Solving large 3-D electromagnetic problems is challenging. Currently, accurate numerical methods are used to solve Maxwells equations in the frequency domain, which leads to solve dense linear systems. Thanks to recent advances on fast direct solvers by the means of compression techniques, we have developed a solver capable of handling systems with millions of complex unknowns and thousands of right hand sides suited for our Petascale machine.

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CP7

Batched Matrix-Matrix Multiplication Operations for Intel® Xeon® Processor and Intel® Xeon Phi™ Co-Processor

Many numerical algorithms such as sparse solvers and finite element method rely on a number of matrix-matrix multiplication operations that can be performed independently. In this talk, we present the new interfaces and implementation details of the batched matrix-matrix multiplication routines in Intel® Math Kernel Library 11.3. Compared to the optimized non-batched counterparts, batched routines provide 8× and 15× speedups on average for Intel® Xeon® processor and Intel® Xeon Phi™ coprocessor respectively.

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CP7

Data Sparse Technique

In this talk we will describe how H-matrix data sparse techniques can be implemented in a parallel hybrid sparse linear solver based on algebraic non overlapping domain decomposition approach. Strong-hierarchical matrix arithmetic and various clustering techniques to approximate the local Schur complements will be investigated, aiming at reducing workload and memory consumption while complying with structures of the local interfaces of the sub-domains. Utilization of these techniques to form effective global preconditioner will be presented.

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CP7

A Newly Proposed BLAS Extension (xGEMMT) to Update a Symmetric Matrix Efficiently

We propose a complement to the Level 3 BLAS xGEMM routine that computes $C := \alpha \times A \times B + \beta \times C$, where C remains symmetric for general A and B matrices. For instance, A may be the product of B^T and a symmetric or diagonal matrix. This new xGEMMT routine provides functionality used in numerous algorithms and within Hessian-based optimization methods. In this talk, we discuss the subtleties of implementing and optimizing xGEMMT in the Intel® Math Kernel Library.

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CP8

Eigenvalue Condition Numbers of Polynomial Eigenvalue Problems under Möbius Transformations

We study the effect of Möbius transformations on the sensitivity of polynomial eigenvalues problems (PEP). More precisely, we compare eigenvalue condition numbers for a PEP and the correspondent eigenvalue condition numbers for the same PEP modified with a Möbius transformation. We bound this relationship with factors that depends on the condition number of the matrix that induces the Möbius transformation and on the eigenvalue whose normwise condition number we consider, and establish sufficient conditions where Möbius transformations do not alter significantly the condition numbers.

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CP8

Computation of All the Eigenpairs for a Particular Kind of Banded Matrix

For a particular kind of banded matrix which is characterized by the band width, we propose a new algorithm for computing all the eigenpairs effectively. Though the intended matrix has complex eigenvalues, our algorithm can compute all the complex eigenpairs only by the arithmetic of real numbers. We also present an error analysis and numerical examples for the proposed algorithm.

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CP8

Fixed-Point Singular Value Decomposition Algorithms with Tight Analytical Bounds

This work presents an analytical approach for finding the ranges of the variables in fixed-point singular value decomposition algorithm based on upper bound for the spectral norm of input matrix. We show that if each element of a matrix is divided by the upper bound for spectral norm, then unvarying and tight ranges for the variables in the algorithm are obtained. Thus overflow is avoided for all range of input matrices with reduced hardware cost.

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CP8

A Novel Numerical Algorithm for Triangularizing Quadratic Matrix Polynomials

For any monic linearization $\lambda I + A$ of a quadratic matrix polynomial, Tisseur and Zaballa [SIAM J. Matrix Anal. Appl., 34-2 (2013), pp. 312-337] show that there exists a nonsingular matrix $[U\ AU]$ that transforms A to a companion linearization of a (quasi)-triangular quadratic matrix polynomial. We observe that the matrix $[U\ AU]$ may be ill-conditioned while U is perfectly-conditioned. To conquer the ill conditioning challenge, we design a numerical algorithm without the orthonormal characteristic of U.

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CP8

A Fiedler-Like Approach to Spectral Equivalence of Matrix Polynomials

In this talk we extend the notion of Fiedler pencils to square matrix polynomials of the form $P(\lambda) = \sum_{i=0}^{k} A_i \phi_i(\lambda)$ where $\{\phi_i(\lambda)\}_{i=0}^{k}$ is either a Bernstein, Newton, or Lagrange basis. We use this new notion to provide a systematic way to easily generate large new families of matrix pencils that are spectrally equivalent to $P(\lambda)$, and consequently, for solving the polynomial eigenproblem $P(\lambda)x = 0, x \neq 0$. Time permitting, we will discuss some numerical properties of these matrix pencils.

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CP8

On First Order Expansions for Multiplicative Perturbation of Eigenvalues

Let A be a matrix with any Jordan structure, and λ an eigenvalue of A whose largest Jordan block has size n. We present first order eigenvalue expansions under multiplicative perturbations $\widehat{A} = (I + \varepsilon C)\, A\, (I + \varepsilon B)$ using Newton Polygon. Explicit formulas for the leading coefficients are obtained, involving the perturbation matrices

and appropriately normalized eigenvectors of A. If $\lambda \neq 0$, the perturbation in the eigenvalue is of order of $\varepsilon^{\frac{1}{n}}$, while if $\lambda = 0$, it is generically of order $\varepsilon^{\frac{1}{n-1}}$.

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CP9

Approximating the Leading Singular Triplets of a Large Matrix Function

Given a large square matrix A and a sufficiently regular function f, we are interested in the approximation of the leading singular values and corresponding vectors of $f(A)$, and in particular of $\|f(A)\|$, where $\|\cdot\|$ is the induced matrix 2-norm. Since neither $f(A)$ nor $f(A)v$ can be computed exactly, we introduce and analyze an inexact Golub-Kahan-Lanczos bidiagonalization procedure. Particular outer and inner stopping criteria are devised to cope with the lack of a true residual.

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CP9

Inverse Probing for Estimating $diag(f(A))$

Computing $diag(f(A))$ where $f(A)$ is a function of a large sparse matrix can be computationally difficult. Probing attempts to solve this by using matrix polynomials to determine the structure of $f(A)$. However, these matrix polynomials can converge slowly, causing probing to fail. To avoid this, we propose a new method which we term Inverse Probing, that directly approximates the structure of $f(A)$ based on a small sample of columns of $f(A)$. We show that this is more effective than probing in most situations.

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CP9

The Waveguide Eigenvalue Problem and the Tensor Infinite Arnoldi Method

We present a new iterative algorithm for nonlinear eigenvalue problems (NEPs), the tensor infinite Arnoldi method, which is applicable to a general class of NEPs. Moreover we show how to specialize the algorithm to a specific NEP: the waveguide eigenvalue problem, which arises from a finite-element discretization of a partial-differential equation used in the study waves propagating in periodic medium. The algorithm is successfully applied to solve benchmark problems as well as complicated waveguides.

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CP9

Verified Solutions of Delay Eigenvalue Problems with Multiple Eigenvalues

Consider computing error bounds for numerical solutions of nonlinear eigenvalue problems arising from delay-differential equations: given $A, B \in C^{n\times n}$ and $\tau \geq 0$, find $\lambda \in C$ and $x \in C^n \setminus \{0\}$ such that

$$(\lambda I - A - Be^{-\tau\lambda})x = 0,$$

where I is the identity matrix, for giving reliability of the solutions. The author previously proposed an algorithm for computing the error bounds. However, this is not applicable when λ is multiple. We hence propose an algorithm which is applicable even in this case.

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CP9

Taylor's Theorem for Matrix Functions and Pseudospectral Bounds on the Condition Number

We generalize Taylor's theorem from scalar functions to matrix functions, obtaining an explicit expression for the remainder term. Consequently we derive pseudospectral bounds on the remainder which can be used to obtain an upper bound on the condition number of the matrix function. Numerical experiments show that this upper bound can be calculated very quickly for $f(A) = A^t$, almost three orders of magnitude faster than the current state-of-the-art method.

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CP9

Contour Integration Via Rational Krylov for Solving Nonlinear Eigenvalue Problems

The Cauchy integral reformulation of the nonlinear eigenvalue problem $A(\lambda)x = 0$ has led to subspace methods

for nonlinear eigenvalue problems, where approximations of contour integration by numerical quadrature play the role of rational filters of the subspace. We show that in some cases this filtering of the subspace by rational functions can be efficiently performed by applying a restarted rational Krylov method. We illustrate that this approach increases computational efficiency. Furthermore, locking of converged eigenvalues can in the rational Krylov method be performed in a robust way.

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CP10

A Block Gram-Schmidt Algorithm with Reorthogonalization and Conditions on the Tall, Skinny Qr

The talk considers block the Gram-Schmidt with reorthogonalization (BCGS2) algorithm discussed in [J. Barlow and A. Smoktunowicz, Reorthogonalized Block Classical Gram-Schmidt, *Num. Math.* ,123:398–423, 2013.] for producing the QR factorization of a matrix X that is partitioned into blocks. A building block operation for BCGS2 is the "tall-skinny QR' factorization (TSQR) which is assumed to be a backward stable factorization. However, that assumption excludes some possible TSQR algorithms, in particular, a recent TSQR algorithm in [I.Yamazaki, S. Tomov, and J. Dongarra. Mixed-Precision Cholesky QR factorization and Its Case Studies on Multicore CPU with mulitiple GPUS. to appear, *SIAM J. Sci. Computing*, 2015]. It is shown that the weaker stability conditions satisfied by the Yamazaki et al. algorithm are sufficient for BCGS2 to produce a conditionally backward stable factorization.

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CP10

Block Methods for Solving Banded Symmetric Linear Systems

Several years ago we discovered an algorithm for factoring banded symmetric systems of equations which required half the number of multiplications and 2/3 the space of the existing algorithms that ignored symmetry. The algorithm reduced that matrix to a sequence of 1 x 1 and 2 x 2 pivots. To prevent fillin and to promote stability a sequence of 2 x 2 planar transformations are necessary when using 2 x 2 pivots which greatly complicates a block approach.

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CP10

On the Factorization of Symmetric Indefinite Matrices into Anti-Triangular Ones

A factorization of a symmetric indefinite matrix, $A = QMQ^T$, with Q orthogonal and M symmetric block antitriangular (BAT) is described in [1], relying only on orthogonal transformations and revealing the inertia of the matrix. In [2] a block algorithm performing all operations almost entirely in level 3 BLAS is developed, featuring a more favorable memory access pattern. In the same paper a lack of reliability is noticed in computing the inertia. In this talk we describe a new implementation of the BAT factorization and compare it to the other implementations in terms of stability and reliability.

1 N. Mastronardi, P. Van Dooren, The antitriangular factorization of symmetric matrices, SIMAX 34 2013 173-196.

2 Z. Bujanovic, D. Kressner, A block algorithm for computing antitriangular factorizations of symmetric matrices, Numer Algor, to appear.

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CP10

Gram-Schmidt Process with Respect to Bilinear Forms

Gram-Schmidt orthogonalization process is probably the most popular and frequently used scheme to obtain mutually orthogonal vectors. In this contribution we consider orthogonalization schemes with respect to the symmetric bilinear forms and skew-symmetric bilinear forms.We analyze their behavior in finite precision arithmetic and give bounds for the loss of orthogonality between the computed vectors.

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CP10

Roundoff Error Analysis of the Choleskyqr2 and Related Algorithms

Cholesky QR is an ideal QR factorization algorithm from the viewpoint of high performance computing, but it has rarely been used in practice due to numerical instability. Recently, we showed that by repeating Cholesky QR twice, we can greatly improve the stability. In this talk, we present a detailed error analysis of the algorithm, which we call CholeskyQR2. Numerical stability of related algorithms, such as the block Gram-Schmidt method using CholeskyQR2, is also discussed.

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CP10

Mixed-Precision Orthogonalization Processes

Orthogonalizing a set of dense vectors is an important computational kernel in subspace projection methods for solving large-scale problems. In this talk, we discuss our efforts to improve the performance of the kernel, while maintaining its numerical accuracy. Our experimental results demonstrate the effectiveness of our approaches.

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CP11

A New Asynchronous Solver for Banded Linear Systems

Banded linear systems occur frequently in mathematics and physics. A solution approach is discussed that decomposes the original linear system into q-subsystems, where q is the number of superdiagonals. Each system is solved asynchronously, followed by a $q \times q$ constraint matrix problem, and a final superposition. Reduction to a lower triangular system is never required, so the method can be fast when q-processors are available. Numerical experiments using Matlab and Fortran are also discussed.

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CP11

The Inverse of Two Level Topelitz Operator Matrices

The celebrated Gohberg-Semencul formula provides a formula for the inverse of a Toeplitz matrix based on the entries in the first and last columns of the inverse, under certain nonsingularity conditions. In this talk we will present similar formulas for two-level Toeplitz matrices and will provide a two variable generalization of the Gohberg-Semencul formula in the case of a positive definite two-level Toeplitz matrix with a symbol of the form $f(z_1, z_2) = P(z_1, z_2)^* - 1 P(z_1, z_2)^{-1} = R(z_1, z_2)^{-1} R(z_1, z_2)^* - 1$ for $z_1, z_2 \in \mathbb{T}$, where $P(z_1, z2)$ and $R(z_1, z2)$ are stable operator valued polynomials of two variables. In addition, we propose an approximation of the inverse of a multilevel Toeplitz matrix with a positive symbol, and use it as the initial value for a Hotelling iteration to compute the inverse. Numerical results are included.

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CP11

Recursive, Orthogonal, Radix-2, Stable Dct-Dst Algorithms and Applications

Discrete Fourier Transformation is engaged in image processing, signal processing, speech processing, feature extraction, convolution etc. In this talk, we address completely recursive, radix-2, stable, and solely based discrete cosine transformation (DCT) and discrete sine transformation (DST) algorithms having sparse, orthogonal, rotation, rotation-reflection, and butterfly matrices. We also present image compression results and signal transform designs based on the completely recursive DCT and DST algorithms having sparse and orthogonal factors.

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CP11

Structured Condition Numbers for the Solution of Parameterized Quasiseparable Linear Systems

We derive relative condition numbers for the solution of quasiseparable linear systems with respect to relative perturbations of the parameters in the quasiseparable and in the Givens-vector representations of the coefficient matrix of the system. We compare these condition numbers with the unstructured one and provide numerical experiments showing that the structured condition numbers we present can be small in situations where the unstructured one is huge.

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CP11

Local Fourier Analysis of Pattern Structured Operators

Local Fourier Analysis (LFA) is a well known tool for analysing and predicting the convergence behavior of multigrid methods. When first introduced, LFA required operators with constant coefficients. This requirement has been relaxed in different ways, e.g., to analyze the complete two-grid method. We continue in this manner by extending the applicability of LFA by introducing a framework for analyzing pattern structured operators.

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CP11

A Fast Structured Eigensolver for Toeplitz Matrices

Abstract not available at time of publication.

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CP12

Solving Dense Symmetric Indefinite Linear Systems on GPU Accelerated Architectures

We present new implementations for dense symmetric indefinite factorizations on multicore processors accelerated by a GPU. Though such algorithms are needed in many scientific applications, obtaining high performance of the factorization on the GPU is difficult because of the cost of symmetric pivoting. To improve performance, we explore different techniques that reduce communication and synchronization between the CPU and GPU. We present performance results using Bunch-Kaufmann, Aasen and RBT methods.

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CP12

A Parallel Divide-and-Conquer Algorithm for Computing the Moore-Penrose Inverses on Gpu

The massive parallelism of the platforms known as Compute Unified Device Architecture (CUDA) makes it possible to achieve dramatic runtime reductions over a standard CPU in many applications at a very affordable cost. However, traditional algorithms are serial in nature and can't take advantage of the multiprocessors that CUDA platforms provide. In this paper, we present a divide-and-conquer algorithm for computing the Moore-Penrose inverse $A^{\dagger}$ of a general matrix A. Our algorithm consists of two phases. The first phase uses a parallel algorithm to orthogonally reduce a general matrix A to a bi-diagonal matrix B while the second one computes the Moore-Penrose of B using a divide-and-conquer approach. Then the Moore-Penrose inverse of A is finally constructed from the results of these two phases. Numerical tests show the dramatic speedup of our new approach over the traditional algorithms.

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CP12

Exploring Qr Factorization on Gpu for Quantum Monte Carlo Simulation

Evaluation of probability computed as determinant of a dense matrix of wave functions is a computational kernel in QMCPack. This matrix undergoes a rank-one update if the event is accepted. Sherman-Morrison formula is used to update the inverse of this matrix. The explicit inverse is recomputed occasionally to maintain numerical stability. QR factorization maintains stability without refactorization. This effort explores low-rank updates to QR factorization on GPU to replace this computational kernel.

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CP12

Comparing Hybrid and Native GPU Acceleration for Linear Algebra

Accelerating dense linear algebra using GPUs admits two models: hybrid CPU-GPU and GPU-only. The hybrid model factors the panel on the CPU while updating the trailing matrix on the GPU, concentrating the GPU on high-performance matrix multiplies. The GPU-only model performs the entire computation on the GPU, avoiding costly data transfers to the CPU. We compare these two approaches for three QR-based algorithms: QR factorization, rank revealing QR, and reduction to Hessenberg.

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CP12

Efficient Eigensolver Algorithm on Accelerator Based Architecture

The enormous gap between the high-performance capabilities of GPUs and the slow interconnect between them has made the development of numerical software that is scalable across multiple GPUs extremely challenging. We describe a successful methodology on how to address the challenges -starting from our algorithm design, kernel optimization and tuning, to our programming model- in the development of a scalable high-performance symmetric eigenvalue and singular value solver.

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CP12

Batched Matrix Computations on Hardware Accelerators Based on GPUs.

We will present techniques for small matrix computations on GPUs and their use for energy efficient, high-performance solvers. Work on small problems delivers high performance through improved data reuse. Many numerical libraries and applications need this functionality further developed. We describe the main factorizations LU,QR, and Cholesky for a set of small dense matrices in parallel. We achieve significant acceleration and reduced energy consumption against other solutions. Our techniques are of interest to GPU application developers in general.

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CP13

Recycling Krylov Subspace Methods for Sequences of Linear Systems with An Application to Lattice Qcd

Many problems in engineering, numerical simulations in physics etc. require the solution of long sequences of slowly changing linear systems. As an alternative to GCRO-DR, we propose an algorithm that uses an oblique projection, in the spirit of truly deflated GMRES, for deflating the eigenvalues of smallest magnitude. This oblique projection requires approximations to right *and left* eigenvectors, and we propose a way of getting the approximations to the left eigenvectors, without having to build a Krylov subspace with respect to A^H, which saves a lot of work. We will show that the new algorithm is numerically comparable to the GCRO-DR algorithm and in addition, we further improve our results for the lattice QCD application by exploiting non-trivial symmetries.

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CP13

Generalized Jacobi Matrices and Band Algorithms

Jacobi matrices, i.e. symmetric tridiagonal matrices with positive subdiagonal entries, represent thoroughly studied objects connected to the Lanczos tridiagonalization, the Golub-Kahan bidiagonalization, the Gauss quadrature, etc. In this presentation, we study recently introduced ρ-wedge-shaped matrices that can be viewed as a generalization of Jacobi matrices. The definition is motivated by the structure of output matrices in the band generalization of the Golub-Kahan bidiagonalization and the band Lanczos algorithm.

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CP13

Symmetric Inner-Iteration Preconditioning for Rank-Deficient Least Squares Problems

Several steps of stationary iterative methods with a symmetric splitting matrix serve as inner-iteration preconditioning. We give a necessary and sufficient condition such that the inner-iteration preconditioning matrix is definite, show that short recurrence type Krylov subspace methods preconditioned by the inner iterations determine a least squares solution and the minimum-norm solution of linear systems of equations, whose coefficient matrices may be rank-deficient, and give bounds for these methods.

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CP13

On Solving Linear Systems Using Adaptive Strategies for Block Lanczos Method

Block Methods based on conjugate directions improve arithmetic intensity and rate of convergence. When these methods are used for the resolution of algebraic linear systems $Ax = b$ (A symmetric positive definite) a drawback is the need to find an adequate block size. In this work we discuss and present results of several strategies for adaptively updating the size of the block based on Ritz values and a threshold for determining when the rule applies.

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CP13

On Rotations and Approximate Rational Krylov Subspaces

Rational Krylov subspaces are useful in many applications. These subspaces are built by not only matrix vector products but also by inverses of a matrix times a vector. This results in significant faster convergence, but on the other hand often creates numerical issues. It is shown that rational Krylov subspaces under some assumptions are retrieved without any explicit inversion or system solves involved. Instead the necessary computations are done implicitly using information from an enlarged Krylov subspace. In this talk the generic building blocks underlying rational Krylov subspaces: rotations, twisted QR-factorizations, turnovers, fusions, are introduced. We will illustrate how to shrink a large Krylov subspace by unitary similarity transformations to a smaller subspace without -if all goes well- essential data loss. Numerical experiments support our claims that this approximation can be very good and as such can lead to time savings when solving particular ODE's.

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CP13

Improving Thick-Restarting Lanczos Method by Subspace Optimization For Large Sparse Eigenvalue Problems

The Thick-Restart Lanczos method is an effective method for large sparse eigenvalue problems. In this work, we propose and study a subspace optimization technique to accelerate this method. The proposed method augments the Krylov subspace with a certain number of vectors from the previous restart cycle and then apply the Rayleigh-Ritz procedure in the new subspace. Numerical experiments show that our method can converges two or three times faster than the Lanczos method.

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CP14

Ca-Ilu Preconditioner

In this talk, we present a new parallel preconditioner called CA-ILU. It performs ILU(k) factorization in parallel and is applied as preconditioner without communication. Block Jacobi and Restrictive Additive Schwartz preconditioners are compared to this new one. Numerical results show that CA-ILU(0) outperforms BJacobi and is close to RAS in term of iterations whereas CA-ILU, with complete LU on each block, does for both of them but uses a lot of memory. Thus CA-ILU(k) takes advantages of both in term of memory consumption and iterations.

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CP14

The Truncation of Low-Rank Preconditioner Updates with Applications

Rather than recomputing preconditioners for a sequence of linear systems, it is often cheaper to update the preconditioner. Here we consider low-rank preconditioner updates and truncating those updates to keep them cheap. We consider applications from nonlinear PDEs and Electronic Structure Calculations.

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CP14

Interpretation of Algebraic Preconditioning As Transformation of the Discretization Basis

In numerical solution of PDEs it is convenient to consider discretization and preconditioning closely linked together. As suggested by several techniques used throughout decades, preconditioning can always be linked with transformation of the discretization basis. It has been shown recently that effective algebraic preconditioners can be interpreted as the transformation of the discretization basis and, simultaneously, as the change of inner product on corresponding Hilbert space. This contribution will present recent work in this direction.

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CP14

Reusing and Recycling Preconditioners for Sequences of Matrices

For sequences of related linear systems, computing a new preconditioner for each system can be expensive. We can reuse a fixed preconditioner, but as the matrix changes this approach can become ineffective. We can alternatively apply cheap updates to the preconditioner. This presentation discusses the benefits of reusing and recycling preconditioners and proposes an update scheme we refer to as a Sparse Approximate Map. Applications include the QMC method, model reduction, tomography, and Helmholtz-type problems.

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CP14

Lu Preconditioners for Non-Symmetric Saddle Point Matrices with Application to the Incompressible Navier-Stokes Equations

The talk focuses on threshold incomplete LU factorizations for non-symmetric saddle point matrices. The research is motivated by the numerical solution of the linearized incompressible Navier–Stokes equations. The resulting preconditioners are used to accelerate the convergence of a Krylov subspace method applied to finite element discretizations of fluid dynamics problems in three space dimensions. We shall discuss the stability of the factorization for generalized saddle point matrices and consider an extension for non-symmetric matrices of the Tismenetsky–Kaporin incomplete factorization. We demonstrate that in numerically challenging cases of higher Reynolds number flows one benefits from using this two-parameter modification of a standard threshold ILU preconditioner. The performance of the ILU preconditioners is studied numerically for a wide range of flow and discretization parameters, and the efficiency of the approach is shown if threshold parameters are chosen suitably. The practical utility of the method is further demonstrated for the haemodynamic problem of simulating a blood flow in a right coronary artery of a real patient.

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CP14

Right Preconditioned MINRES using Eisenstat-SSOR for Positive Semidefinite Systems

Consider solving symmetric positive semidefinite systems. We use MINRES because CG does not necessarily converge for inconsistent systems. We use right preconditioning because it is easier to preserve the equivalence of the problem for inconsistent systems. We apply Eisenstats trick to economize the right SSOR preconditioned MINRES. Numerical experiments show that the method is more efficient and robust compared to no-preconditioned and right scaling preconditioned MINRES.

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CP15

Ky Fan Theorem Applied to Randić Energy

Let G be an undirected simple graph of order n with vertex set $V = \{v_1, \ldots, v_n\}$. Let d_i be the degree of the vertex v_i. The Randić matrix $\mathbf{R} = (r_{i,j})$ of G is the square matrix of order n whose (i,j)-entry is equal to $1/\sqrt{d_i\, d_j}$ if the vertices v_i and v_j are adjacent, and zero otherwise. The Randić energy is the sum of the absolute values of the eigenvalues of $\mathbf{R}$. Let $\mathbf{X}$, $\mathbf{Y}$, and $\mathbf{Z}$ be matrices, such that $\mathbf{X} + \mathbf{Y} = \mathbf{Z}$. Ky Fan established an inequality between the sum of singular values of $\mathbf{X}$, $\mathbf{Y}$, and $\mathbf{Z}$. We apply this inequality to obtain bounds on Randić energy. Some results are presented considering the energy of a symmetric partitioned matrix, as well as an application to the coalescence of graphs.

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CP15

The Linear Transformation that Relates the Canonical and Coefficient Embeddings of Ideals in Cyclotomic Integer Rings

The geometric embedding of an ideal in the algebraic integer ring of some number field is called an ideal lattice. Ideal lattices and the shortest vector problem (SVP) are at the core of many recent developments in lattice-based cryptography. We utilize the matrix of the linear transformation that relates two commonly used geometric embeddings to provide novel results concerning the equivalence of the SVP in these ideal lattices arising from rings of cyclotomic integers.

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CP15

Coupled Sylvester-Type Matrix Equations and Block Diagonalization

We prove Roth's type theorems for systems of matrix equations including an arbitrary mix of Sylvester and $\star$-Sylvester equations, in which also the transpose or conjugate transpose of the unknown matrices appear. In full generality, we derive consistency conditions by proving that such a system has a solution if and only if the associated set of 2×2 block matrix representations of the equations are block diagonalizable by (linked) equivalence transformations. Various applications leading to several particular cases have already been investigated in the literature, some recently and some long ago. Solvability of these cases follow immediately from our general consistency theory. We also show how to apply our main result to systems of Stein-type matrix equations.

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CP15

Generalized Inverses of Copositive Matrices, Self-Conditional Positive Semidefinite Matrices and Inheritance Properties

A symmetric matrix $A \in \mathbb{R}^{n\times n}$ is called *copositive* if $x^T Ax \geq 0$ for all $x \geq 0$, where the ordering of vectors is the standard component wise ordering. $A \in \mathbb{R}^{n\times n}$ is said to be *copositive of order* $n-1$ if all the $(n-1)\times(n-1)$ principal minors of A are copositive. Let $A \in \mathbb{R}^{n\times n}$ be a copositive matrix of order $n-1$. A rather well known result states that A is not copositive if and only if A is invertible and that all the entries of the inverse of A are nonpositive. Recently, we have proved a version of this result for singular matrices, using the group generalized inverse of A. Among other things, this talk will showcase this result.

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CP15

The Principal Rank Characteristic Sequence and the Enhanced Principal Rank Characteristic Sequence

The *enhanced principal rank characteristic sequence* of an $n \times n$ symmetric matrix B is $\ell_1 \ell_2 \cdots \ell_n$, where ℓ_k is `A` (respectively, `N`) if all (respectively, none) the principal minors of order k are nonzero; if some but not all are nonzero, then $\ell_k =$ `S`. Results regarding the attainability of certain classes of sequences are introduced, and restrictions for some subsequences to appear in an attainable sequence are discussed.

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CP15

A Characterization of Minimal Surfaces in the Lorentz Group L3

In this talk we establish the equation for the Gaussian Curvature of a minimal surface in the Lorentz Group $\mathbb{L}^3$. Using the Gauss equation we prove that minimal surfaces in $\mathbb{L}^3$ with constant contact angle have non-positive Gaussian curvature. Also, we provide a congruence theorem for minimal surfaces immersed in the Lorentz space $\mathbb{L}^3$.

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CP16

Linear Algebra Provides a Basis for Elasticity Without Stress Or Strain

Linear algebra can describe the energy of deformation of hyper-elastic materials in terms of a single deformation gradient tensor without the need to define stress or strain. Positions of points replace strain and force replaces stress. The model is appropriate for both infinitesimal and finite deformations, isotropic and anisotropic materials, quasi-static and dynamic elastic responses.

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CP16

Bounds on Algebraic, Discretization, and Total Numerical Approximation Errors for Linear Diffusion PDEs

We present a posteriori error estimates that allow to give a guaranteed bound on the algebraic and discretization errors for conforming finite element approximations of the Laplace equation. This extends the results of [Ern, Vohralík 2013] which allow to estimate the different components of the error and to guarantee an upper bound on the total approximation error. The efficiency of the bounds is discussed and extensive numerical results for higher-order finite element approximations are presented.

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CP16

Iterative Method for Mildly Overdetermined Least-Squares Problems with a Helmholtz Block

We present a matrix-free iterative method to solve least-squares problems, which contain a Helmholtz discretization. This type of problems arises in quadratic-penalty methods for PDE-constrained optimization. The problems of interest have multiple-right hand sides. The proposed strategy includes preconditioning to induce and exploit an identity + low-rank system matrix structure. Randomization and subsampling of one of the blocks in the least-squares problem is used to reduce the computational cost.

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CP16

On the Backward Stability of Chebyshev Rootfinding Via Colleague Matrix Eigenvalues

In this work, we analyze the backward stability of the polynomial rootfinding problem solved with colleague matrices. In other words, given a scalar polynomial $p(x)$ or a matrix polynomial $P(x)$ expressed in the Chebyshev basis, the question is to determine whether the whole set of computed eigenvalues of the colleague matrix, obtained with a backward stable algorithm are the set of roots of a nearby polynomial or not. We derive a first order backward error analysis of the polynomial rootfinding algorithm using colleague matrices adapting the geometric arguments in [A. Edelman and H. Murakami, *Polynomial roots for companion matrix eigenvalues*, Math. Comp., 1995] to the Chebyshev basis. We show that, if the norm of the coefficients of the polynomial are bounded by a moderate number, computing its roots via the eigenvalues of its colleague matrix using a backward stable eigenvalue algorithm is backward stable.

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CP16

Companion Matrices of Hermite-Birkhoff Inter-

polants

In computational mathematics, we sometimes have to deal with polynomials that are not represented in the monomial basis. They are given by values of a function and/or its derivatives of various orders at some points called nodes or sample points. This case often leads to solving a Hermite-Birkhoff interpolation problem. The present work unifies various aspects of the Newton, Hermite and Birkhoff bases. We study the companion pencils as an efficient tool for computing roots of such polynomials.

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CP16

Fixing Gauge and Rank Deficiency

Gauge fixing is a powerful concept for handling redundant degrees of freedom in Lagrangian mechanics. The challenge is finding logically consistent and mathematically tractable procedures for fixing the gauge. Working in the context of gradients of scalar potentials demonstrated how fixing the gauge also fixes rank deficient linear systems by restoring them to full rank. Also presented is an analytic derivation of gauge conditions and simplistic geometric methods for identifying gauge conditions beyond one dimension.

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CP17

Matrix-Free Krylov Subspace Methods for Solving a Riemannian Newton Equation

We consider an optimization problem on the Stiefel manifold which is equivalent to the singular value decomposition. The Riemannian Newton method for the problem has been proposed, but the Newton equation is expressed by a system of matrix equations which is difficult to solve directly. In this talk, we apply matrix-free Krylov subspace methods to a sparse linear system into which the Newton equation is rewritten. Numerical experiments show the effectiveness of our proposed method.

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CP17

Approximating the Cardinality of a Vector to Handle Cardinality Constraints in Optimization

An obvious, often loose, lower bound of cardinality of a vector, i.e. the number of nonzero elements, is the squared ratio of norm one over Euclidian norm. From this bound, we derive an estimate of the cardinality by maximizing a Rayleigh ratio involving a positive definite matrix with a simple structure, leading to an analytical formula for estimating the cardinality. Numerical experiments show estimation errors systematically smaller than those obtained with the initial bound.

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CP17

Primal and Dual Algorithms for the Ball Covering Problem

Consider the convex optimization problem of finding a Euclidean ball of minimum radius that covers m Euclidean balls with fixed centers and radii in $\Re^n$. We propose two directional search methods in which search paths (rays or two-dimensional hyperbolas in $\Re^n$) are constructed by intersecting bisectors (hyperboloids in $\Re^n$) and the step size is determined explicitly. We prove interesting properties about pairwise intersection of n-dimensional hyperboloids to achieve finite convergence.

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CP17

Finding the Nearest Valid Covariance Matrix: a Fx Market Case

We consider the problem of finding a valid covariance matrix in the FX market given an initial non-PSD estimate of such a matrix. The standard no-arbitrage assumption implies additional linear constraints on such matrices, which automatically makes them singular. As a result, such a problem is not well-posed while the PSD-solution is not strictly feasible. In order to deal with this issue, we described a low-dimensional face of the PSD cone that contains the feasible set. After projecting the initial problem onto this face, we come out with a reduced problem, which turns out to be well posed and of a smaller scale. We show that after solving the reduced problem the solution to the initial problem can be uniquely recovered in one step.

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CP17

Convergence of Newton Iterations for Order-Convex Matrix Functions

In stochastic problems and some physical problems, it is important that solving the elementwise minimal nonnegative solvent of a nonlinear matrix equation. A lot of such equations have properties of differentiable order-convex functions. Using the properties of differentiable order-convex functions, We will show that the Newton iterations for the equations are well-defined and converge to the elementwise minimal nonnegative solvent. Finally, it is given numerical experiments of the iterations for the equations.

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CP17

Modulus-Type Inner Outer Iterative Methods for Nonnegative Constrained Least Squares Problems

For the solution of large sparse nonnegative constrained least squares (NNLS) problems, a new iterative method is proposed by using conjugate gradient least squares method for inner iterations and the modulus iterative method in the outer iterations for solving linear complementarity problem resulting from Karush-Kuhn-Tucker conditions of NNLS. Convergence analysis is presented and numerical experiments show the proposed methods outperform the projected gradient methods.

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CP18

Tropical Bounds for the Eigenvalues of Block Structured Matrices

We establish a log-majorization inequality, which relates the moduli of the eigenvalues of a block structured matrix with the tropical eigenvalues of the matrix obtained by replacing every block entry of the original matrix by its norm. This inequality involves combinatorial constants depending on the size and pattern of the matrix. Its proof relies on diagonal scalings, constructed from the optimal dual variables of a parametric optimal assignment problem.

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CP18

Coherency Preservers

We will present a description of continuous coherency preservers on hermitian matrices. Applications in mathematical physics will be discussed.

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CP18

A Connection Between Comrade Matrices and Reachability Matrices

In this paper is explained a connection between comrade matrices and reachability matrices. This work is done by orthogonal polynomials, companion matrices and their connections with reachability matrices. Firstly an algebraic structure is introduced by these matrices. Then some properties of these matrices are described such as determinant, eigenvalues and eigenvectors. The fields are restricted to that $\mathbb{F} = \mathbb{R}$ or $\mathbb{C}$, namely real and complex numbers respectively. Characteristic polynomial of the companion matrix C is related by

$$p(x) = x^n - c_{n-1}x^{n-1} - \ldots - c_1 x - c_0 \in \mathbb{F}[x]. \quad (1)$$

Let $A \in \mathbb{F}^{n\times n}$, $\mathbf{b} \in \mathbb{F}^n$, the matrix

$$R(A, \mathbf{b}) = [\mathbf{b}, A\mathbf{b}, \ldots, A^{n-1}\mathbf{b}] \in \mathbb{F}^{n\times n},$$

is the reachability matrix of the pair (A, b). Also, A is the comrade matrix similar as C by an invertible matrix Q_n i.e.

$$A = Q_n C Q_n^{-1}.$$

Easily, it is shown

$$R(C, \mathbf{b}) = Q_n^{-1} R(A, Q_n \mathbf{b}).$$

The generating polynomial is defined of $\mathbf{b} = [b_0, b_1, \ldots, b_{n-1}]^T \in \mathbb{F}^{n\times 1}$ *by* $\mathbf{b}(x) = \sum_{k=0}^{n-1} b_k x^k$ then

$$R(C, \mathbf{b}) = \sum_{k=0}^{n-1} b_k R(C, \mathbf{e_k}) = \sum_{k=0}^{n-1} b_k C^k = \mathbf{b}(C) = Q_n^{-1} R(A, Q_n \mathbf{b}) \quad (2)$$

where $\mathbf{e_k}$ stands for the $(k+1)$th unit vector in the standard basis of $\mathbb{F}^{n\times 1}$. Now, an algebraic structure is introduced of

$$\mathcal{S}(A) = \{Q_n^{-1} R(A, Q_n \mathbf{b}) | \mathbf{b} \in \mathbb{F}^{n\times 1}\},$$

that is proven $\mathcal{S}(A) \simeq \mathbb{F}[x]/ \prec d(x) \succ$. Determinants, eigenvalues and eigenvectors are described of this connection. Also the colleague matrices and Chebyshev polynomials are investigated of this connection.

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CP18

Maximal Lower Bounds in Loewner Order

We show that the set of maximal lower bounds of two symmetric matrices with respect to Loewner order can be identified to the quotient set $O(p,q)/(O(p)\times O(q))$. Here, (p,q) denotes the inertia of the difference of the two matrices, $O(p)$ is the p-th orthogonal group, and $O(p,q)$ is the indefinite orthogonal group arising from a quadratic form with inertia (p,q). We discuss the application of this result to the synthesis of ellipsoidal invariants of hybrid dynamical systems.

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CP19

Coupled Preconditioners for the Incompressible Navier-Stokes Equations

After linearization and discretization of the incompressible Navier Stokes equations one has to solve block-structured indefinite linear systems. In this talk we consider SIMPLE-type preconditioners as proposed in [1]. It appears that this type of preconditioners can lead to a considerable acceleration of the solver and are weakly depending on the number of grid points and Reynolds number. Recently, the augmented Lagrangian method becomes popular [2]. The method is more expensive per iteration but independent of the grid size and Reynolds number for academic problems. The third preconditioner is the so-called 'grad-div' preconditioner. We also define modified versions of the SIMPLE and 'grad-div' preconditioners. In this talk we investigate their performance for academic problems [3].

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CP19

On Some Algebraic Issues of Domain Decomposition Approaches

Various domain decomposition approaches are considered with regard to parallel solution of very large sparse systems of linear algebraic equations arising from some finite element or finite volume approximations of complicated boundary value problems on non-structured grids. The proposed methods include automatic construction of the balanced subdomains with or without a parametrized overlapping, different type of interface conditions on internal boundaries of subdomains, augmented iterative additive Schwarz algorithm in Krylov subspaces, multi-preconditioning techniques and aggregation. The work focuses on experimental analysis of performance of the aforementioned methods. The implementation of the proposed approaches was done on the basis of hybrid parallel programming and taking into account sparse matrix structure and with using the compressed sparse row format of the matrix representation. The experiments have been performed for a representative set of test problems.

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CP19

Robust Incomplete Factorization Preconditioner with Mixed-Precision for Parallel Finite Element Analysis

In our previous study, localized IRIF(0) and IRIF(1) preconditioners were proposed to solve the equation system in the frame work of the parallel FEM. This research aims to apply the mixed precision algorithm to this preconditioning method. As the numerical results, matrices given from shell structures were solved. It has been shown that the mixed-precision IRIF(0) and IRIF(1) are effective in reducing the processing time by 40% while preserving the number of iterations.

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CP19

Efficient Simulation of Fluid-Structure Interactions Using Fast Multipole Method

Regularized Stokes formulation has been shown to be very effective at modeling fluid-structure interactions when the fluid is highly viscous. However, its computational cost grows quadratically with the number of particles immersed in the fluid. We demonstrate how kernel-independent fast multipole method can be applied to significantly improve the efficiency of this method, and present numerical results for simulating the dynamics of a large number of elastic rods immersed in 3D stokes flows.

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CP19

Block Preconditioners for An Incompressible Magnetohydrodynamics Problem

We focus on preconditioning techniques for a mixed finite element discretization of an incompressible magnetohydrodynamics (MHD) problem. Upon discretization and linearization, a 4x4 non-symmetric block-structured linear system needs to be (repetitively) solved. One of the principal challenges is the presence of a skew-symmetric term that couples the fluid velocity with the electric field. Our proposed technique exploits the block structure of the underlying linear system, utilizing and combining effective preconditioners for the mixed Maxwell and Navier-Stokes

subproblems. The preconditioner is based on dual and primal Schur complement approximations to yield a scalable solution method. Large scale numerical results demonstrate the effectiveness of our approach.

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CP19

The WR-HSS Method and Its Subspace Acceleration for the Unsteady Elliptic Problem

We consider the numerical methods for the unsteady elliptic problem with Dirichlet boundary condition. Taking into account the idea of Hermitian/skew-Hermitian (HS) splitting, a class of waveform relaxation methods is established based on the HS splitting of the linear differential operator in the corresponding differential equations, i.e., the WR-HSS method. Furthermore, the subspace acceleration of the WR-HSS method is also considered. Finally, the theoretical and numerical behaviors of the above methods are carefully analyzed.

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MS1

Functions of Matrices with Kronecker Sum Structure

Functions of large and sparse matrices with tensor structure arise in a number of scientific and engineering applications. In this talk we focus on functions of matrices in Kronecker sum form. After discussing some recent results on the decay behavior of such matrix functions, we will describe efficient Krylov subspace techniques for evaluating a function of a matrix times a vector. The results of numerical experiments will be discussed.

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MS1

First-Order Riemannian Optimization Techniques for the Karcher Mean

The Karcher mean is a matrix function of several positive definite matrices which represents their geometric mean. It is the unique minimum over the set of positive definite matrices of a real function related to a Riemannian structure of this set. We explore first-order optimization algorithms, showing that exploiting the geometric structure leads to a considerable acceleration. Moreover, we present a new strategy which appears to be faster than the existing algorithms.

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MS1

Error Estimation in Krylov Subspace Methods for Matrix Functions

Using the Lanczos method to approximate $f(A)b$, there is no straightforward way to measure the error of the current iterate. Therefore, different error estimators have been suggested, all of them specific to certain classes of functions. We add a technique to compute error bounds for Stieltjes functions, using an integral representation of the error. These bounds can be computed essentially for free, with cost independent of the iteration number and the dimension of A.

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MS1

A High Performance Algorithm for the Matrix Sign Function

The talk will described a blocked (partitioned) algorithm for the matrix sign function, along with performance results that compare the existing algorithm to the new one. The algorithm is a blocked version of the Higham's stabilized version of the Parlett-Schur matrix-sign algorithm for triangular matrices.

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MS2

Mpgmres-Sh : Multipreconditioned GMRES for Shifted Systems

We propose using the Multipreconditioned Generalized Minimal Residual (MPGMRES) method to solve shifted linear systems $(A+\sigma_j I)x_j = b$ for $j = 1, \ldots, N_\sigma$ with multiple shift-and-invert preconditioners. The multipreconditioned space is obtained by applying the preconditioners to all search directions and searching for a minimum norm solution over a larger subspace. We show that for thie particular problem this space grows linearly and discuss our implementation on systems arising from hydraulic tomography and matrix function computations.

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MS2

Nested Krylov Methods for Shifted Linear Systems

Most algorithms for the simultaneous solution of shifted linear systems make use of the shift-invariance property of the underlying Krylov spaces. This particular comes into play when preconditioning is taken into account. We propose a new iterative framework for the solution of shifted systems that uses an inner multi-shift Krylov method as a preconditioner within a flexible outer Krylov method. Shift-invariance is preserved if the inner method yields collinear residuals.

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MS2

One Matrix, Several Right Hand Sides: Efficient Alternatives to Block Krylov Subspace Methods

Matrix-block vector products are more efficient than a sequence of matrix-vector products on current architectures. This is why methods for linear systems with several, s say, right hand sides gained renewed interest recently. We investigate short recurrence alternatives to known block Krylov subspace methods and, in particular, variants of BiCG and QMR which need just one (not s) multiplications with the transposed matrix.

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MS2

Iterative Methods for Solving Shifted Linear Systems Built Upon a Block Matrix-vector Product

We discuss methods for simultaneous solving a family of shifted linear systems of the form

$$(A + \sigma_j I)x_{\sigma_j} = b_{\sigma_j} \quad j = 1, 2, \ldots, L \quad \text{with} \quad A \in \mathbb{C}^{n \times n}.$$

We explore methods built upon Krylov subspace iterations which employ a block matrix-vector product as their core operation. We demonstrate that by carefully designing these block-iterative methods, we can overcome some restrictions present in many existing techniques, i.e., the requirement that right-hand sides be collinear, incompatibility with many preconditioners, and difficulty of integration with subspace recycling techniques.

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MS3

Linearizations of Hermitian Matrix Polynomials Preserving the Sign Characteristic

The sign characteristic of a Hermitian matrix polynomial $P(\lambda)$ is a set of signs attached to the real eigenvalues of $P(\lambda)$, which is crucial for determining the behavior of systems described by Hermitian matrix polynomials. In this talk we present a characterization of the Hermitian strong linearizations that preserve the sign characteristic of a given Hermitian matrix polynomial and identify several families of such linearizations that can be easily constructed from the coefficients of the matrix polynomial.

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MS3

Low Rank Perturbations of Canonical Forms

In this talk, we will review some know results that describe the change of the following canonical forms under low rank perturbations:

- The Jordan canonical form of a square matrix.
- The Weierstrass canonical form of a regular matrix pencil.
- The Kronecker canonical of a singular matrix pencil without full rank.
- The Smith form of a regular matrix polynomial.

We will also present some recent results on the change of the Weierstrass canonical form of regular matrix pencils under low rank perturbations.

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MS3

Matrix Polynomials in Non-Standard Form

Matrix polynomials $P(\lambda)$ and their associated eigenproblems are fundamental for a variety of applications. Certainly the standard (and apparently most natural) way to express such a polynomial has been

$$P(\lambda) \;=\; \lambda^k A_k + \lambda^{k-1} A_{k-1} + \cdots + \lambda A_1 + A_0\,,$$

where $A_i \in \mathbb{F}^{m\times n}$. However, it is becoming increasingly important to be able to work directly and effectively with polynomials in the non-standard form

$$Q(\lambda) \;=\; \phi_k(\lambda)A_k + \phi_{k-1}(\lambda)A_{k-1} + \cdots + \phi_1(\lambda)A_1 + \phi_0(\lambda)A_0\,,$$

where $\{\phi_i(\lambda)\}_{i=0}^k$ is some other basis for the space of all scalar polynomials of degree at most k. This talk will describe some new approaches to the systematic construction of families of linearizations for matrix polynomials like $Q(\lambda)$, with emphasis on the classical bases associated with the names Newton, Hermite, Bernstein, and Lagrange.

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MS3

A Diagonal Plus Low Rank Family of Linearizations for Matrix Polynomials

We present a family of linearizations for an $m \times m$ matrix polynomial $P(x) = \sum_{i=0}^{d} P_i x^i$ that have the form $A(x) = D(x) + UV^t$ with $D(x)$ diagonal. The diagonal term $D(x)$ is a $dm \times dm$ matrix and U and V are $dm \times m$. Moreover, $D(x)$ can be chosen almost arbitrarily and U and V can be computed from $P(x)$ and $D(x)$. We show that appropriate choices of $D(x)$ lead to linearizations with very good numerical properties. We provide a cheap strategy to determine good choices for $D(x)$.

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MS4

Undergraduate Research in Linear Algebra 4

Abstract not available at time of publication.

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MS4

Student Research on Infinite Toeplitz Matrices

A Toeplitz matrix A has constant entries down each diagonal. So the whole matrix is determined by those numbers a_k. Then those numbers are the coefficients in the function $a(\theta) = \Sigma a_k e^{ik\theta}$. This symbol function is the superconvenient way to study the infinite matrix. The student project started by factoring $a(\theta)$ into lower times upper (negative and positive powers), leading to $A = LU$. (Hugo Woerdeman has studied the much harder 2-level problem when $a(\theta, \phi)$.) Then the student Liang Wang moved to the Radon Transform Matrix – with neat results that are still to be published.

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MS4

Research in Linear Algebra with Undergraduates

I will discuss the benefits and difficulties and general issues in working with *undergraduate* students on research projects in Linear Algebra. I will share results from projects with students from the past few years, including a Sinkhorn-Knopp fixed point problem

$$\vec{x} = \left(A^T (A\vec{x})^{(-1)}\right)^{(-1)}$$

(where for $\vec{x} = (x_1, \ldots, x_n)$, $\vec{x}^{(-1)} = (1/x_1, \ldots, 1/x_n)$), an approximation of derivatives using the LU factorization of Vandermonde Matrices, and mosaicking with digital images.

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MS4

Undergraduate Research Projects in Linear Algebra

Linear Algebra lends itself well for undergraduate research projects as with one or two terms of Linear Algebra classes a variety of research projects are accessible. In addition, problems can often be explored by numerical and symbolic computations. In this talks we discuss some successful projects from the past, some ongoing ones, as well as some future possibilities. The focus will be on matrix completion problems and questions regarding determinantal representations of multivariable polynomials.

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MS5

Exploiting Sparsity in Parallel Sparse Matrix-Matrix Multiplication

In this talk, we discuss graph and hypergraph partitioning based models and methods proposed to exploit the sparsity of SpGEMM computations for achieving efficiency on

distributed memory architectures for different parallelization schemes. All models rely on one-dimensional partitioning of both input matrices. In these models, partitioning constraint encodes balancing computational loads of processors, whereas partitioning objective of minimizing cutsize corresponds to increasing locality within each processor and reducing volume of interprocessor communication. We further address latency issues in these models. The performance of these models will be discussed through an MPI-based parallel SpGEMM library developed for this purpose.

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MS5

Generalized Sparse Matrix-Matrix Multiplication and Its Use in Parallel Graph Algorithms

We present experimental results for optimized implementations of various (1D, 2D, 3D) parallel SpGEMM algorithms and their applications to graph problems such as triangle counting, betweenness centrality, graph contracting, and Markov clustering. We quantify the effects of in-node multithreading and the implementation trade-offs involved. We will also present a new primitive, masked SpGEMM, that avoids communication when the output structure (or an upper bound on it) is known beforehand. Masked SpGEMM has applications to matrix-based triangle counting and enumeration.

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MS5

Hypergraph Partitioning for Sparse Matrix-Matrix Multiplication

We model sparse matrix-matrix multiplication using an input-specific hypergraph, where nets of the hypergraph correspond to nonzero entries and vertices correspond to nonzero scalar multiplications. The communication cost of a parallel algorithm corresponds to the size of the cut of a multi-way partition of the hypergraph. We will discuss the efficiency of various algorithms for input matrices from several applications in the context of this and related hypergraph models.

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MS5

The Input/Output Complexity of Sparse Matrix Multiplication

We consider the problem of multiplying sparse matrices (over a semiring) where the number of non-zero entries is larger than main memory. In this paper we generalize the upper and lower bounds of Hong and Kung (STOC'81) to the sparse case. Our bounds depend of the number N of nonzero entries in A and C, as well as the number Z of nonzero entries in AC. We show that AC can be computed using $\tilde{O}\left(\frac{N}{B}\min\left(\sqrt{\frac{Z}{M}}, \frac{N}{M}\right)\right)$ I/Os, with high probability. This is tight (up to polylogarithmic factors) when only semiring operations are allowed, even for dense rectangular matrices: We show a lower bound of $\Omega\left(\frac{N}{B}\min\left(\sqrt{\frac{Z}{M}}, \frac{N}{M}\right)\right)$ I/Os.

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MS6

Eigenvector Norms Matter in Spectral Graph Theory

We investigate the role of eigenvector norms in spectral graph theory to various combinatorial problems including the densest subgraph problem, the Cheeger constant, among others. We introduce randomized spectral algorithms that produce guarantees which, in some cases, are better than the classical spectral techniques. In particular, we will give an alternative Cheeger sweep (graph partitioning) algorithm which provides a linear spectral bound for the Cheeger constant at the expense of an additional factor determined by eigenvector norms. Finally, we apply these ideas and techniques to problems and concepts unique to directed graphs.

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MS6

Local Clustering with Graph Diffusions and Spectral Solution Paths

Eigenvectors of graph-related matrices are intimately connected to diffusion processes that model the spread of information across a graph. Local Cheeger inequalities guarantee that localized diffusions like the personalized PageRank eigenvector and heat kernel identify small, good-conductance clusters. We provide constant-time algorithms for computing a generalized class of such diffusions, apply their solution paths to produce refined clusters, and prove that these diffusions always identify clusters of con-

stant size.

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MS6

Signed Laplacians and Spectral Clustering Via Quotient Space Metrics

Signed Laplacians represent the structure of graphs whose edges possess signatures, i.e., certain group actions. They are quite useful for many purposes, e.g., modelling social networks with friend/enemy relationships between its members. We investigate the spectral clustering method for signed Laplacians. Like in the traditional spectral algorithms, the eigenvectors are used to map the graph vertices into unit spheres. We show that, by using the metrics of certain quotient spaces of the spheres, e.g., projective spaces, one can cluster the graph vertices to find interesting signature-related substructures. In particular, this provides a spectral approach to Harary's structural balance theory. The approach also unify the (higher order) Cheeger type inequalities for the small and large eigenvalues of the usual unsigned Laplacians, which encode the connectivity and bipartiteness properties of the underlying graphs, respectively.

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MS6

Eigenvectors of the Nonlinear Graph p-Laplacian and Application in Graph Clustering

We investigate the discrete p-Laplacian operator L_p on connected graphs. We show that many relevant properties of the spectrum of the linear Laplacian can be extended to the nonlinear L_p. In particular we provide a variational characterization of a set of n points of the spectrum of L_p, hence we prove a p-Laplacian nodal domain theorem and some higher-order Cheeger-type inequalities. We interpret the obtained results in the context of graph clustering, proposing few examples and discussing some computational issues.

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MS7

Recovering Planted Subgraphs via Convex Graph Invariants

Extracting planted subgraphs from large graphs is a fundamental question that arises in a range of application domains. In this talk, we outline a computationally tractable approach based on convex optimization to recovery structured planted graphs that are embedded in larger graphs containing spurious edges. (Joint work with Utkan Candogan.)

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MS7

Computationally-Efficient Approximations to Arbitrary Linear Dimensionality Reduction Operators

We examine a fundamental matrix approximation problem, motivated by computational considerations in large-scale data processing: how well can an arbitrary linear dimensionality reduction (LDR) operator (a matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$ with $m < n$) be approximated by a *computationally efficient* surrogate? As one illustrative example, we establish a fundamental result for partial circulant approximations of general matrices. We also examine approximations employing other computationally-efficient "primitives,' and discuss how low-dimensional structure may be exploited in these approximation tasks.

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MS7

More Data, Less Work: Sharp DataComputation Tradeoffs for Linear Inverse Problems

Often one wishes to estimate an unknown but structured signal from linear measurements where the number of measurements is far less that the dimension of the signal. We present a unified theoretical framework for convergence rates of various optimization schemes for such problems. Our framework applies to both convex and nonconvex objectives, providing precise tradeoffs between running time, data, and structure complexity for many optimization problems. Joint with B. Recht and S. Oymak.

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MS7

A Data-dependent Weighted LASSO under Poisson Noise

Sparse linear inverse problems appear in a variety of settings, but often the noise contaminating observations cannot accurately be described as bounded or arising from a Gaussian distribution. Poisson observations in particular are a characteristic feature of several real-world applications. Previous work on sparse Poisson inverse problems encountered several limiting technical hurdles. In

this talk I will describe an alternative, streamlined analysis approach for sparse Poisson inverse problems which (a) sidesteps the technical challenges present in previous work, (b) admits estimators that can readily be computed using off-the-shelf LASSO algorithms, and (c) hints at a general weighted LASSO framework for broader classes of problems. At the heart of this new approach lies a weighted LASSO estimator for which data-dependent weights are based on Poisson concentration inequalities. Unlike previous analyses of the weighted LASSO, the proposed analysis depends on conditions which can be checked or shown to hold in general settings with high probability.

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MS8

Estimating the Condition Number of $f(A)b$

I will present some new algorithms for estimating the condition number of $f(A)b$. Standard condition number estimation algorithms for $f(A)$ require explicit computation of matrix functions and their Fréchet derivatives and are therefore unsuitable for the large, sparse A typically encountered in $f(A)b$ problems. The algorithms proposed here use only matrix-vector multiplications. The number of matrix-vector multiplications required to estimate the condition number is proportional to the square of the number required by the underlying $f(A)b$ algorithm. Numerical experiments demonstrate that the condition estimates are reliable and of reasonable cost.

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MS8

An Algorithm for the Lambert W Function on Matrices

Despite being implicitly defined by the simple equation $z = W(z)\exp(W(z))$, the so-called "Lambert W' function is not straightforward to compute, mainly because of the lack of regularity and logarithm-like properties. The Newton method proves itself worthy for the scalar case, but a trivial extension to matrices suffers from numerical instability and difficulty in choosing a suitable starting matrix. These issues are fixed by deriving a numerically stable, coupled form of the Newton iteration and by employing a blocked Schur decomposition, with suitable starting matrices chosen for each diagonal block. We obtain a robust algorithm that works well in practice.

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MS8

The Leja Method: Backward Error Analysis and Implementation

The Leja method is a well established scheme for computing the action of the matrix exponential. We present a new backward error analysis allowing a more efficient method. From a scalar computation in high precision we predict the necessary number of scaling steps based only on a rough estimate of the field of values or norm of the matrix and the desired backward error. The efficiency of the approach is shown in numerical experiments.

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MS8

An Exponential Integrator for Polynomially Perturbed Linear ODEs

Consider the initial value problem $u'(t) = (\sum_{\ell=0}^{N} \varepsilon^\ell A_\ell)u(t)$, $u(0) = u_0$, where $A_0, A_1, \ldots, A_N \in \mathbb{C}^{n\times n}$ and $u_0 \in \mathbb{C}^n$. We present results that allow us to evaluate $u(t)$ efficiently for several values of ε and t.
We propose a new Krylov subspace method which uses the approximation of the product of the matrix exponential and a vector. The approach is based on the Taylor expansion of the exact solution $u(t)$ with respect to ε. We show that the coefficient vectors of this expansion are given by the matrix exponential of a block Toeplitz matrix. This result can be seen as a generalization of a result given by Najfeld and Havel (1995).
A priori error bounds are derived for the approximation which show a superlinear convergence for any N.

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MS9

Interpolatory Techniques for Model Reduction of Multivariate Linear Systems using Error Estimation

We consider interpolatory techniques for model reduction of multivariate linear systems as they appear in the input output representation of quadratic bilinear systems. Existing interpolatory techniques [C.Gu, QLMOR: a projection-based nonlinear model order reduction approach using quadratic-linear representation of nonlinear systems, 2011], [P.Benner and T.Breiten, Two-sided projection methods for nonlinear model order reduction 2015] for model reduction of quadratic bilinear systems interpolate these generalized transfer functions at some random set of interpolation points or by using the corresponding linear iterative rational Krylov algorithm. The goal here is to propose an approach that identifies a good choice of interpolation points based on the error bound expressions derived recently in [L. Feng, A. C. Antoulas and P. Benner, Some a posteriori error bounds for reduced order modelling of (non-)parameterized linear systems, 2015]. The approach iteratively updates the interpolation points in a predefined sample space by computing the maximum error bound corresponding to the previous set of interpolation points. This results in a greedy type algorithm for model reduction of the generalized transfer functions. Numerical results show the importance of choosing the interpolation points for some benchmark examples.

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MS9

Parallelization of the Rational Arnoldi Method

The rational Arnoldi algorithm is a popular method in scientific computing used to construct an orthonormal basis of a rational Krylov space. Each basis vector is a rational matrix function times the starting vector. Rational functions possess a partial fraction expansion which often allows to compute several basis vectors simultaneously. However, this parallelism may cause instability due to the orthogonalization of ill-conditioned bases. We present and compare continuation strategies to minimize these effects.

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MS9

Solving Linear Systems with Nonlinear Parameter Dependency

We present the CORK method for solving the parametric linear system $A(\sigma)x = b$. The idea is to approximate $A(\sigma)$ by a (rational) matrix polynomial and then extract x from the solution of a large scale problem with affine parameter. Previous work was reported using monomial (GAWE-method) and Chebyshev polynomials (infinite Arnoldi). The CORK framework is a general one that allows for much more freedom in the selection of polynomial or rational polynomial basis.

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MS9

Perfectly Matched Layers and Rational Krylov Subspaces with Adaptive Shifts for Maxwell Systems

The efficient and accurate modeling of waves in inhomogeneous media on unbounded domains is of paramount importance in many different areas in science and engineering. We show that optimal complex scaling and stability-corrected wave functions allow for the efficient computation of wave fields via Krylov subspace techniques. Polynomial and rational Krylov methods are discussed and numerical experiments will illustrate the performance of the proposed Krylov methods.

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MS10

Recent Advances on Inverse Problems for Matrix Polynomials

We summarize several results on inverse eigenstructure problems for matrix polynomials that have been obtained recently and discuss how they complete other results previously known in the literature. These new results are closely connected to the Index Sum Theorem and to the new class of Polynomial Zigzag matrices. In particular, we solve the

most general possible version of complete inverse eigenstructure problem for matrix polynomials.

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MS10

Matrix Functions: The Contributions of Leiba Rodman

In this presentation I will try to review the voluminous contributions to linear algebra made by Leiba Rodman. I will combine this with some new insights into canonical structures for selfadjoint quadratic matrix polynomials.

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MS10

Generic Low Rank Perturbations of Structured Matrices

Recently, the theory of generic structure-preserving rank-one perturbations of matrices that have symmetry structures with respect to some indefinite inner product has been developed. Concerning the case of arbitrary rank k, it was conjectured, but is not immediate, that a generic rank k perturbations can be interpreted as sequence of k generic rank-one perturbations. In this talk, we close this gap by giving an affirmative answer.

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MS10

A Factorized Form of the Inverse Polynomial Matrix Problem

In this talk we consider the problem of constructing a polynomial matrix of degree d with prescribed sets of left and right minimal indices and with prescribed sets of finite elementary divisors, satisfying the degree sum theorem. The use of a factorized form has the advantage that the different structural elements are easily recovered from each of the three factors. The left factor gives the left null space structure, the right factor gives the right null space structure and the middle factor reveals the finite elementary divisors.

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MS11

When Life is Linear Worldwide

In this spring of 2015, Tim Chartier taught a MOOC through Davidson College and edX. The course came in two parts with both teaching applications of linear algebra in computer graphics and data mining. Part 1 taught basics of linear algebra and was targeted to a broad audience. Part 2 taught more advanced concepts such as eigenvectors, Markov Chains, and the SVD. Both parts had activities intended to encourage exploration, discovery, and creativity.

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MS11

Coding the Matrix: Linear Algebra through Computer Science Applications

Starting in 2008, I have been developing and teaching a linear algebra course, *Coding the Matrix*, aimed at computer science students. Concepts are motivated and illustrated using applications from computer science. I view programming as a learning modality; students write programs to develop and reinforce their understanding of concepts and proofs. In the MOOC version, taught twice through Coursera, student programs are submitted to a grader and automatically checked using example data. I'll discuss my experiences.

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MS11

LAFF Long and Prosper?

Linear Algebra: Foundations to Frontiers (LAFF) is a course developed specifically for the edX platform. It encompasses more than 850 pages of notes, 250+ videos, online activities, homeworks with answers, and programming exercises. We took on this activity to a large degree because of the MOOC movement's promise to educate the masses, including those who don't necessarily have access to high quality classes. What is the intended audience? Who showed up to take the course? What is the short term and long term prognosis? Will MOOCs change education as we know it? The fact is that it is too early to tell. We discuss design decisions that underlie our course and early experiences from offering this course in Spring 2014

and Spring 2015.

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MS11

Experience with OpenCourseWare Online Video Lectures

I will share my experience in preparing video lectures for basic mathematics courses. Linear Algebra and also Computational Science came directly from the MIT classroom. Calculus and the new Differential Equations videos were filmed without an audience—I bought a camera and students helped. All are uploaded to OpenCourseWare ocw.mit.edu and to YouTube (where an individual can create a Channel, but most viewers will find videos from established websites). Using a blackboard can still be more effective than slides (but there is a place for slides). Your voice and movements make a human connection that can change lives.

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MS12

Strong Scaling and Stability: SpAMM Acceleration for the Matrix Square Root Inverse and the Heavyside Function

For matrices with decay, incomplete/inexact approximations based on the dropping of small elements leads to a sparse approximation and fast solutions for preconditioners (and even close to full solutions in well-conditioned circumstances) via the SpMM kernel. In this talk, I will develop an alternative strategy for the N-Body multiplication of data local decay matrices, the Sparse Approximate Matrix Multiply (SpAMM), based on recursive Cauchy-Swartz occlusion of sub-multiplicative norms (metric query). The SpAMM kernel is sparse in the multiplication (task) space, via occlusion and culling of small norms (rather than in the vector (data) space), yielding bounds for the product that are multiplicative rather than additive. I will develop a stability analysis for SpAMM accelerated Newton Schulz iterations towards the inverse square root, and show how the convergence of Frechet channels towards idempotence and nilpotence determine stability. I will demonstrate extreme stability under SpAMM approximation for NS iteration with congruential transformation, and show dramatic error cancellation between the nilpotent Frechet derivative and the corresponding skew displacement, which grows as $\mathrm{cond}(Z_k^{-1/2}), with Z_k - > A^{-1/2}$. Finally, I will describe how N-Body structure of the SpAMM algorithm leads to encouraging results for distributed memory implementations, with recent results for a hybrid Charm++/OpenMP approach to task parallelism, yielding strong scaling up to 500 cores per heavy atom for calculation of the matrix Heavyside function in the context of electronic structure theory.

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MS12

Analyzing Spgemm on Gpu Architectures

Mapping sparse matrix-sparse matrix multiplication (SpGEMM) to modern throughput-oriented architectures, such as GPUs, presents a unique set challenges in comparison with traditional CPUs implementations. In this presentation we will present an overview of the architectural issues that must be addressed by SpGEMM operations on GPUs and discuss recent work to address these areas of concern. Specifically we will compare and contrast segmented and flat processing schemes and the impact of each scheme on the expected SpGEMM performance.

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MS12

The Distributed Block-Compressed Sparse Row Library: Large Scale and GPU Accelerated Sparse Matrix Multiplication

The Distributed Block-Compressed Sparse Row (DBCSR) library is designed to efficiently perform block-sparse matrix-matrix multiplication, among other operations. It is MPI and OpenMP parallel, and can exploit accelerators. It is developed as part of CP2K, where it provides core functionality for linear scaling electronic structure theory. The deployed algorithm takes in account the sparsity of the problem in order to reduce the MPI communication. We will discuss performance results and development insights.

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MS12

A Framework for SpGEMM on GPUs and Heterogeneous Processors

This talk will focus on our framework and corresponding algorithms for solving three main challenges (unknown number of nonzeros of the resulting matrix, expensive insertion and load imbalance) of executing SpGEMM on GPUs and emerging heterogeneous processors. See *http://arxiv.org/abs/1504.05022* for a preprint paper of this talk.

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MS13

Active Subspaces in Theory and Practice

Active subspaces are an emerging set of tools for working with functions of several variables. I will motivate dimension reduction in scalar-valued functions of several variables, define the active subspace, and analyze methods for estimating it based on the function's gradient.

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MS13

Sketching Active Subspaces

When gradients are not available, estimating the eigenvectors that define a multivariate function's active subspace is especially challenging. We present a matrix sketching approach that exploits the connection between directional derivatives and linear projections to estimate the eigenvectors with fewer function calls than standard finite differences.

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MS13

Adaptive Morris Techniques for Active Subspace Construction

In this presentation, we discuss the use of adaptive Morris techniques for adaptive subspace construction. In applications ranging from neutronics models for nuclear power plant design to partial differential equations with discretized random fields, the number of inputs can range from the thousands to millions. In many cases, however, the dimension of the active subspace of influential parameters is moderate in the sense that it is less than one hundred. For codes in which adjoints are available, gradient approximations can be used to construct these active subspaces. In this presentation, we will discuss techniques, which are applicable when adjoints are not available or are prohibitively expensive. Specifically, we will employ Morris indices with adaptive stepsizes and step-directions to approximate the active subspace. We illustrate these techniques using examples from nuclear and aerospace engineering.

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MS13

Recovery of Structured Multivariate Functions

Approximation of multivariate functions typically suffers from curse of dimension, i.e. the number of sampling points grows exponentially with the dimension. We pose a structural assumption on the functions to be approximated - namely that they take a form of a ridge, $f(x) = g(Ax)$. We present recovery algorithms for this kind of a problem, including tractability results.

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MS14

Fractional Tikhonov Regularization and the Discrepancy Principle for Deterministic and Stochastic Noise Models

Recently, two different regularization methods called fractional Tikhonov regularization have been introduced, in particular to reduce the over-smoothing of classical Tikhonov regularization. In this talk, we discuss convergence properties of these methods in the classical deterministic setting and show how one can lift these results to the case of stochastic noise models. We compare the reconstruction quality of fractional Tikhonov methods with the classical approach for the discrepancy principle.

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MS14

A Singular Value Decomposition for Atmospheric

Tomography

The image quality of ground based astronomical telescopes suffers from turbulences in the atmosphere. Adaptive Optics (AO) systems use wavefront sensor measurements of incoming light from guide stars to determine an optimal shape of deformable mirrors (DM) such that the image of the scientific object is corrected after reflection on the DM. An important step in the computation of the mirror shapes is Atmospheric Tomography, where the turbulence profile of the atmosphere is reconstructed from the incoming wavefronts. We present several reconstruction approaches and will in particular focus on reconstructions based on a singular value decomposition of the underlying operator.

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MS14

Unbiased Predictive Risk Estimator for Regularization Parameter Estimation in the Context of Iteratively Reweighted Lsqr Algorithms for Ill-Posed Problems

Determination of the regularization parameter using the method of unbiased predictive risk estimation (UPRE) for the LSQR Tikhonov regularization of under determined ill-posed problems is considered and contrasted with the generalized cross validation and discrepancy principle techniques. Examining the UPRE for the projected problem it is shown that the obtained regularized parameter provides a good estimate for that to be used for the full problem with the solution found on the projected space. The results are independent of whether systems are over or underdetermined. Numerical simulations support the analysis and a large scale problem of image restoration validates the use of these techniques.

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MS14

Shape Reconstruction by Photometric Stereo with Unknown Lighting

Photometric stereo is a typical technique in computer vision to extract shape and color information from an object which is observed under different lighting conditions, from a fixed point of view. We will describe a fast and accurate algorithm to approximate the framed object, treating, in particular, the case when the position of the light sources is not known. Numerical experiments concerning an application in archaeology will be illustrated.

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MS15

Sparse Approximate Inverse Preconditioners, Revisited

Preconditioners that are sparse approximations to the inverse of a matrix can be applied very efficiently in parallel. A disadvantage, however, is that they are local–the preconditioning only propagates information from one grid point to nearby grid points, resulting in slow convergence. We investigate applying sparse approximate inverses in an hierarchical basis. The hierarchical basis transformations are also sparse matrix vector products. The method is related to using sparse approximate inverses as multigrid smoothers and to using wavelet bases, which have been investigated in the past. Our goal, however, is to develop a simple method that is easily parallelizable.

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MS15

Iterative Solver for Linear Systems Arising in Interior Point Methods for Semidefinite Programming

Interior point methods for Semidefinite Programming (SDP) face a difficult linear algebra subproblem. We propose an iterative scheme to solve the Newton equation system arising in SDP. It relies on a new preconditioner which exploits well the sparsity of matrices. Theoretical insights into the method will be provided. The computational results for the method applied to large MaxCut and matrix-norm minimization problems will be reported.

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MS15

On Nonsingular Saddle-Point Systems with a Maximally Rank Deficient Leading Block

We consider nonsingular saddle-point matrices whose leading block is maximally rank deficient, and show that the inverse in this case has unique mathematical properties. We then develop a class of indefinite block preconditioners that rely on approximating the null space of the leading block. The preconditioned matrix is a product of two indefinite matrices but under certain conditions the conjugate gradient method can be applied and is rapidly convergent. Spectral properties of the preconditioners are observed and validated by numerical experiments.

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MS15

A Tridiagonalization Method for Saddle-Point and Quasi-Definite Systems

The tridiagonalization process of Simon, Saunders and Yip (1988) applied to a rectangular operator A gives rise to USYMQR, which solves a least-squares problem with A, and USYMLQ, which solves a least-norm problem with A^T. Symmetric saddle-point systems may be viewed as a pair of least-squares/least-norm problems. This allows us to merge USYMQR and USYMLQ into a single method that solves both problems in one pass. We present preconditioned and regularized variants that apply to symmetric and quasi-definite linear systems and illustrate the performance of our implementation on systems coming from optimization and fluid flow.

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MS16

Averaging Block-Toeplitz Matrices with Preservation of Toeplitz Block Structure

In many applications, data measurements are transformed into matrices. To find a trend in repeated measurements, an average of the corresponding matrices is required. We use the barycenter, or minimizer of the sum of squared intrinsic distances, as our averaging operation. This intrinsic distance depends on the chosen geometry for the set of interest. We present an application-inspired geometry for positive definite Toeplitz-Block Block-Toeplitz matrices. Both the corresponding barycenter and an efficient approximation are discussed.

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MS16

Theory and Algorithms of Operator Means

We will consider the theory of matrix and operator means based on the Kubo-Ando and Loenwer theories. We will consider theoretical methods for extending, defining and approximating means of more than two positive operators, in fact means of probability measures supported on the cone of positive operators. The techniques will be motivated by the geometric mean of positive definite matrices and discrete-time gradient flows for geodescally convex potential functions.

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MS16

Using Inverse-free Arithmetic in Large-scale Matrix Equations

Inverse-free arithmetic and permuted Riccati bases have been used recently in the solution of small-scale algebraic Riccati equations, with excellent stability properties. We explore their use to solve large-scale matrix equations: our target is being able to deal with problems where the matrix X has large norm, and hence the columns of $[I; X]$ are an ill-conditioned basis for its column space. For simplicity, we focus on solving Lyapunov equations with the ADI algorithm.

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MS16

Preconditioned Riemannian Optimization for Low-Rank Tensor Equations

Solving partial differential equations on high-dimensional domains leads to very large linear systems. In these cases, the degrees of freedom in the linear system grow exponentially with the number of dimensions, making classic approaches unfeasible. Approximation of the solution by low-rank tensor formats often allows us to avoid this *curse of dimensionality* by exploiting the underlying structure of the linear operator. We propose a truncated Newton method on the manifold of tensors of fixed rank, in particular, *Tensor Train* (TT) / *Matrix Product States* (MPS) tensors. We demonstrate the flexibility of our algorithm by comparing different approximations of the Riemannian Hessian as preconditioners for the gradient directions. Finally, we compare the efficiency of our algorithm with other tensor-based approaches such as the *Alternating Linear Scheme* (ALS).

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MS17

Tensors and Structured Matrices of Low Rank

We present an interesting connection between higher-order tensors and structured matrices, in the context of low-rank approximation. In particular, we show that the tensor low multilinear rank approximation problem can be reformulated as a structured matrix low-rank approximation, the latter being an extensively studied and well understood problem. For simplicity, we consider symmetric tensors.

By imposing simple constraints in the optimization problem, the proposed approach is applicable to general tensors, as well as to affinely structured tensors to find (locally) best low multilinear rank approximation with the same structure.

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MS17

Alternating Least-Squares Variants for Tensor Approximation

The Alternating Least-Squares (ALS) algorithm for CP approximation of tensors has spawned several variants, the best-known of these being ALS with (Tikhonov) regularization. We present a unified description of these variants of ALS, and further generalize it to produce novel variants of the algorithm. One variant, tentatively titled "greased ALS", converges significantly more rapidly than ALS for several test cases. We seek to understand the circumstances under which these variants provide more rapid convergence, and fully understand the reasons for the improvement.

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MS17

Generating Polynomials and Symmetric Tensor Decomposition

For symmetric tensors of a given rank, there exist linear relations of recursive patterns among their entries. Such relations can be represented by polynomials, which are called generating polynomials. The homogenization of a generating polynomial belongs to the apolar ideal of the tensor. A set of generating polynomials can be represented by a matrix, which is called a generating matrix. Generally, a symmetric tensor decomposition can be uniquely determined by a generating matrix satisfying certain conditions. We characterize the sets of such generating matrices and investigate their properties (e.g., the existence, dimensions, nondefectiveness). Using these properties, we propose computational methods for symmetric tensor decompositions. Extensive examples are shown to demonstrate their efficiency.

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MS17

On the Convergence of Higher-order Orthogonality Iteration and Its Extension

The higher-order orthogonality iteration (HOOI) method has been popularly used to find a best low multilinear-rank approximation of a tensor. It often performs well in practice to learn a multilinear subspace. However, little of its convergence behavior has been known. In this talk, I will present a greedy way to implement the HOOI method and show its subsequence convergence to a stationary point without any assumption. Assuming a nondegeneracy condition, I will further show its global sequence convergence result, which guarantees global optimality if the starting point is sufficiently close to a globally optimal solution. The results are then extended to the multilinear SVD with missing values.

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MS18

Communication-optimal Loop Nests

Scheduling an algorithm's operations to minimize communication can reduce its runtime and energy costs. We study communication-efficient schedules for a class of algorithms including many-body and matrix/tensor computations and, more generally, loop nests operating on array variables subscripted by linear functions of the loop iteration vector. We derive lower bounds on communication between levels in a memory hierarchy and between parallel processors, and present communication-optimal schedules that attain these bounds in many cases.

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MS18

A Computation and Communication-Optimal Parallel Direct 3-Body Algorithm

We present a new 3-way interactions N-body (3-body) algorithm that is both computation and communication optimal. Its optional replication factor, c, saves c^3 in communication latency (number of messages) and c^2 in bandwidth (volume). We also extend the algorithm to support k-way interactions with cutoff distance. The 3-body algorithm demonstrates 99% efficiency on tens of thousands of cores, showing strong scaling properties with order of magnitude speedups over the naïve algorithm.

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MS18

Communication Lower Bounds for Distributed-Memory Computations

We present a new approach to the study of the communication requirements of distributed computations. This approach advocates for the removal of the restrictive assumptions under which earlier lower bounds on communication complexity were derived, and prescribes that lower bounds rely only on a mild assumption on work distribution in order to be significant and applicable. This approach is illustrated by providing tight communication lower bounds for several fundamental problems, such as matrix multipli-

cation.

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MS18

Minimizing Communication in Tensor Contraction Algorithms

Accurate numerical models of electronic correlation in molecules are derived in terms of tensors that represent multi-orbital functions and consequently contain permutational symmetries. Traditionally, contractions of such symmetric tensors exploit only the symmetries in the set of tensor element products. I will present an algebraically-restructured method that requires fewer operations for many such contractions of symmetric tensors. Additionally, I will present communication lower bounds that contain surprising new insights for both approaches.

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MS19

Numerical Tensor Algebra in Modern Quantum Chemistry and Physics

I will review the role of tensor operations in quantum simulations, and in particular, the challenges of numerical computation in the matrix product state and tensor network representations. Issues of parallelization and numerical stability will be discussed, especially for tensor networks with cycles.

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MS19

Efficient Algorithms for Transition State Calculations

Transition states are fundamental to understanding the reaction dynamics qualitatively. To date various methods of first principle location of transition states have been developed. In the absence of the knowledge of the final structure, the minimal-mode following method climbs up to a transition state without calculating the Hessian matrix. In this talk, we introduce a locally optimal search direction finding algorithm and an iterative minimizing method for the translation which improve the rotational step by a factor and the translational step a quantitative scale. Numerical experiments demonstrate the efficiency of our proposed algorithms. This is joint work with Jing Leng, Zhi-Pan Liu, Cheng Shang and Xiang Zhou.

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MS19

Compression of the Electron Repulsion Integral Tensor

The electron repulsion integral tensor has ubiquitous application in quantum chemistry calculation. In this talk, we discuss some recent progress on compressing the electron repulsion tensor into the tensor hypercontraction format with cubic scaling computational cost. (joint work with Lexing Ying)

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MS19

Reduced Density Matrix Methods in Theoretical Chemistry and Physics

The energy of an N-electron quantum system can be expressed as a functional of the two-electron reduced density matrix (2-RDM). In 2-RDM methods the 2-RDM of an N-electron system is directly computed without the wave function. In this lecture recent theoretical and computational advances as well as examples from chemistry and condensed-matter physics will be discussed.

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MS20

On Powers of Certain Positive Matrices

A matrix is called totally positive (resp. nonnegative) if all of its minors are positive (resp. nonnegative). It is known that such matrices are closed under conventional multiplication, but not necessarily closed under entry-wise or Hadamard multiplication. On the other hand, a real matrix is called positive definite (resp. semidefinite) if it is symmetric and has positive (resp. nonnegative) principal minors. In this case, such matrices need not be closed under matrix multiplication, but are closed under Hadamard multiplication. In this talk, we will survey existing work and discuss some current advances on continuous Hadamard and conventional powers of both totally positive and positive definite matrices (along with their closures), in the spirit of identifying a critical exponent in either situation, should one exist.

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MS20

Perron-Frobenius Theory of Generalizations of Nonnegative Matrices

An eventual property is one that is attained by all powers of a matrix beyond some power, so a matrix is eventually positive if A^k is entrywise positive for all $k \geq k_0$, This talk will survey Perron-Frobenius theory of positive and nonnegative matrices and and how it extends to generalizations of nonnegative matrices, especially those defined by eventual properties.

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MS20

Inverses of Acyclic Matrices and Parter Sets

An important result of Gantmacher and Krein describes the inverses of symmetric, irreducible and invertible tridiagonal matrices. In the early 2000s, Nabben extended this by describing the inverses of invertible matrices, M, whose graph is a given tree T under the assumption that each diagonal entry of M^{-1} is positive. These are closely related to the important class of ultrametric matrices. We establish a similar description for arbitrary trees T without the condition on the diagonal entries, and relate this to the Parter-sets of M, i.e. subsets α of vertices such that the nullity of the matrix obtained from M by deleting the rows and columns indexed by α is the cardinality of α.

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MS20

Geometric Mapping Properties of Semipositive Matrices

Semipositive matrices map a positive vector to a positive vector. The geometric mapping properties of semipositive matrices exhibit parallels to the theory of cone preserving and cone mapping matrices: For a semipositive matrix A, there exist a positive proper polyhedral cone K_1 and a positive polyhedral cone K_2 such that $AK_1 = K_2$. The set of all nonnegative vectors mapped by A to the nonnegative orthant is a proper polyhedral cone; as a consequence, A belongs to a proper polyhedral cone comprising semipositive matrices. When the powers A^k have a common semipositivity vector, then A has a positive eigenvalue. When the spectral radius of A is the sole peripheral eigenvalue and the powers of A are semipositive, A leaves a proper cone invariant.

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MS21

Vector Etrapolation for Image Restoration

Abstract not available at time of publication.

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MS21

Psf Reconstruction for Extremely Large Telescopes

Objects on the sky appear blurred when observed by a ground based telescope due to diffraction of light and turbulences in the atmosphere. Mathematically the relation between the real object and its observed image can be described as a convolution with the so called point spread function (PSF). Even though the to-be-built generation of extremely large telescopes (ELTs) use adaptive optics (AO) systems to reduce the effects of the atmosphere, still some residual blurring remains. The PSF serves as quality measure for the AO system and thus needs to be very accurate. As the PSF cannot be measured directly, a reconstruction form the data of the AO system is necessary. In this talk, an efficient algorithm for PSF reconstruction for the European ELT (E-ELT) is presented. The reconstruction process is based on splitting the PSF in one part calculated on the fly from observation data and a second part that can only be obtained from simulation. Especially for the latter one, a good model of the atmosphere is needed and due to the size of the E-ELT all calculations have to be made as efficient as possible even though simulations can be done beforehand. On the fly computations need to be fast and using little memory as the measurements are usually taken at a frequency of 500 Hz, leading to a huge amount of data just for one single night. In addition, astronomers want to evaluate the current observations conditions using the PSF and thus need it almost on time. We show how to use an efficient representation, leading to a sparse matrix. The reconstructed PSF can be used for improvement of the observed images. We opt for a blind deconvolution scheme to also improve the quality of the reconstructed PSF. Again the choice of an efficient representation, now for the observed image, is crucial to get a sparse linear system. Finally, a blind deconvolution algorithm taking care of the features of ground based astronomy is presented.

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MS21

Randomized Tensor Singular Value Decomposition

The tensor Singular Value Decomposition (t-SVD) proposed by Kilmer and Martin [2011] has been applied successfully in many fields, such as computed tomography, facial recognition, and video completion. In this talk, I will present a probabilistic method that can produce a factorization with similar properties to the t-SVD, but is stable and more computationally efficient on very large datasets. This method is an extension of a well-known randomized matrix method. I will present the details of the algorithm, theoretical results, and provide experimental results for two specific applications.

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MS21

Multidirectional Subspace Expansion for Single-Parameter and Multi-Parameter Tikhonov Regu-

larization

Tikhonov regularization is often used to approximate solutions of linear discrete ill-posed problems when the observed or measured data is contaminated by noise. Multi-parameter Tikhonov regularization may improve the quality of the computed approximate solutions. We propose a new iterative method for large-scale multi-parameter Tikhonov regularization with general regularization operators based on a multidirectional subspace expansion.

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MS22

Fast Iterative Solvers for a Coupled Cahn-Hilliard/Navier-Stokes System

We consider a diffuse interface model that governs the hydrodynamics of two-phase flows. Our research builds on the work of Garcke, Hinze and Kahle. Our contribution concerns the fully iterative solution of the arising large and sparse linear systems. This is based on preconditioning techniques we have developed for Cahn–Hilliard variational inequalities. Block preconditioners using an effective Schur complement approximation are presented. Numerical results illustrate the efficiency of the approach.

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MS22

Preconditioning a Mass-Conserving DG Discretization of the Stokes Equations

While there is a long history of work on conforming finite-element discretizations of the Stokes and Navier-Stokes equations, using H(div)-conforming elements for the velocity has recently emerged as a way to ensure strong enforcement of the incompressibility condition at the element scale. In this talk, we explore the applicability of classic block preconditioning and monolithic multigrid methods for Stokes-like saddle-point problems to one such discretization, using BDM elements for the velocities.

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MS22

A Multilevel Preconditioner for Data Assimilation with 4D-Var

Large-scale variational data assimilation problems are common in numerical weather prediction. The 4D-Var method is frequently used to calculate a forecast model trajectory that best fits the available observations to within the observational error over a period of time. This results in a large-scale nonlinear weighted least-squares problem, typically solved by a Gauss-Newton method. We will discuss using a multilevel preconditioner within 4D-Var to reduce memory requirements and increase computational efficiency.

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MS22

Asynchronous Optimized Schwarz Methods

Optimized Schwarz Methods are domain decomposition methods, where one imposes Robin conditions on the artificial interfaces. The Robin parameter can be optimized to obtain very fast convergence. We present an asynchronous version of this method, where the problem in each subdomain is solved using whatever boundary data is locally available and with no synchronizations with other processes. We prove convergence of the method, and illustrate its efficiency on large three-dimensional problems. (Joint work with Frédéric Magoulès and Cédric Venet, École Centrale Paris).

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MS23

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MS23

Preconditioners for Linear Systems Arising From The Eddy Current Problem

We consider the preconditioning techniques for the structued systems of linear equations arising from the finite element discretization of the eddy current problem. A class of positive definite and positive semidefinite splittings is proposed to solve such linear systems. This kind of matrix splitting, as well as its relaxed variants, can be used as the preconditoners for Krylov subspace methods. The performance of the preconditioners is illustrated by numerical examples.

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MS23

An Alternating Positive Semidefinite Splitting Preconditioner for Saddle Point Problems from Time-harmonic Eddy Current Models

For the saddle point problem arising from the finite element discretization of the hybrid formulation of the time-harmonic eddy current problem, we propose an alternating positive semidefinite splitting preconditioner which is based on two positive semidefinite splittings of the saddle point matrix. It is proved that the corresponding alternating positive semidefinite splitting iteration method is unconditionally convergent. We show that the new preconditioner is much easier to implement than the block alternating splitting implicit preconditioner proposed in [Z.-Z. Bai, Numer. Linear Algebra Appl., 19 (2012), 914–936] when they are used to accelerate the convergence rate of Krylov subspace methods such as GMRES. Numerical examples are given to show the effectiveness of our proposed preconditioner.

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MS23

Title Not Available at Time of Publication

In this talk, we focus on solving a class of complex linear systems arising from distributed optimal control with time-periodic parabolic equations. A block alternating splitting (BAS) iteration method and preconditioner are presented. The convergence theory of the BAS iteration and the spectral properties of the BAS preconditioned matrix are discussed. Numerical experiments are presented to illustrate the efficiency of the BAS iteration as a solver as well as a preconditioner for Krylov subspace methods.

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MS24

Localization and Reconstruction of Brain Sources Using a Constrained Tensor-based Approach

This talk addresses the localization and reconstruction of spatially distributed sources from ElectroEncephaloGraphic (EEG) signals. The occurrence of several amplitude modulated spikes originating from the same epileptic region are used to build a space-time-spike tensor from the EEG data. A Canonical Polyadic (CP) decomposition of this tensor is computed such that the column vectors of one loading matrix are linear combinations of a physics-driven dictionary. A performance study on realistic simulated EEG data of the proposed tensor-based approach is provided.

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MS24

On the Uniqueness of Coupled Matrix Block Diagonalization in the Joint Analysis of Multiple Datasets

Uniqueness of matrix (or tensor) factorizations is necessary in order to achieve interpretability and attribute physical meaning to factors. In this work, we discuss new uniqueness results on a coupled matrix block diagonalization model. This model is associated with the joint blind source separation of multiple datasets, where each datasets is a linear mixture of statistically independent multidimensional components.

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MS24

The Decomposition of Matrices

There are well-known matrix decompositions: LU-decomposition, SVD-decomopostion and QR-decomposition. In this talk we will discuss new types of matrix decompositions. We will use algebraic geometry to show that every matrix can be decomposed into the product of finitely many Toeplitz or Hankel matrices. Our method can also recover LU-decomposition and QR-decompositon for generic matrices. This is a joint work with Lim Lek-Heng.

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MS24

"Sequentially Drilled" Joint Congruence Decom-

positions (SeDJoCo): The Simple Case and the Extended Case

We present the formulation and several associated properties of a particular congruence transformations, which we term "Sequentially Drilled" Joint Congruence (SeDJoCo) decompositions and Extended SeDJoCo decompositions. In its basic form, SeDJoCo is defined as follows: Given an ordered set of K (conjugate-)symmetric target-matrices of dimensions KxK, find a KxK transformation matrix, such that when the k-th target-matrix is multiplied by the transformation matrix on the left, and by its (conjugate) transpose on the right, the resulting matrix is drilled on its k-th column (and k-th row), namely, all elements in that column are zeros, except for the diagonal ((k,k)-th) element. We show that this problem is closely related to Maximum Likelihood (ML) Independent Component Analysis (ICA) in some contexts, as well as to the problem of Coordinated Beamforming (CBF) in multi-user Multiple-Inputs Multiple-Outputs (MIMO) communications. We show that a sufficient condition for existence of a solution to this problem is that all the target matrices be positive definite. We also present some iterative solutions. We then proceed to describe the Extended SeDJoCo, in which, for some M, an ordered set of KM2 target matrices (each of dimensions KxK) is considered, and M transformation matrices are sought, satisfying a more complicated set of congruence transformations. This extended version is closely related to ML Independent Vector Analysis (IVA), an emerging extension of ICA which considers M mixtures, with correlations between sources participating in different mixtures. It is also related to CBF in the context of multicast Multi-Users MIMO.

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MS25

Network Oblivious Algorithms

Network obliviousness is a framework for design of algorithms that can run efficiently on machines with different parallelism and communication capabilities. Algorithms are specified only in terms of the input size and evaluated on a model with two parameters, capturing parallelism and communication latency. Under broad conditions, optimality in the latter model implies optimality in Decomposable BSP. Optimal network-oblivious algorithms are given for a few key problems. Limitations of non-oblivious broadcast are established.

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MS25

Characterizing the Communication Costs of Sparse Matrix Multiplication

Parallel sparse matrix-matrix multiplication is a key computational kernel in scientific computing. Although its running time is typically dominated by the cost of interprocessor communication, little is known about these communication costs. We propose a hypergraph model for this problem, in which vertices represent nonzero scalar multiplications, hyper-edges represent data, and the optimal vertex partition represents a communication-minimizing, load-balanced distribution of work. We demonstrate the potential of this model and similar coarser ones for deriving communication lower bounds.

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MS25

Data Movement Lower Bounds for Computational Directed Acyclic Graphs

Abstract not available at time of publication.

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MS25

Using Symmetry to Schedule Algorithms

Presented with a machine with a new interconnect topology, designers use intuition about the geometry of the algorithm and the machine to design time and communication-efficient schedules that map the algorithm onto the machine. Is there a systematic procedure for designing such schedules? We explore a new algebraic approach with a view towards automating schedule design. Specifically, we describe how the "symmetry" of matrix multiplication can be used to derive schedules for different network topologies.

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MS26

O(N) Density Functional Theory Calculations: The

Challenge of Going Sparse

To reduce computational complexity in Density Functional Theory calculations with wave functions, a special representation of the solution is required. Sparse solutions, which retain the accuracy of traditional approaches are possible but present many challenges. Nonetheless, they also offer many opportunities to solve much larger and more realistic problems in material sciences, and to scale on much larger high performance computing platforms. In this talk, we will discuss our recent developments using real-space discretizations. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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MS26

Randomized Estimation of Spectral Densities of Large Matrices Made Accurate

In physics, it is sometimes desirable to compute the spectral density of a Hermitian matrix A. In many cases, the only affordable operation is matrix-vector multiplication, and stochastic based methods can be used to estimate the DOS. The accuracy of stochastic algorithms converge as $O(1/\sqrt{N_v})$, where N_v is the number of stochastic vectors. I will introduce a new method called spectrum sweeping, which is a stochastic method and the convergence rate can be much faster than $O(1/\sqrt{N_v})$ for modest choice of N_v.

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MS26

Challenges and Opportunities for Solving Large-scale Eigenvalue Problems in Electronic Structure Calculations

Realistic first-principle quantum simulations applied to large-scale atomistic systems, pose new challenges in the design of numerical algorithms that are both capable of processing a considerable amount of generated data, and achieving significant parallel scalability on modern high end computing architectures. In this presentation, we explore variations of the FEAST eigensolver that can considerably broaden the perspectives for addressing such difficulties.

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MS26

Towards Large and Fast Density Functional Theory Calculations

Electronic structure calculations based on Density Functional Theory (DFT) have been remarkably successful in describing material properties and behavior. However, the large computational cost associated with these simulations has severely restricted the size of systems that can be routinely studied. In this talk, previous and current efforts of the speaker to develop efficient real-space formulations and parallel implementations for DFT will be discussed. These include linear scaling methods applicable to both insulating and metallic systems.

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MS27

Arrangements of Equal Minors in the Positive Grassmannian

We investigate the structure of equalities and inequalities between the minors of totally positive matrices. We show that collections of equal minors of largest value are in bijection with sorted sets, which earlier appeared in the context of alcoved polytopes. We also prove in many cases that collections of equal minors of smallest value are exactly weakly separated sets. Such sets are closely related to the positive Grassmannian and the associated cluster algebra.

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MS27

Preserving Positivity for Matrices with Sparsity Constraints

Functions preserving positivity have been investigated by analysts and linear algebraists for much of the last few decades. It is well known from the work of Rudin and Schoenberg that functions (applied entrywise) which are analytic and absolutely monontonic preserve positivity for all positive definite matrices of any size. The emergence of data science has raised new questions in the field of positivity. In this talk we investigate maps which preserve positivity when various sparsity, rank and other constraints are imposed. As a consequence, we extend the results of Rudin and Schoenberg with modern motivations in mind. (Joint with B. Rajaratnam and A. Khare)

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MS27

Critical Exponents and Positivity

We classify the powers that preserve positivity, when applied entrywise to positive semidefinite (psd) matrices with rank and sparsity constraints. This is part of a broad pro-

gram to study positive entrywise functions on distinguished submanifolds of the cone. In our first main result, we completely classify the powers preserving Loewner properties on psd matrices with fixed dimension and rank. This includes the case where the matrices have negative entries. Our second main result characterizes powers preserving positivity on matrices with zeros according to a chordal graph. We show how preserving positivity relates to the geometry of the graph, thus providing interesting connections between combinatorics and analysis. The work has applications in regularizing covariance/correlation matrices, where entrywise powers are used to separate signal from noise, while minimally modifying the entries of the original matrix. (Based on joint work with D. Guillot and B. Rajaratnam.)

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MS27

The Jordan Form of An Irreducible Eventually Nonnegative Matrix

A square complex matrix A is eventually nonnegative if there exists a positive integer k_0 such that for all $k \geq k_0$, $A^k \geq 0$. We say a matrix is strongly eventually nonnegative if it is eventually nonnegative and has an irreducible nonnegative power. We present some results about the Jordan forms of strongly eventually nonnegative matrices and the Jordan forms of irreducible, eventually nonnegative matrices.

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MS28

Dynamic Network Centrality with Edge Multidamping

Dynamic centrality measures provide a numerical tool for the identification of key players in a network whose edges are evolving over time. In this talk we consider a Katz-type centrality measure modified to accommodate the dynamical aspect of the network. We study the significance of an edge attenuation parameter to the ordinal rankings at a given time. We introduce a concept of edge multidamping allowing for a time-dependent variant of the standard Katz parameter.

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MS28

Solving Graph Laplacians for Complex Networks

The graph Laplacian is often used in network analysis. Therefore, solving linear systems and eigensystems for graph Laplacians is of great practical interest. For large problems, iterative solvers such as preconditioned conjugate gradients are needed. We show that Jacobi and Gauss-Seidel preconditioning are remarkably effective for power-law graphs. Support-graph (combinatorial) preconditioners can reduce the number of iterations further but may not be faster in practice. Finally, we discuss and show preliminary results for a recent theoretically almost-optimal algorithm by Kelner et al.

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MS28

On Growth and Form of Networks

A new spectral scaling method to detecting topological irregularities in networks is introduced. It is based on the communicability function and the principal eigenvector of the adjacency matrix of a network. The relation between the spatial efficiency of a network, measured by means of the communicability angles, and the topological heterogeneities is found. We then analyse the growing of Erdos-Renyi random graphs, networks growing with modularity, fractal networks, and networks growing under spatial constraints.

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MS28

Using the Heat Kernel of a Graph for Local Algorithms

The heat kernel is a fundamental tool in extracting local information about large graphs. In fact, the heat kernel can be restricted to a few entries which are enough to summarize local structure. In this talk, I will present an efficient algorithm for approximating the heat kernel of a graph. I will also present two local algorithms using the approximation procedure; a local cluster detection algorithm, and a local Laplacian linear solver.

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MS29

Constraint Preconditioning for the Coupled Stokes-Darcy System

We propose the use of constraint preconditioned GMRES for the solution of the linear system arising from the finite element discretization of coupled Stokes-Darcy flow. We

provide spectral and field-of-values bounds for the preconditioned system which are independent of the underlying mesh size. We present several numerical experiments in 3D that illustrate the effectiveness of our approach.

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MS29

Krylov Methods in Adaptive Finite Element Computations

Since decades modern technological applications lead to challenging PDE eigenvalue problems, e.g., vibrations of structures, modeling of photonic gap materials, analysis of the hydrodynamic stability, or calculations of energy levels in quantum mechanics. Recently, a lot of research is devoted to the so-called Adaptive Finite Element Methods (AFEM). In most AFEM approaches the underlying algebraic problems, i.e., linear systems or eigenvalue problems, are of large dimension which makes the Krylov subspace methods of particular importance. The goal of this work is to analyze the influence of the accuracy of the algebraic approximation, e.g. inexact Krylov method on the adaptivity process. Moreover, we discuss how to reduce the computational effort of the iterative solver by adapting the size of the Krylov subspace. Based on perturbation results in $H^1(\Omega)$- and $H^{-1}(\Omega)$-norm derived in [1] and a standard residual a posteriori error estimator a balancing AFEM algorithm is proposed. [1] U. L. Hetmaniuk and R. B. Lehoucq. Uniform accuracy of eigenpairs from a shift-invert Lanczos method. *SIAM J. Matrix Anal. Appl.*, 28:927–948, 2006.

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MS29

Near-Krylov for Eigenvalues and Linear Equations Including Multigrid and Rank-1

We look at several eigenvalue and linear equations computations that involve near-Krylov subspaces. Included are two-grid methods that are more robust than standard multigrid and methods for Rank-1 updates of large matrices. Recycling methods for changing matrices are also considered. We analyze some of the properties of near-Krylov subspaces that are used by these methods.

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MS29

Efficient Iterative Algorithms for Linear Stability Analysis of Incompressible Flows

Linear stability analysis of a dynamical system entails finding the rightmost eigenvalue for a series of eigenvalue problems. For large-scale systems, it is known that conventional iterative eigenvalue solvers are not reliable for computing this eigenvalue. A recently developed and more robust method, Lyapunov inverse iteraiton, involves solving large-scale Lyapunov equations, which in turn requires the solution of large, sparse linear systems analogous to those arising from solving the underlying partial differential equations. This study explores the efficient implementation of Lyapunov inverse iteration when it is used for linear stability analysis of incompressible flows. Efficiencies are obtained from effective solution strategies for the Lyapunov equations and for the underlying partial differential equations. Solution strategies based on effective preconditioning methods and on recycling Krylov subspace methods are tested and compared, and a modified version of a Lyapunov solver is proposed that achieves significant savings in computational cost.

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MS30

Squish Scalings

Given non-negative matrices $A, L, U \in \mathbb{R}^{n\times n}$ we show how to compute a scalar $\alpha \in \mathbb{R}$ and a diagonal matrix $D \in \mathbb{R}^{n\times n}$ such that

$$L/\beta \leq \alpha D^{-1} A D \leq U\beta,$$

for the least possible $\beta \in \mathbb{R}$. The entities in A are 'pushed down' by the upper bound U and 'pushed up' thy the lower bound L. Hence squish scaling. Squish scalings are computed using max-plus algebra and have applications in graph theory and eigenvalue computation.

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MS30

Using Matrix Scaling to Identify Block Structure

We can apply a two-sided diagonal scaling to a nonnegative matrix to render it into doubly stochastic form if and only if the matrix is fully indecomposable. The scaling often reveals key structural properties of the matrix as the effects of element size and connectivity are balanced. Exploiting key spectral properties of doubly stochastic matrices, we will show how to use the scaling to reveal hidden block structure in matrices without any prior knowledge.

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MS30

Hungarian Scaling of Polynomial Eigenproblems

We study the behaviour of the eigenvalues of a parametric matrix polynomial P in a neighbourhood of zero. If we suppose that the entries of P have Puiseux series expansions we can build an auxiliary matrix polynomial Q whose entries are the leading exponents of those of P. We show that preconditioning P via a diagonal scaling based

on the tropical eigenvalues of Q can improve conditioning and backward error of the eigenvalues.

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MS30

Max-Balancing Hungarian Scalings

A Hungarian scaling is a two-sided diagonal scaling of a matrix, which is typically applied along with a permutation to sparse indefinite nonsymmetric linear system before calling a direct or iterative solver. A Hungarian scaled and reordered matrix has all its entries of modulus less than or equal to one and entries of modulus one on the diagonal. We use max-plus algebra to characterize the set of all Hungarian scalings for a given matrix and show that max-balancing a Hungarian scaled matrix yields the most diagonally dominant Hungarian scaled matrix possible. We also propose an approximate max-balancing Hungarian scaling whose computation is embarrassingly parallel.

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MS31

A High-Accuracy SR1 Trust-Region Subproblem Solver for Large-Scale Optimization

In this talk we present an SR1 trust-region subproblem solver for large-scale optimization. This work makes use of the compact representation of an SR1 matrix and a QR factorization to obtain the eigenvalues of the SR1 matrix. Optimality conditions are used to find a high accuracy solution to each subproblem even in the so-called "hard case". Numerical results will be presented.

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MS31

Compact Representation of Quasi-Newton Matrices

Very large systems of linear equations arising from quasi-Newton methods can be solved efficiently using the compact representation of the quasi-Newton matrices. In this talk, we present a compact formulation for the entire Broyden convex class of updates for limited-memory quasi-Newton methods and how they can be used to solve large-scale trust-region subproblems with quasi-Newton Hessian approximations.

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MS31

Obtaining Singular Value Decompositions in a Distributed Environment

Matrix decompositions like the singular value decompositions are important analysis tools for processing and analyzing large amounts data. It is thus important to develop stable robust approaches to efficiently processing large datasets in a distributed environment. We present results for processing both sparse and dense data for big data problems. We further explore the efficiency of some promising approximate optimization-based approaches that provide more flexibility in customizing the canonical problem formulation.

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MS31

Linear Algebra Software in Nonlinear Optimization

We discuss some practical issues associated with sequential quadratic programming (SQP) methods for large-scale nonlinear optimization. In particular, we focus on SQP methods that can exploit advances in linear algebra software. Numerical results are presented for the latest version of the software package SNOPT when utilizing third-party linear algebra software packages.

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MS32

Low-Rank Cross Approximation Methods for Reduction of Parametric Equations

The low-rank decomposition of matrices and tensors is a known data compression technique. One of the problems is to build a low-rank representation, given a procedure to evaluate a particular element of a tensor. The cross approximation algorithms select a few entries to construct the low-rank factorization. However, these methods assume that each fixed element of a tensor is a single number, and that different elements can be evaluated independently on each other. For stochastic PDEs this is not the case: each parameter point produces a vector of the discrete solution of the PDE. This would hinder the performance of the cross algorithms, since a large portion of data is likely to be wasted. We extend the TT cross algorithm to approximate many tensors simultaneously in the same low-rank format. Besides, for a linear SPDE we can use the computed low-rank factors as model reduction bases, and increase the efficiency further.

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MS32

Hierarchical Low Rank Approximation for Extreme Scale Uncertainty Quantification

We consider the problem of uncertainty quantification for extreme scale parameter dependent problems where an underlying low rank property of the parameter dependency is assumed. For this type of dependency the hierarchical Tucker format offers a suitable framework to approximate a given output function of the solutions of the parameter dependent problem from a number of samples that is linear in the number of parameters. In particular we can a posteriori compute the mean, variance or other interesting statistical quantities of interest. In the extreme scale setting it is already assumed that the underlying fixed-parameter problem is distributed and solved for in parallel. We provide in addition a parallel evaluation scheme for the sampling phase that allows us on the one hand to combine several solves and on the other hand parallelise the sampling.

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MS32

Interpolation of Inverse Operators for Preconditioning Parameter-Dependent Equations and Projection-Based Model Reduction Methods

We present a method for the construction of preconditioners for large systems of parameter-dependent equations, where an interpolation of the matrix inverse is computed through a projection of the identity with respect to random approximations of the Frobenius norm. Adaptive interpolation strategies are then proposed for different objectives in the context of projection-based model order reduction methods: error estimation, projection on a given approximation space, or recycling of computations.

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MS32

Stochastic Galerkin Method for the Steady State Navier-Stokes Equations

We study steady state Navier-Stokes equations in the context of stochastic finite element discretizations. We assume that the viscosity is given in terms of a generalized polynomial chaos (gPC) expansion. We formulate the model and linearization schemes using Picard and Newton iterations in the framework of the stochastic Galerkin method, and compare the results with that of stochastic collocation and Monte Carlo methods. We also propose a preconditioner for systems of equations solved in each step of the stochastic (Galerkin) nonlinear iteration and we demonstrate its effectiveness in a series of numerical experiments.

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MS33

Global and Local Methods for Solving the Gravitational Lens Equation

The effect of gravitational microlensing can be modeled by the lens equation $R(z) - \bar{z}$, where $R(z)$ is a complex rational function. The zeros of this function correspond to images of a distant light source, created by the action of gravity on light. We discuss the numerical solution of the lens equation, including a reformulation as a rootfinding problem of a polyanalytic polynomial, and discuss local optimization methods in the complex variables z and $\bar{z}$.

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MS33

Fast and Stable Computation of the Roots of Polynomials

A stable algorithm to compute the roots of polynomials in the monomial basis is presented. Implicit QR steps are executed on a suitable representation of the iterates, which remain unitary plus low rank. The computational complexity is reduced to a minimum by exploiting the redundancy present in the representation allowing to ignore the low rank part. By ignoring the low rank part the remaining computations are solely based on rotations and thus unitary.

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MS33

Stable Polefinding-Rootfinding and Rational Least-Squares Fitting Via Eigenvalues

One way of finding the poles/roots of a meromorphic function is rational interpolatation, followed by rootfinging for

the denominator. This is a two-step process and the type of the rational interpolant is required as input. Moreover, the numerical stability has remained largely uninvestigated. This work introduces an algorithm with the features: (i) automatic detection of the numerical type (ii) pole/root-finding via a generalized eigenvalue problem in a one-step fashion, and (iii) backward stability, defined appropriately.

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MS33

Resultant Methods for Multidimensional Rootfinding Are Exponentially Unstable

Hidden-variable resultant methods are a class of algorithms for the solution of systems of polynomial equations. When the number of variable is 2, when care is taken, they can be competitive. Yet, in higher dimensions they are known to miss solutions, calculate roots to low precision, and introduce spurious ghost solutions. We show that the popular hidden-variable resultant method based on the Cayley resultant is inherently and spectacularly numerically unstable, by a factor that grows exponentially with the dimension. We also show the ill-conditioning of the Sylvester resultant for solving systems of two bivariate polynomial equations. This provides a rigorous explanation of the numerical difficulties that practitioners are frequently reporting.

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MS34

Singular Values and Vectors under Random Perturbation

Computing the singular values and singular vectors of a large matrix is a basic task in high dimensional data analysis with many applications in computer science and statistics. In practice, however, data is often perturbed by noise. A natural question is the following. How much does a small perturbation to the matrix change the singular values and vectors? Classical (deterministic) theorems, such as those by Davis-Kahan, Wedin, and Weyl, give tight estimates for the worst-case scenario. In this talk, I will consider the case when the perturbation is random. In this setting, better estimates can be achieved when our matrix has low rank. This talk is based on joint work with Van Vu and Ke Wang.

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MS34

The Stochastic Block Model and Communities in Sparse Random Graphs: Detection at Optimal Rate

We consider the problem of communities detection in sparse random graphs. Our model is the so-called Stochastic Block Model, which has been immensely popular in the recent statistics literature. Let $X_1, ...X_k$ be vertex sets of size n each (where k is fixed and n is large). One draws random edges inside each X_i with probability p/n, and between X_i and X_j with probability q/n, for some constants p and q. Given one instance of this sparse random graph, our goal is to recover the sets X_i as correctly as possible. We are going to present a fast spectral algorithm which does this job at the optimal rate (namely the relation between p, q and the number of mistakes in the recovery is optimal). Our algorithm is based on spectral properties of random sparse matrices and is easy to implement. We will also discuss several related works and algorithms and an open question concerning perturbation of random matrices.

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MS34

Robust Tensor Decomposition and Independent Component Analysis

ICA is a classical model of unsupervised learning originating and widely used in signal processing. In this model, observations in n-space are obtained by an unknown linear transformation of a signal with independent components. The goal is to learn the the transformation and thereby the hidden basis of the independent components. In this talk, we'll begin with a polynomial-time algorithm called Fourier PCA, for underdetermined ICA, the setting where the observed signal is in a lower dimensional space than the original signal, assuming a mild, verifiable condition on the transformation. The algorithm is based on a robust tensor decomposition method applied to a higher-order derivative tensor of the Fourier transform and its analysis uses the anticoncentration of Gaussian polynomials. The running time and sample complexity are polynomial, but of high constant degree, for any constant error; a MATLAB implementation of the algorithm appears to need 10^4 samples for 10-dimensional observations. We then present a more efficient recursive variant for the fully determined case of standard ICA, which needs only a nearly linear number of samples and has polynomial time complexity. Its analysis is based on the gaps between the roots of polynomials of Gaussian random variables.

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MS34

Applications of Matrix Perturbation Bounds with Random Noise in Matrix Recovery Problems

The general matrix recovery problem is the following: A is a large unknown matrix. We can only observe its noisy version A+E, or in some cases just a small part of it. We would like to reconstruct A or estimate an important parameter as accurately as possible from the observation. In a recent work, we study how much the singular value or singular vector of data matrix will change under a small perturbation. We show that better estimates can be achieved if the data matrix is low rank and the perturbation is random, improving the classical perturbation results. In this talk, I would like to discuss some applications of our results in the matrix recovery problems. This is joint work with Sean O'Rourke and Van Vu.

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MS35

A Hybrid LSMR Algorithm for Large-Scale Tikhonov Regularization

We develop a hybrid iterative approach for computing solutions to large-scale ill-posed inverse problems via Tikhonov regularization. We consider a hybrid LSMR algorithm, where Tikhonov regularization is applied to the LSMR subproblem rather than the original problem. We show that, contrary to standard hybrid methods, hybrid LSMR iterates are not equivalent to LSMR iterates on the directly regularized Tikhonov problem. Instead, hybrid LSMR leads to a different Krylov subspace problem. We show that hybrid LSMR shares many of the benefits of standard hybrid methods such as avoiding semiconvergence behavior. In addition, since the regularization parameter can be estimated during the iterative process, it does not need to be estimated a priori, making this approach attractive for large-scale problems. We consider various methods for selecting regularization parameters and discuss stopping criteria for hybrid LSMR, and we present results from image processing.

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MS35

Lanczos Bidiagonalization with Subspace Augementation for Discrete Inverse Problems

The regularizing properties of Lanczos bidiagonalization were studied and advocated by many researchers, including Dianne O'Leary. This approach is powerful when the underlying Krylov subspace captures the dominating components of the solution. In some applications the regularized solution can be further improved by augmenting the Krylov subspace with a low-dimensional subspace that represents specific prior information. Inspired by earlier work on GMRES we demonstrate how to carry these ideas over to the Lanczos bidiagonalization algorithm.

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MS35

A Flexible Regression Model for Count Data

Poisson regression is a popular tool for modeling count data and is applied in a vast array of applications. Real data, however, are often over- or under-dispersed and, thus, not conducive to Poisson regression. We instead propose a regression model based on the ConwayMaxwell-Poisson (COM-Poisson) distribution to address this problem. The COM-Poisson regression generalizes the well-known Poisson and logistic regressions, and is suitable for fitting count data with a wide range of dispersion levels.

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MS35

Solving Eigenvalue and Linear System Problems on GPU for Three-Dimentional Photonic Device Simulations

Solutions of discretized Maxwell's equations are essential to three-dimensional photonic device simulations. For full bandgap diagrams of photonic crystals, we demonstrate how the wanted interior eigenvalues can be computed in a ultrafast manner by the nullspace free algorithm on a multiple-GPU cluster. For linear systems in frequency-domain simulation, we explore the homogeneous and periodic structures to develop a domain decomposition type algorithm. The algorithm significantly reduces the memory usage with satisfactory scalability and acceleration performance.

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MS36

Rotated Block Two-by-Two Preconditioners Based on Pmhss

Motivated by the HSS iteration method, to solve the distributed control problem we have proposed modified HSS (MHSS) as well as preconditioned and modified HSS

(PMHSS) iteration methods. Theoretical analyses and numerical experiments have shown the effectiveness of these iteration methods when used either as linear solvers or as matrix preconditioners for Krylov subspace methods. Moreover, we have developed the PMHSS iteration method to block two-by-two matrices of non-Hermitian sub-blocks, resulting in the additive-type and the rotated block triangular preconditioners. Spectral analyses and numerical computations have shown that these preconditioners can significantly accelerate the convergence rates of the Krylov subspace iteration methods when they are used to solve the block two-by-two linear systems, and the inexact variants these preconditioners are as effective and robust as the corresponding exact ones.

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MS36

Optimal Order Multigrid Preconditioners for Linear Systems Arising in the Semismooth Newton Method Solution Process of a Class of Control-Constrained Problems

We introduce multigrid preconditioners for the semismooth Newton solution process of certain optimal control problems with control-constraints. Each semismooth Newton iteration essentially requires inverting a principal submatrix of the matrix entering the normal equations of the associated unconstrained optimal control problem. Using a piecewise constant discretization of the control space and non-conforming coarse spaces, we show that, under reasonable geometric assumptions, the preconditioner approximates the inverse of the desired matrix to optimal order.

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MS36

The Iterative Solution of Systems from Pde Constrained Optimization: An Overview

In this, the introductory talk of the minisymposium "Linear Algebra for PDE-constrained optimization", we set the scene by introducing the PDE-constrained optimization problem and describe a few of the ways such problems can be discretized, give the resulting linear systems. Solving this linear system is typically the bottleneck in codes that solve such problems, and fast and efficient iterative methods to do this are the topic of this session. We describe a number of the common methods to solve such systems, and set the scene for the rest of the talks in the minisymposium.

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MS36

Inexact Full-space Methods for PDE-constrained Optimization

We discuss a hierarchy of inexact full-space methods for large-scale optimization known as matrix-free sequential quadratic programming (SQP) methods. The hierarchy is based on the increasing complexity of linear systems and, consequently, the increasing flexibility in the design of efficient linear solvers and preconditioners. We examine the solver performance on large-scale optimization problems with linear and nonlinear PDE constraints, related to the optimal design of acoustic fields and optimal control of radiative heat transfer.

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MS37

Eigenvalues and Beyond

Spectral graph partitioning and graph-based signal processing are mathematically based on the spectral decomposition of the graph Laplacian. Computing the full eigenvalue decomposition is impractical, since the graph Laplacian can be of an enormous size. Thus, iterative approaches are of great importance such as, e.g., approximate low-pass filters resulted from Chebyshev and Krylov based iterations. We present an overview of some of our recently published results in this area.

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MS37

Implementation of LOBPCG for Symmetric Eigenvalue Problems in SLEPc

SLEPc is a parallel library that provides a collection of eigenvalue solvers such as Krylov-Schur and Jacobi-Davidson. We have recently added an implementation of LOBPCG, the Locally Optimal Block Preconditioned Conjugate Gradient method [Knyazev, SIAM J. Sci. Comput. 23 (2001)]. In this talk we discuss several implementation details, such as locking, block-orthogonalization, and multi-vector operations, and compare the performance with the solver provided in BLOPEX (which is also interfaced in SLEPc).

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MS37

Spectrum Slicing by Polynomial and Rational Function Filtering

Filtering techniques are presented for solving eigenvalue large Hermitian problems by spectrum slicing. Polynomial filtering techniques can be quite efficient in the situation where the matrix-vector product operation is inexpensive and when a large number of eigenvalues is sought, as is the case in electronic structure calculations for example. Rational filtering techniques will also be described with a focus on showing the advantages of such filters obtained by a least-squares approach.

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MS37

Techniques for Computing a Large Number of Eigenpairs of Sparse, Hermitian Matrices

Computing a large number, m, of extreme or interior eigenvalues of sparse Hermitian matrices remains an outstanding problem in many applications, including materials science and lattice QCD. Current state-of-the-art methods are limited by the cost of the orthogonalization or the Rayleigh Ritz step which grows cubicly with m. We present a window approach that uses high degree polynomials to avoid both steps, at the expense of more matrix-vector products.

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MS38

Data Sparse Techniques for Parallel Hybrid Solvers

In this talk we will describe how H-matrix data sparse techniques can be implemented in a parallel hybrid sparse linear solver based on algebraic non overlapping domain decomposition approach. Strong-hierarchical matrix arithmetic and various clustering techniques to approximate the local Schur complements will be investigated, aiming at reducing workload and memory consumption while complying with structures of the local interfaces of the sub-domains. Utilization of these techniques to form effective global preconditioner will be presented.

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MS38

Title Not Available at Time of Publication

Abstract not available at time of publication.

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MS38

Fast Solvers for H^2 Matrices Using Sparse Algebra

We will present a new class of preconditioners for sparse matrices, based on hierarchical matrices. Similar to the incomplete LU algorithm, this preconditioner controls the sparsity of the matrix as the LU factorization is progressing. However, low-rank approximations instead of thresholding are used to remove the fill-in. This solver also shares similarities with algebraic multigrid in its use of multiple scales to represent the problem. Many variants of these new preconditioners exist. We will focus on variants that use either a domain decomposition approach (simpler to implement), or multifrontal approach (optimal but more difficult to program). These solvers were shown to guarantee a bounded number of iterations independent of the matrix size N. The cost of the preconditioner is $O(r^2N)$ where r is the rank used in the approximation. r has a slow dependence on N (logarithmic or slower).

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MS38

A Tensor Train Decomposition Solver for Integral Equations on Two and Three Dimensions

We present an efficient method based on TT (tensor train) decomposition for solving volume and boundary integral equations in 2D and 3D. This method proceeds by interpreting the corresponding matrix as a high-dimensional tensor, exploiting a matrix-block low-rank structure to produce a highly compressed approximation of the inverse. For a variety of problems, computational cost and storage needed to construct a preconditioner are very low, compared to existing methods, with experimentally observed complexity $O(\log N)$ or lower. Once computed, it allows for a fast $O(N \log N)$ solve. For volume and boundary integrals in simple geometries, our method yield a practical fast $O(N)$ direct solver. For boundary integrals in complex geometries, we show that a low accuracy approximation can be reliably used as a preconditioner.

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MS39

Approximating Kernel Matrix with Recursive Low-Rank Structure

Given a positive-definite function ϕ and a set of n points $\{x_i\}$, a kernel matrix Φ has the (i,j) element being $\phi(x_i, x_j)$. Kernel matrices play an important role in Gaussian process modeling and are widely used in statistics and machine learning. A challenge, however, is that many calculations with these matrices are $O(n^3)$. We present an approximation with a recursive low-rank structure that preserves the positive definiteness of the matrix. A benefit of the structure is that it allows an $O(n)$ cost for many matrix computations of interest. We also present bounds to characterize the asymptomatic convergence of the approximation.

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MS39

A Robust Algebraic Schur Complement Preconditioner Based on Low Rank Corrections

In this talk we discuss LORASC, a robust algebraic preconditioner for solving sparse linear systems of equations involving symmetric and positive definite matrices. The graph of the matrix is partitioned by using k-way partitioning with vertex separators into N disjoint domains and a separator formed by the vertices connecting the N domains. The obtained permuted matrix has a block arrow structure. The preconditioner relies on the Cholesky factorization of the first N diagonal blocks and on approximating the Schur complement corresponding to the separator block. The approximation of the Schur complement involves the factorization of the last diagonal block and a low rank correction obtained by solving a generalized eigenvalue problem or a randomized algorithm. The preconditioner can be build and applied in parallel. Numerical results on a set of matrices arising from the discretization by the finite element method of linear elasticity models illustrate the robusteness and the efficiency of our preconditioner.

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MS39

A Comparison of Different Low-Rank Approximation Techniques

Linear solvers and preconditioners based on structured matrices have gained popularity in the past few years. In particular, Hierarchically Semi-Separable (HSS) matrices, Hierarchically Off-Diagonal Low-Rank (HODLR) matrices and Block Low-Rank (BLR) matrices have been used to design both dense and direct solvers. In this presentation we compare these three techniques from a theoretical and practical standpoint, using large dense and sparse problems from real applications.

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MS39

An Algebraic Multilevel Preconditioner with Low-Rank Corrections for General Sparse Symmetric Matrices

In this talk we present a multilevel Schur low rank (MSLR) preconditioner for general sparse symmetric matrices. This preconditioner exploits a low-rank property that is satisfied by the difference between the inverses of the local Schur complements and specific blocks of the original matrix and computes an approximate inverse of the original matrix following a tree structure. We demonstrate its efficiency and robustness through various numerical examples.

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MS40

Spectral Clustering with Tensors

Two of the fundamental analyses of networks are clustering (partitioning, community detection) and the frequency of network motifs, or patterns of links between nodes. However, these analyses are disjoint as community structure is typically defined by link relationships and ignore motifs. Here, we unify these two ideas through motif-based spectral clustering. Our framework represents motifs through adjacency tensors and uses Markov chains derived from these tensors to find motif-based clusters.

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MS40

Spacey Random Walks, Tensor Eigenvalues, and Multilinear PageRank

This presentation will present an overview of the minisymposia. Then we'll introduce the spacey-random walk, a new type of stationary distribution that gives rise to a tensor eigenvalue problem. We'll conclude by discussing the multilinear PageRank vector and conditions when the PageRank eigenvector is unique and easy to compute.

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MS40

Eigenvalues of Tensors and a Second Order Markov Chain

It is possible to generalize the notion of eigenvalues of matrices to eigenvalues of tensors, from both algebraic and geometric perspectives. Many interesting properties of eigenvalues of matrices have analogues for eigenvalues of tensors. Especially, there are Perron-Frobenius type theorems for eigenvalues of nonnegative tensors. The theory can be applied to study a particular second order Markov chain model. This talk will present some attempts along this way.

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MS40

The Anatomy of the Second Dominant Eigenvalue in a Transition Probability Tensor — The Power Iteration for Markov Chains with Memory

Though ineffective for general eigenvalue computation, the power iteration has been of practical usage for computing the stationary distribution of a stochastic matrix. For a Markov chain with memory m, the transition "matrix" becomes an order-m tensor. Under suitable tensor products, the evolution of the chain with memory toward the limiting probability distribution can be interpreted as two types of power-like iterations — one traditional and the other shorter alternative. What is not clear is the makeup of the "second dominant eigenvalue" that affects the convergence rate of the iteration, if the method converges at all. Casting the power method as a fixed-point iteration, this paper examines the local behavior of the nonlinear map and identifies the cause of convergence or divergence. Equipped with this understanding, it is found that there exists an open set of irreducible and aperiodic transition probability tensors where the short-cut type of power iterates fail to converge.

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MS41

Solving the Bethe-Salpeter Eigenvalue Problem using Low-rank Tensor Factorization and a Reduced Basis Approach

The Bethe-Salpeter equation (BSE) is a reliable model for estimating the absorption spectra in molecules on the basis of accurate calculation of the excited states from first principles. Direct diagonalization of the BSE matrix is intractable due to the $\mathcal{O}(N^6)$ complexity w.r.t. the atomic orbitals basis set. We present a new approach, yielding a complexity of $\mathcal{O}(N^3)$, based on a low-rank tensor approximation of the dense matrix blocks and a reduced basis approach.

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MS41

Fast Direct Solvers as Preconditioners for Time Evolution Problems

For problems involving time evolution of geometries, the cost of a time step is often dominated by the cost of solv-

ing an integral equation. Typically, iterative solution techniques requiring many iterations are used as the computation of a direct solver is too expensive to be done at each time step. This talk will illustrate the potential of creating a high accuracy approximate inverse for a reference geometry as preconditioner for the evolved geometries.

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MS41

Hierarchical Matrix Factorization of the Inverse.

Given a sparse matrix, its LU-factors, inverse and inverse factors typically suffer from substantial fill-in, leading to non-optimal complexities in their computation as well as their storage. We will focus on the construction and representation of the (LU-) factors of the inverse of a matrix. We introduce a blockwise approach that permits to replace (exact) matrix arithmetic through (approximate but efficient) $\mathcal{H}$-arithmetic. We conclude with numerical results to illustrate the performance of different approaches.

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MS41

H-Matrices for Elliptic Problems: Approximation of the Inverses of FEM and BEM Matrices.

Typically, the inversion or factorization of a rank-structured matrix cannot be performed exactly. A basic question, therefore, is whether the inverse or the factors can at least be approximated well in the chosen target format. For the format of $\mathcal{H}$-matrices (introduced by W. Hackbusch), which are blockwise low-rank matrices, we show that indeed the inverses of Galerkin matrices arising in FEM and in BEM can be approximated at an exponential rate in the block rank.

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MS42

Matrix Computations and Text Summarization

Automatic text summarization is an approach to addressing information overload. Machine-generated summaries are applied to a range of genres from newswire to scientific reports. A user is presented with the key elements, extracted from one or more documents and arranged to be both coherent and nonredundant. This talk will focus on matrix computations in text summarization, including Markov models, the QR decomposition, nonnegative matrix factorization and robust regression.

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MS42

Towards Textbook Multigrid for the Helmholtz Equation

The paper [H.C. Elman, O. G. Ernst and D. P. O'Leary: A multigrid method enhanced by Krylov subspace iteration for discrete Helmholtz equations] introduced a novel way of combining Krylov subspace iterations with a standard multigrid V-cycle to obtain a robust solver for the Helmholtz equation which scales favorably with the wave number parameter. It also gave a simple model problem eigenvalue analysis which explained why the standard multigrid V-cycle will, in general, fail for the large wavenumber case. In this talk we present some advances that have been made since then, and show how a similar analysis can be used to examine the behavior of the Wave-Ray Method of Brand and Livshits.

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MS42

Symmetric Tensor Analysis

A symmetric tensor is a multiway array that is invariant under permutation of its indices. We consider the problem of decomposing a real-valued symmetric tensor as the sum of symmetric outer products of real-valued vectors, including the consideration of constraints such as nonnegativity and orthogonality. Application of standard numerical optimization methods can be used to solve these problems. We also consider the data structures for efficiently storing symmetric tensors and the related decompositions.

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MS42

Blocks, Curves, and Splits: A Glimpse into the O'Leary Toolbox

Along with mathematical results, Dianne O'Leary's body of work includes a wide variety of numerical algorithms, techniques, and strategies that can, in her words, be viewed as "tools in our virtual toolbox". Among these are blocks that capture relationships in form, structure, and sparsity; curves that adaptively trace an enlightening, improving path; and splits that partition unknowns and equations to improve speed, accuracy, and flexibility. This talk will present an overview of her work from this perspective, beginning with her earliest days as a PhD student.

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MS43

Solving Large Scale NNLS Problems Arising In Computer Vision

Given a set of images of a scene, the problem of reconstructing the 3D structure of the scene and estimating the pose of the camera(s) when acquiring these images can be formulated as non-linear least squares problem. Relatively small instances (tens of images) of this problem lead to Jacobians with thousands of columns and tens of thousands of rows. I will describe some new techniques for efficiently

solving problems with hundreds of thousands of images. These techniques combine ideas from Domain Decomposition, data clustering and truncated Newton methods.

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MS43

Modulus Iterative Methods for Least Squares Problems with Box Constraints

For the solution of large sparse box constrained least squares problems (BLS), a new iterative method is proposed using generalized SOR method for the inner iterations, and the accelerated modulus iterative method for the outer iterations for the solution of the linear complementarity problem resulting from the Karush-Kuhn-Tucker condition of the BLS problem. Theoretical convergence analysis is presented. Numerical experiments show the efficiency of the proposed method with less iteration steps and CPU time compared to projection methods.

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MS43

LU Preconditioning for Full-Rank and Singular Sparse Least Squares

Sparse QR factorization is often the most efficient approach to solving sparse least-squares problems $\min \|Ax-b\|$, especially since the advent of Davis's SuiteSparseQR software. For cases where QR factors are unacceptably dense, we consider sparse LU factors from LUSOL for preconditioning an iterative solver such as LSMR. LUSOL computes factors of the form $P_1AP_2 = LU$, with permutations chosen to preserve sparsity while ensuring L is well-conditioned. For full-rank problems, one can right-precondition with either U or B, where B is a basis from the rows of A defined by P_1 [Saunders, 1979]. More recently, Duff and Arioli have recommended that B be chosen to have maximum volume. We experiment with LUSOL and LSMR on many realistic examples. For singular problems we make use of LUSOL's threshold rook pivoting option, and investigate whether threshold complete pivoting increases the volume of B in a useful way.

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MS43

The State-of-the-Art of Preconditioners for Sparse Linear Least Squares

In recent years, a number of different preconditioning strategies have been proposed for use in solving $m \times n$ overdetermined large sparse linear least squares problems. However, little has been done in the way of comparing their performances in terms of efficiency, robustness and applicability. In this talk, we briefly review the different preconditioners and present a numerical evaluation of them using a large set of problems arising from practical applications.

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MS44

A Structure-preserving Lanczos Algorithm for the Complex J-symmetric Eigenproblem

A structure-preserving Lanczos algorithm for the eigenproblem $H_C x = \lambda x$ with

$$H_C = \begin{bmatrix} A & C \\ D & -A^T \end{bmatrix}$$

and $n \times n$ complex matrices $A, C = C^T, D = D^T$ will be considered. Matrices H_C are called complex-J-symmetric where $J = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}$ and I_n is the $n \times n$ identity. The eigenvalues of H_C display a symmetry: they appear in pairs $(\lambda, -\lambda)$. The structure-preserving algorithm is based on similarity transformations with $2n \times 2n$ complex symplectic matrices S_C, $S_C^T J S_C = J$. These matrices form the automorphism group associated with the Lie algebra of complex-J-symmetric matrices. The similarity transformation $S_C^{-1} H_C S_C$ yields a complex-J-symmetric matrix.

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MS44

Structure Preserving Algorithms for Solving the Bethe–Salpeter Eigenvalue Problem

In the numerical computation of electron-hole excitations,

we need to solve a complex J-symmetric eigenvalue problem arising from the discretized Bethe–Salpeter equation. In general all eigenpairs are of interest in this dense eigenvalue problem. We develop new algorithms by investigating the connection between this problem and the Hamiltonian eigenvalue problem. Compared to several existing approaches, our algorithm is fully structure preserving, and is easily parallelizable. Computational experiments demonstrate the efficiency and accuracy of our algorithm.

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MS44

Preconditioned Locally Harmonic Residual Methods for Interior Eigenvalue Computations

This talk describes a Preconditioned Locally Harmonic Residual (PLHR) method for computing several interior eigenpairs of a generalized Hermitian eigenvalue problem, without traditional spectral transformations, matrix factorizations, or inversions. PLHR is based on a short-term recurrence, easily extended to a block form, computing eigenpairs simultaneously. The method takes advantage of Hermitian positive definite preconditioning. We also discuss generalizations of PLHR on non-Hermitian eigenproblems and cases where only an indefinite preconditioner is at hand. We demonstrate that PLHR is an efficient and robust option for interior eigenvalue calculation, especially if memory requirements are tight.

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MS44

Preconditioned Solvers for Nonlinear Hermitian Eigenproblems with Variational Characterization

Large-scale nonlinear Hermitian eigenproblems of the form $T(\lambda)v = 0$ satisfying the standard variational characterization arises in a variety of applications. We review some recent development of numerical methods for solving eigenproblems of this type, including variants of preconditioned conjugate gradient (PCG) methods for extreme eigenvalues, and preconditioned locally minimal residual (PLMR) methods for interior eigenvalues. We discuss the development of search subspaces, projection and extractions, preconditioning, deflation, and convergence analysis of these methods. Numerical experiments demonstrate the efficiency and competitiveness of our algorithms.

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MS45

Fast Hierarchical Randomized Methods for the Approximation of Large Covariance Matrices

We propose a new efficient algorithm for performing hierarchical kernel MVPs in $\mathcal{O}(N)$ operations called the Uniform FMM (UFMM), an FFT accelerated variant of the black box FMM by Fong and Darve. The UFMM is used to speed up randomized low-rank methods thus reducing their computational cost to $\mathcal{O}(N)$ in time and memory. Numerical benchmarks include low-rank approximations of covariance matrices for the simulation of stationary random fields on very large distributions of points.

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MS45

Algebraic Operations with $\mathcal{H}^2$-Matrices

We present a family of algorithms that perform approximate algebraic operations on $\mathcal{H}^2$-matrices. These algorithms allow us to compute approximations of factorizations, inverses, and products of $\mathcal{H}^2$-matrices in almost linear complexity with respect to the matrix dimension. Compared to previous methods, our approach is based on *local low-rank updates* that can be carried out in linear complexity. All other matrix operations can be expressed by these updates and simple matrix-vector products, and we obtain a fast and flexible technique for, e.g., constructing robust preconditioners for integral and elliptic partial differential operators.

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MS45

Fast Numerical Linear Algebra for Kohn-Sham Density Functional Theory via Compression

In this talk we discuss algorithms for accelerating the solution of the non-linear eigenvalue and eigenvector problem in Kohn-Sham density functional theory. Solving this problem self consistently requires the repeated computation and application of various linear algebraic operators. As part of this talk we demonstrate how to construct a localized, and hence sparse, representation of basis functions that allows for reductions in the overall computational cost.

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MS45

Comparison of FMM and HSS at Large Scale

We perform a direct comparison between the fast multipole method (FMM) and hierarchically semi separable (HSS) matrix-vector multiplication for Laplace, Helmholtz, and Stokes kernels. Both methods are implemented with distributed memory, thread, and SIMD parallelism, and the runs are performed on large Cray systems such as Edison (XC30, 133,824 cores) at NERSC and Shaheen2 (XC40, 197,568 cores) at KAUST.

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MS46

A Stable and Efficient Matrix Version of the Fast Multipole Method

It is well known that Fast Multipole Method (FMM) is very efficient for evaluating matrix-vector products involving discretized kernel functions. In contrast, hierarchically semiseparable (HSS) representations provide a fast and stable way for many matrix operations, especially direct factorizations. However, HSS forms have always been constructed based on algebraic compression(e.g., SVD) of off-diagonal blocks. In this work, we show how to directly obtain an HSS representation from the matrix derived in FMM.

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MS46

Some Recent Progress on Algorithms for FMM Matrices

There are simple time efficient $O(N^2)$ algorithms for converting a general dense matrix to FMM form using a prior partition tree. We show that there is a surprise as far as memory efficiency goes, and present a $O(N^{1.5})$ working memory algorithm and a corresponding worst case family of partition trees. It is an open question whether there is a construction algorithm that only requires $O(N)$ work space. On another front, there is a simple $O(N)$ flops algorithm to multiply two HSS forms exactly. However the corresponding question for FMM forms has remained open. We show how to close it.

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MS46

Fast Linear Solvers for Weakly Hierarchical Matrices

In recent years, we have seen the development of a new class of linear solvers and preconditioners based on hierarchical low-rank approximations of matrices. Such solvers have been very successful and can solve problems that are currently intractable or very expensive using conventional preconditioners such as block diagonal, incomplete LU, algebraic multigrid, etc. However, the computational cost of these solvers currently fails to scale linearly with the size of the matrix. This is true in particular for 3D elliptic partial differential equations. In this talk, we will present a new version of these fast solvers that scale like O(N) for general situations. We will see how these solvers are able to represent dense matrices using (slightly larger) sparse matrices, and how the fill-in that appears during the LU factorization of these sparse matrices can be removed, so that the algebra remains sparse throughout the process. As a result of this new approach, all steps are O(N), even in 3D. This results in very fast linear solvers that scale favorably with the problem size.

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MS46

MHS Structures for the Direct Solution of Multi-Dimensional Problems

We propose multi-layer hierarchically semiseparable

(MHS) structures for the efficient factorizations of dense matrices arising from multi-dimensional discretized problems. The problems include discretized integral equations and dense Schur complements in the factorizations of discretized PDEs. Unlike existing work on hierarchically semiseparable (HSS) structures which are essentially 1D structures, the MHS framework integrates multiple layers of rank and tree structures. We lay theoretical foundations for MHS structures and justify the feasibility of MHS approximations for these dense matrices. Rigorous rank bounds for the low-rank structures are given. Representative subsets of mesh points are used to illustrate the multi-layer structures as well as the structured factorization. Systematic fast and stable MHS algorithms are proposed, particularly convenient direct factorizations. The new structures and algorithms can yield direct solvers with nearly linear complexity and linear storage for solving some practical 2D and 3D problems.

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MS47

A Semi-Tensor Product Approach for Probabilistic Boolean Networks

Modeling genetic regulatory networks is an important issue in systems biology. Various models and mathematical formalisms have been proposed in the literature to solve the capture problem. The main purpose in this paper is to show that the transition matrix generated under semi-tensor product approach (Here we call it the probability structure matrix for simplicity) and the traditional approach (Transition probability matrix) are similar to each other. And we shall discuss three important problems in Probabilistic Boolean Networks (PBNs): the dynamic of a PBN, the steady-state probability distribution and the inverse problem. Numerical examples are given to show the validity of our theory. We shall give a brief introduction to semi-tensor and its application. After that we shall focus on the main results: to show the similarity of these two matrices. Since the semi-tensor approach gives a new way for interpreting a BN and therefore a PBN, we expect that advanced algorithms can be developed if one can describe the PBN through semi-tensor product approach.

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MS47

Positive Diagonal Scaling of a Nonnegative Tensor to One with Prescribed Slice Sums

Given a nonnegative 3-tensor $T = [t_{i,j,k}]$ of dimensions m, n, p, when one can rescale it by three positive vectors $x = (x_1, \ldots, x_m), y = (y_1, \ldots, y_n), z = (z_1, \ldots, z_p)$, such that the tensor $[x_i y_j z_k t_{i,j,k}]$ has given row, column and depth slice sums r_i, c_j, d_k. Here

$$r_i = \sum_{j,k=1}^{n,p} x_i y_j z_k t_{i,j,k},\ c_j = \sum_{i,k=1}^{m,p} x_i y_j z_k t_{i,j,k},\ d_k = \sum_{i,j=1}^{m.n} x_i y_j z_k t_{i,j,k}$$

for $i = 1, \ldots, m, j = 1, \ldots, m, k = 1, \ldots, l$. We give a neccesary and sufficient condition and state a corresponding minimizing problem of a convex function that gives a solution to the diagonal scaling. These results generalize to any d-mode nonnegative tensors. References: S. Friedland, Positive diagonal scaling of a nonnegative tensor to one with prescribed slice sums, *Linear Algebra Appl.*, vol. 434 (2011), 1615-1619.

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MS47

Open Problems and Concluding Discussions

In this final session of our mini-symposia, we will present a summary of the results from all of the other presenters as well as invite them to submit slides for an open problem discussion. The point is to identify a few key problems that could be solved to move the field forward.

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MS47

The Laplacian Tensor of a Multi-Hypergraph

Given a uniform multi-hypergraph $\mathcal{H}$, we define a new hyper-adjacency tensor $\mathbb{A}(\mathcal{H})$ and use it to define the Laplacian $\mathbb{L}(\mathcal{H})$ and the signless Laplacian $\mathbb{Q}(\mathcal{H})$. We prove $\mathbb{L}(\mathcal{H})$ and $\mathbb{Q}(\mathcal{H})$ are positive semi-definite for connected even uniform multigraphs. Some analysis on the largest and smallest H and Z-eigenvalues of $\mathbb{L}(\mathcal{H})$ are given as well as a comparison of other adjacency tensors.

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MS48

Basker: A Scalable Sparse Direct Linear Solver for Many-Core Architectures

In this talk, we describe challenges related to the implementation of a scalable direct linear solver on many-core architectures. Basker focuses on solving irregular systems such as those from circuit simulation. These systems may require full partial pivoting, and cannot be reorder for efficient use of BLAS3 operations. We attempt to mitigate these issues by using a parallel implementation of Gilbert-Peierls method, while developing with Kokkos, which is a framework that allows for portability on emerging many-core architectures.

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MS48

Parallel Iterative Incomplete Factorizations and Triangular Solves

We present asynchronous fine-grained parallel algorithms for computing incomplete LU (ILU) factorizations and performing the corresponding sparse triangular solves. The ILU algorithm computes all the non-zeros of the factors in parallel (asynchronously) using an iterative method. The triangular solves can be performed approximately using another iterative method. We present several modifications from previous work that improve the robustness of the method. We show results from Intel Xeon Phi and GPU using the Kokkos library.

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MS48

A Sparse Direct Solver for Distributed Memory GPU and Xeon Phi Accelerated Systems

In this talk, we presents the first sparse direct solver for distributed memory systems comprising hybrid multicore CPU and Intel Xeon Phi co-processors or GPUs. It builds on the algorithmic approach of SuperLUDist, which is right-looking and statically pivoted. Our contribution is a novel algorithm, called the HALO. The name is shorthand for *highly asynchronous lazy offload*; it refers to the way the algorithm combines highly aggressive use of asynchrony with accelerated offload, lazy updates, and data shadowing (*a la* halo or ghost zones), all of which serve to hide and reduce communication, whether to local memory, across the network, or over PCIe. We further augment HALO with a model-driven autotuning heuristic that chooses the intra-node division of labor among CPU and accelerator components. When integrated into HALO and evaluated on a variety of realistic test problems in both single-node and multi-node configurations, the resulting implementation achieves speedups of up to 2.5× over an already efficient multicore CPU implementation, and achieves up to 83% of a machine-specific upper-bound that we have estimated.

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MS48

Parallel Multilevel Incomplete LU Factorization Preconditioner with Variable-Block Structure

In this talk, we describe a distributed-memory implementation of a variable-block multilevel algebraic recursive iterative preconditioner for general non-symmetric linear systems. The preconditioner construction detects automatically exact or approximate dense blocks in the coefficient matrix and exploits them to achieve better reliability and computation density. To find such a dense-block structure, a graph-compression algorithm has been developed, which requires only one easy-to-use parameter. We present a study of the numerical performance and parallel scalability using additive Schwarz and Schur complement type preconditioners on a variety of general linear systems as well as in the analysis of turbulent Navier-Stokes equations.

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MS49

Solving Sequential Strongly Underdetermined Systems Using Sherman-Morrison Iterations

We are interested in repeatedly solving a regularized linear least squares problem of the form where data become sequentially available. We assume we are given a strongly underdetermined matrix and a Tikhonov type regularization term. Using the Sherman-Morrison-Woodbury formula we were able to develop a fast solver which can compete with methods base on Cholesky factorization and iterative methods such as LSQR, CGLS, and LSMR.

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MS49

A Tensor-Based Dictionary Approach to Tomographic Image Reconstruction

The problem of low-dose tomographic image reconstruction is investigated using dictionary priors learned from training images. The reconstruction problem is considered as a two phase process: in phase one, we construct a tensor dictionary prior from our training data (a process formulated as a non-negative tensor factorization problem), and in phase two, we pose the reconstruction problem in terms of recovering expansion coefficients in that dictionary. Experiments demonstrate the potential utility of our approach.

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MS49

Some Inverse Problems in Optical Imaging for Remote Sensing

Hyperspectral, Light Detection and Ranging (LiDAR), and Polarimetric imaging are the pervasive optical imaging modalities in remote sensing. Here, we describe methods for deblurring and analyzing 3D images of these types, as well as 4D compressive spectro-polarimetric snapshot images.

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MS49

Efficient Iterative Methods for Quantitative Susceptibility Mapping

Quantitative Susceptibility Mapping (QSM) is a MRI technique that allows to image magnetic properties of tissue. QSM is applied more and more widely, for example, in neuroscience, where iron concentration serves as a biomarker of certain neurological diseases. While the tissues susceptibility cannot be measured directly it can be reconstructed by solving a highly ill-posed inverse problem. In this talk, we will present iterative methods for QSM reconstruction and their efficient implementation using Julia. We formulate QSM as a PDE constrained optimization problem with a non-smooth regularizer based on total variation (TV). Special emphasis will be put on iterative all-at-once methods for handling the PDE-constraints.

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MS50

Domain Decomposition Algorithms for Large Hermitian Eigenvalue Problems

In this talk we will discuss Domain-Decomposition (DD) type methods for large Hermitian eigenvalue problems. This class of thechniques rely on spectral Schur complements combined with Newton's iteration. The eigenvalues of the spectral Schur complement appear in the form of branches of some functions, the roots of which are eigenvalues of the original matrix. It is possible to extract these roots by a number of methods which range from a form or approximate Rayleigh iteration to an approximate inverse iteration, in which a Domain Decomposition framework is used. Numerical experiments in parallel environments will illustrate the numerical properties and efficiency of the method.

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MS50

A Contour Integral-based Parallel Eigensolver with Higher Complex Moments

Large-scale eigenvalue problems arise in wide variety of scientific and engineering applications such as nano-scale materials simulation, vibration analysis of automobiles, data analysis, etc. In such situation, high performance parallel eigensolvers are required to exploit distributed parallel computational environments. In this talk, we present a parallel eigensolver (SS method) for large-scale interior eigenvalue problems. This method has a good parallel scalability according to a hierarchical structure of the method. We also present parallel software for computing eigenvalues and corresponding eigenvectors in a given region or interval. We illustrate the performance of the software with some numerical examples.

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MS50

On the Orthogonality of Eigenvectors Obtained from Parallel Spectral Projection Methods

A number of recent eigensolvers have been devised with the aid of some approximate projectors to invariant subspaces. One of the major advantages on the use of these approximate spectral projectors is the natural parallelism they present. Different independent processing tasks can work on different parts of the spectrum in parallel. It is well known that exact eigenvectors from Hermitian problems are mutually orthogonal. On the other hand, some initial studies cast doubts on the numerical orthogonalities of the vectors computed independently when spectral projection

methods are applied in a parallel setting. In this talk we will present several practical approaches to maintain orthogonalities without explicit reorthogonalization between independent tasks.

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MS50

A Contour-Integral Based Algorithm for Counting the Eigenvalues Inside a Region in the Complex Plane

In many applications, the information about the number of eigenvalues inside a given region is required. In this paper, we propose a contour-integral based method for this purpose. The new method is motivated by two findings. Recently, some contour-integral based methods were developed for estimating the number of eigenvalues inside a region in the complex plane. But our method is able to count the eigenvalues inside the given region exactly. An appealing feature of our method is that it can integrate with recently developed contour-integral based eigensolvers to determine whether all desired eigenvalues are found by these methods. Numerical experiments are reported to show the viability of our new method.

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MS51

Parallel Algorithms for Computing Functions of Matrix Inverses

Functions of entries of inverses of matrices like all diagonal entries of a sparse symmetric indefinite matrix inverse or its trace arise in several important computational applications such as density functional theory, covariance matrix analysis or when evaluating Green's functions in computational nanolelectronics. We will utilize an algorithm for selective inversion by Lin et al. (TOMS 2011) for approximately computing selective parts of a sparse symmetric matrix inverse. Its overall performance will be demonstrated for selected numerical examples and we will sketch parallelization aspects for raising the computational efficiency.

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MS51

A Parallel Multifrontal Solver and Preconditioner Using Hierarchically Semiseparable Structured Matrices

We present a sparse solver or preconditioner using hierarchically semi-separable (HSS) matrices to approximate dense matrices that arise during sparse matrix factorization. Using HSS, rank structured matrices with low-rank off-diagonal blocks, reduces fill-in and for many PDE problems, it leads to a solver with lower computational complexity than the pure multifrontal method. For HSS construction, we use a novel randomized sampling technique. Hybrid shared and distributed memory parallel results are presented.

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MS51

Iterative Construction of Non-Symmetric Factored Sparse Approximate Preconditioners

Factored sparse approximate inverses (FSAI) play a key-role in the efficient algebraic preconditioning of sparse linear systems of equations. For SPD problems remarkable results are obtained by building the FSAI non-zero pattern iteratively during its computation. Unfortunately, an equivalent algorithm is still missing in the non-symmetric case. In the present contribution we explore the possibility of iteratively computing FSAI for non-symmetric matrices by using a incomplete Krylov subspace bi-orthogonalization procedure.

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MS51

Monte Carlo Synthetic Acceleration Methods for Sparse Linear Systems

Stochastic linear solvers based on Monte Carlo Synthetic Acceleration are being studied as a potentially resilient alternative to standard methods. Our work has shown that for certain classes of problems, these methods can also demonstrate performance competitive with modern techniques. In this talk we will review recent developments in Monte Carlo solvers for linear systems. Our work targets large, distributed memory systems by adapting Monte Carlo techniques developed by the transport community to solve sparse linear systems arising from the discretization of partial differential equations.

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MS52

A Matrix Equation Approach for Incremental Linear Discriminant Analysis

Abstract not available at time of publication.

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MS52

Riccati Equations Arising in Stochastic Control

The numerical treatment of the infinite dimensional stochastic linear quadratic control problem requires solving large-scale Riccati equations. We investigate the convergence of these Riccati operators to the finite dimensional ones. Moreover, the coefficient matrices of the resulting Riccati equation have a given structure (e.g. sparse, symmetric or low rank). We proposed an efficient method based on a low-rank approach which exploit the given structure. The performance of our method is illustrated by numerical results.

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MS52

Splitting Schemes for Differential Riccati Equations

I will consider the application of exponential splitting schemes to large-scale differential Riccati equations of the form

$$\dot{P} = A^T P + PA + Q - PSP. \tag{3}$$

These numerical methods consider the affine and nonlinear parts of the equation separately, thereby decreasing the necessary computational effort. I will focus on implementation issues and how to utilize low-rank structure. I will also consider several natural generalizations such as time-dependent or implicit problems.

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MS52

Conditioning Number of Solutions of Matrix Equations in Stability Analysis

Abstract not available at time of publication.

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MS53

Kolmogorov Widths and Low-Rank Approximation of Parametric Problems

This talk is concerned with error estimates for low-rank approximation of diffusion equations with several parameters. In particular, we focus on estimates of Kolmogorov n-widths of such solution manifolds, which also allow conclusions to be drawn concerning the performance achievable by model reduction based on the reduced basis method. Moreover, we discuss numerical schemes for the computation of low-rank approximations of such problems. Our theoretical bounds are illustrated by numerical experiments, and the results indicate in particular a surprisingly strong dependence on particular structural features of the problems.

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MS53

A Greedy Method with Subspace Point of View for Low-Rank Tensor Approximation in Hierarchical Tucker Format.

The goal is to approximate high-order tensors in subspace-based low-rank formats. A strategy is proposed for computing adapted nested tensor subspaces in a greedy fashion. The best approximation in these subspaces is then computed with a DMRG-like algorithm, again usign a greedy strategy, allowing an automatic rank adaptation with a reduced complexity compared to standard DMRG. A heuristic error indicator based on singular values enables to capture a possible anisotropy of the tensor of interest.

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MS53

Tensor Krylov Methods

High dimensional models with parametric dependencies can be challenging to simulate. We use tensor Krylov techniques to reduce the parametric model, combining both moment matching and interpolatory model reduction in the parameter space. If a low rank tensor formulation is possible, this approach is competitive with classic parametric model reduction. Furthermore, we look at models containing stochastic parameters and construct a reduced model that outputs the mean over these parameters within the domain of interest.

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MS53

An Adaptive Tensor Method for High-Dimensional Parametric PDEs

We apply the recently developed Tensor Train (TT) format for tensor decomposition to high-dimensional parametric PDEs [Oseledets, Tensor-Train Decomposition, 2011, SIAM J. Sci. Comput. 33, pp. 2295-2317]. Adaptive solvers have been introduced independently [Eigel et al., Adaptive Stochastic Galerkin FEM, Comput. Method. Appl. M. 270, pp. 247-269] but computational cost grows exponentially with the number of dimensions. In particular, the proposed error estimators become unfeasable very quickly for larger problems. The TT format breaks this *curse of dimensionality* and allows for the treatment of these problems. We solve the discretized problem iteratively using the well-known Alternating Least Squares (ALS) algorithm [Holtz et al., The alternating linear scheme for tensor optimisation in the TT format, SIAM J. Sci. Comput. 34, pp. A683-A713] . Furthermore, we exploit the component structure of the tensor format. The error estimation can be computed far more efficiently this way. Numerical results support this approach by showing higher accuracy even for problems of far greater size than previously discussed.

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MS54

Steady-state Analysis of a Multi-class MAP/PH/c Queue with Acyclic PH Retrials

A multi-class c-server retrial queueing system in which customers arrive according to a class-dependent Markovian arrival process (MAP) is considered. Service and retrial times follow class-dependent phase-type (PH) distributions. A necessary and sufficient condition for ergodicity is given. A Lyapunov function is used to obtain a finite state space with a given steady-state probability mass. The truncated system is described as a multi-dimensional Markov chain and a Kronecker representation of its generator matrix is analyzed numerically.

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MS54

The Computation of the Key Properties of Markov Chains using a Variety of Techniques

Techniques for finding the stationary distribution, the mean first passage times and the group inverse of finite irreducible Markov chains is presented. We extend the technique of [Kohlas J., Numerical computation of mean first passage times and absorption probabilities in Markov and semi-Markov models, Zeit fur Oper Res, 30, (1986), 197-207], include some new results involving perturbation techniques as well as some generalised matrix inverse procedures. Accuracies are compared using some test problems in the literature.

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MS54

General Solution of the Poisson Equation for QBDs

If T is the transition matrix of a finite irreducible Markov chain and b is a given vector, the Poisson equation $(I - T)x = b$ has a unique solution, up to an additive constant, given by $x = (I - T)^{\#}b + \alpha 1$, for any α scalar, where 1 is the vector of all ones and $H^{\#}$ denotes the group inverse of H. This does not hold when the state space is infinite. We consider the Poisson equation $(I - P)u = g$, where P is the transition matrix of a Quasi-Birth-and-Death (QBD) process with infinitely many levels, g is a given infinite–dimensional vector and u is the unknown vector. By using the block tridiagonal and block Toeplitz structure of P, we recast the problem in terms of a set of matrix difference equations. We provide an explicit expression of the general solution, relying on the properties of Jordan triples of matrix polynomials and on the solutions of suitable quadratic matrix equations. The uniqueness and boundedness of the solutions are discussed, according to the properties of the right–hand side g.

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MS54

Complex Nonsymmetric Algebraic Riccati Equations Arising in Markov Modulated Fluid Flows

Motivated by the transient analysis of stochastic fluid flow models, we introduce a class of complex nonsymmetric algebraic Riccati equations. The existence and uniqueness of the extremal solutions to these equations are proved. Numerical methods for the extremal solutions are discussed.

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MS55

Recovering Sparsity in a Krylov Subspace Framework

For many ill-posed inverse problems, such as image restoration, the regularized solution may benefit from the inclu-

sion of sparsity constraints, which involve terms evaluated in the 1-norm. Our goal is to efficiently approximate the 1-norm terms by iteratively reweighed 2-norm terms. After presenting some new results on the regularizing properties of Krylov subspace methods, we describe a couple of new approaches to enforce sparsity within a Krylov subspace framework.

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MS55

Structure Preserving Reblurring Preconditioners for Image Deblurring

In the context of image deblurring, we extend a preconditioning technique proposed in [Dell'Acqua et al., JCAM 2013] to a more general method whose preconditioners inherit the boundary conditions of the problem without losing in computational cost. Furthermore, following the idea developed in [Donatelli, Hanke, IP 2013], we introduce a nonstationary version of the proposed method providing further improvements in terms of iterations and quality of reconstruction. Numerical comparisons with the aforementioned techniques are given.

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MS55

SVD Approximations for Large Scale Imaging Problems

A fundamental tool for analyzing and solving ill-posed inverse problems is the singular value decomposition (SVD). However, in imaging applications the matrices are often too large to be able to efficiently compute the SVD. In this talk we present an efficient approach to compute an approximate SVD, which exploits Kronecker product and tensor structures that arise in imaging applications.

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MS55

Arnoldi Methods for Image Deblurring with Anti-Reflective Boundary Conditions

We consider image deblurring with anti-reflective boundary conditions and a nonsymmetric point spread function, and compare several iterative Krylov subspace methods used with with reblurring right or left preconditioners. The purpose of the preconditioner is not to accelerate the rate of convergence, but to improve the quality of the computed solution and to increase the robustness of the regularization method. Right preconditioned methods based on the Arnoldi process are found to perform well.

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MS56

The Use of Stochastic Collocation Methods to Understand Pseudo-Spectra in Linear Stability Analysis

Eigenvalue analysis is a well-established tool for stability analysis of dynamical systems. However, it is also known that there are situations where eigenvalues miss some important features of physical models. For example, in models of incompressible fluid dynamics, there are examples where eigenvalue analysis predicts stability but transient simulations exhibit significant growth of infinitesmal perturbations. This behavior can be predicted by pseudo-spectral analysis. In this work, we show that an approach similar to pseudo-spectral analysis can be performed inexpensively using stochastic collocation methods and the results can be used to provide quantitive information about the nature and probability of instability.

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MS56

Large-Scale Eigenvalue Calculations in Scientific Problems

We will consider the problem of computing a relatively large number of eigenvalues of a large sparse and symmetric matrix on distributed-memory parallel computers. The problem arises in several scientific applications, such as electronic structure calculations. We will discuss the use of spectrum slicing and multiple shift-invert Lanczos in computing the eigenvalues. This is joint work with Hasan Metin Aktulga, Lin Lin, Christopher Haine, and Chao Yang.

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MS56

Accurate Computations of Eigenvalues of Diagonally Dominant Matrices with Applications to Differential Operators

In this talk, we present an algorithm that computes all eigenvalues of a symmetric diagonally dominant matrix to high relative accuracy. We further consider using the algorithm in an iterative method for a large scale eigenvalue problem and we show how smaller eigenvalues of finite difference discretizations of differential operators can be computed accurately. Numerical examples are presented to demonstrate the high accuracy achieved by the new algorithm.

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MS56

Convergence of the Truncated Lanczos Approach for the Trust-Region Subproblem

The Trust-Region Subproblem plays a vital role in various other applications. The truncated Lanczos approach proposed in [Gould, Lucidi, Roma and Toint, SIAM J. Optim., 9:504–525 (1999)] is a natural extension of the Lanczos method and mimics the Rayleigh-Ritz procedure. In this paper, we analyze the convergence of the truncated Lanczos approach and reveals its convergence behavior in theory. Numerical examples are reported to support our analysis.

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MS57

Low-Rank Approximation Preconditioners for Symmetric and Nonsymmetric Systems

This talk will present a few preconditioning techniques based on low-rank approximations, designed for the general framework of the domain decomposition (DD) approach and distributed sparse matrices. The DD decouples the matrix and yields two variants of preconditioners. The first is an approximate inverse of the original matrix based on a low-rank correction that exploits the Sherman-Morrison-Woodbury formula. The second method is based on the Schur complement technique and it is based on approximating the inverse of the Schur complement. Low-rank expansions are computed by the Lanczos/Arnoldi procedure with reorthogonalization. Numerical experiments with Krylov subspace accelerators will be presented for symmetric indefinite systems and nonsymmetric systems. These methods were found to be more efficient and robust than ILU and multilevel ILU-type preconditioners.

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MS57

An Algebraic Multigrid Method for Nonsymmetric Linear Systems

Linear systems with multiple physical unknowns pose a challenge for standard multigrid techniques, particularly when the coupling between the unknowns is strong. We present our efforts to develop an AMG-preconditioned Krylov solver for nonsymmetric systems of linear equations. The preconditioner is designed to represent the coupling between the physical variables and account for the underlying physics of the system. We present performance results for the solver on challenging flow and transport applications.

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MS57

Aggressive Accelerator-Enabled Local Smoothing Via Incomplete Factorization, with Applications to Preconditioning of Stokes Problems with Heterogeneous Viscosity Structure

Hybrid supercomputers offer attractive performance per Watt, yet present communication-related bottlenecks. We investigate "heavy smoothing' with multigrid preconditioners; aggressive coarsening with accelerator-enabled smoothing can reduce communication, maintaining scalability and admitting a tradeoff between local work and non-local communication. We examine local polynomial smoothing as well as the Chow-Patel fine-grained ILU decomposition. Our work aims to provide portable software contributions within ViennaCL, PETSc, and pTatin3D. We apply the smoothers to ill-conditioned systems from lithospheric dynamics.

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MS57

Preconditioned Iterative Methods for Solving In-

definite Linear Systems

Sparse symmetric indefinite linear systems of equations arise in many practical applications. A preconditioned iterative method is frequently the method of choice. In the talk we consider both general indefinite systems and saddle-point problems and we summarize our work along these lines based on the recently adopted limited memory approach. A number of new ideas proposed with the goal of improving the stability, robustness and efficiency of the resulting preconditioner will be mentioned.

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MS58

The s-Step Lanczos Method and its Behavior in Finite Precision

The s-step Lanczos method can reduce communication by a factor of $O(s)$ versus the classical approach. By translating results of the finite-precision block process back onto the individual elements of the tridiagonal matrix, we show that the bounds given by Paige [*Lin. Alg. Appl.*, 34:235–258, 1980] apply to the s-step case under certain assumptions. Our results confirm the importance of the s-step basis conditioning and motivate approaches for improving finite precision behavior while still avoiding communication.

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MS58

Sparse Approximate Inverse Preconditioners for Communication-Avoiding Bicgstab Solvers

Communication-avoiding formulations of Krylov solvers can reduce communication costs by taking s steps of the solver at the same time. In this work, we address the lack of preconditioners for communication-avoiding Krylov solvers. We derive a preconditioned variant of the s-step BiCGStab iterative solver and demonstrate the effectiveness of Sparse Approximate Inverse (SAI) preconditioners in improving the convergence rate of the preconditioned s-step BiCGStab solver while maintaining the reduction in communication costs.

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MS58

Enlarged Krylov Subspace Methods for Reducing Communication

We introduce a new approach for reducing communication in Krylov subspace methods that consists of enlarging the Krylov subspace by a maximum of t vectors per iteration, based on the domain decomposition of the graph of A. The enlarged Krylov projection subspace methods lead to faster convergence in terms of iterations and parallelizable algorithms with less communication, with respect to Krylov methods. We present three enlarged CG versions, MSDO-CG, LRE-CG and SRE-CG.

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MS58

Preconditioning Communication-Avoiding Krylov Methods

Krylov subspace projection methods are the most widely-used iterative methods for solving large-scale linear systems of equations. Communication-avoiding (CA) techniques can improve Krylov methods' performance on modern computers. However, in practice CA-Krylov methods suffer from lack of good preconditioners that can work seamlessly in a communication-avoiding fashion. I will outline a domain decomposition like framework for a family of preconditioners that are suitable for CA Krylov methods. Within this framework, we can envision multiple preconditioners that can work seamlessly with a CA-Krylov method. I will present the first few preconditioners we have developed so far and present results comparing these preconditioned CA techniques to traditional methods.

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MS59

Low-rank Tensor Approximation of Singular Functions

We study the *quantized tensor train* approximation of singular functions, which are given, in low-order discretizations, by coefficient tensors. The functions of interest are analytic but with singularities on the boundary of the domain. Such functions arise, for example, as solutions of linear second-order elliptic problems, where the singularities are inherited from the data or occur due to the nonsmoothness of the domain. We show that the QTT approximation achieves, theoretically and algorithmically, the optimal approximation accuracy ε with polylogarithmic ranks $\mathcal{O}(\log^{\kappa} \varepsilon^{-1})$. That renders the low-rank QTT representation, which is amply adaptive and non-specific to the particular class of functions, comparable or even superior to special techniques such as *hp* approximations. CS was supported by the European Research Council (ERC) under AdG 247277.

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MS59

A Variant of Alternating Least Squares Tensor Completion in TT-Format

We fit a low rank tensor $A \in \mathbb{R}^{\mathcal{I}}$, $\mathcal{I} = \{1, \ldots, n\}^d$, to a given set $\{M_i \in \mathbb{R} \mid i \in P\}$, $P \subset \mathcal{I}$ being unchangeable. Considered is the TT-format with target rank r (rank adaption is realizable), while $M \in \mathbb{R}^{\mathcal{I}}$ (e.g. certain multivariate functions) is assumed rank structured. A SOR-type solver ADF with $\mathcal{O}(r^2 d \#P)$ computational complexity (r^2 lower than alternating least squares (ALS)) is presented, working with $\#P = cdnr^2 \sim \log(\#\mathcal{I})$ samples. As good results as for ALS, yet a significantly lower runtime are observed rank $r = 4, \ldots, 20$, given $d \leq 50$, $n \leq 100$ and $c \geq 2$.

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MS59

Low Rank Approximation of High Dimensional Functions Using Sparsity Inducing Regularization

Approximation of high dimensional stochastic functions using functional approaches is often limited by the so called curse of dimensionality. In literature, approximation methods often rely on exploiting particular structures of high dimensional functions. One such structure which is increasingly found to be applicable in these functions is sparsity on suitable basis. Also, these functions exhibit optimal low rank representation and can be approximated in suitable low rank tensor subsets. In this work, we exploit sparsity within low rank representation to approximate high dimensional stochastic functions in a non intrusive setting using few sample evaluations. We will illustrate this approach on suitable examples arising in computational sciences and engineering.

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MS59

Riemannian Optimization for High-Dimensional Tensor Completion

Tensor completion aims to reconstruct a high-dimensional data set with a large fraction of missing entries. Assuming low-rank structure in the underlying data allows us to cast the problem into an optimization problem restricted to the manifold of fixed-rank TT tensors. We present a Riemannian nonlinear conjugate gradient scheme scaling linearly with the number of dimensions. In numerical experiments, we show the effectiveness of our approach and compare to adaptive sampling techniques such as cross-approximation.

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MS60

Rank-Structured PDE Solvers

We describe a "superfast" Cholesky code based on CHOLMOD, organized around level 3 BLAS for speed. We combine sparsity and low-rank structure and directly factor low-rank blocks using randomized algorithms. For a nearly-incompressible elasticity problem, CG with our rank-structured Cholesky converges faster than with incomplete Cholesky and the ML multigrid preconditioner, both in iteration counts and in run time. At 10^6 degrees of

freedom, we use 3 GB of memory; exact factorization takes 30 GB.

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MS60

Approximation of Real Eigenvalues of Some Structured Nonsymmetric Matrices

Matrix Sign iteration is an efficient algorithm for general eigenvalue problem, but we explore its application to approximation of real eigenvalues of structured matrices with further application to real polynomial root-finding. Our formal analysis and extensive tests show that the approach is quite promising.

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MS60

Linear Time Eigendecomposition and SVD Algorithms

We present a set of superfast (nearly O(n) complexity in time and storage) algorithms for finding the full singular value decomposition or selected eigenpairs for a (nonsymmetric) rank-structured matrix. These algorithms rely on tools from Hierarchically Semiseperable (HSS) matrix theory, as well as the Fast Multipole Method (FMM), randomization, and additional tools. We further show how these algorithms can be used in applications, such as PDE solvers. This is joint work with Jianlin Xia.

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MS60

Butterfly Factorizations

The butterfly factorization is a data-sparse representation of the butterfly algorithm. It can be constructed efficiently if either the butterfly algorithm is available or the entries of the matrix can be sampled individually. For an $N \times N$ matrix, the resulting factorization is a product of $O(\log N)$ sparse matrices, each with $O(N)$ non-zero entries. The application complexity of this factorization is $O(N \log N)$ with a prefactor significantly smaller than the original butterfly algorithm.

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PP1

On the Global Convergence of the Cyclic Jacobi Methods for the Symmetric Matrix of Order 4

We prove the global convergence of the general cyclic Jacobi method for the symmetric matrix of order four. In particular, we study the method under the strategies that enable full parallelization of the method. These strategies, unlike the serial ones, can force the method to be very slow/fast within one cycle, depending on the underlying matrix. This implies that for the global convergence proof one has to consider several adjacent cycles.

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PP1

BFGS-like Updates of Constraint Preconditioners for Saddle Point Linear Systems Arising in Convex Quadratic Programming

Constraint preconditioners (CP) have revealed very effective in accelerating iterative methods to solve saddle-point type linear systems arising in unconstrained optimization problems. To avoid a large part of the costly application of CP we propose to selectively compute and update it via suitable low-rank BFGS-like modifications. We show under which conditions the new updated preconditioner guarantees convergence of the PCG method and test it onto a class of large-size problems taken from the CUTE repository.

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PP1

Pivotality of Nodes in Reachability Problems Using Avoidance and Transit Hitting Time Metrics

We propose a "pivotality" measure of how easy it is to reach a node t from a node s. This measure attempts to capture how pivotal a role that some intermediate node k plays in the reachability from node s to node t in a given network. We propose two metrics, the avoidance and transit hitting times, and show how these can be computed from the fundamental matrices associated with the appropriate random walk matrices.

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PP1

A Constructive Proof of Upper Hessenberg Form for Matrix Polynomials

We present a constructive proof that every $n \times n$ matrix polynomial can be reduced to an upper Hessenberg matrix rational. The proof relies on a pseudo inner product to be defined over the vector space of n tuples whose elements are rational functions. Armed with this pseudo inner product we proceed to apply Arnoldi and Krylov type subspace methods to obtain an upper Hessenberg matrix rational whose eigenvalues are the same as the original matrix polynomial. We present a numerical technique for computing the eigenvalues of an upper Hessenberg matrix rational and one numerical example.

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PP1

A New Parallel Sparse Linear Solver

We will present a new parallel sparse linear solver based on hierarchical matrices. The algorithm shares some elements with the incomplete LU factorization, but uses low-rank approximations to remove fill-ins. In addition, it uses multiple levels, in a way similar to multigrid, to achieve fast global convergence. Empirically, the current implementation has nearly linear complexity on equations arising from the discretization of elliptic PDE, making it very efficient to solve large problems. Moreover, the task dependency graph of this algorithm has a tree structure that we exploit in our MPI parallelization of the algorithm. Lastly, because fill-ins are strictly controlled by the algorithm, communication is needed only when boundary nodes are eliminated on every process. Preliminary performance and scalability results of the solver will be demonstrated by our numerical experiments.

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PP1

Towards Batched Linear Solvers on Accelerated Hardware Platforms

Many applications need computations on very large number of small matrices, especially for GPUs, which are currently known to be about four to five times more energy efficient than multicore CPUs. We describe the development of the main one-sided factorizations that work for a set of small dense matrices in parallel. Our approach is based on representing the algorithms as a sequence of batched BLAS routines for GPU-only execution.

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PP1

Improved Incremental 2-Norm Condition Estimation of Triangular Matrices

Basically two incremental techniques to estimate the 2-norm condition number of triangular matrices were introduced, one using left and one using right approximate singular vectors. With incremental we mean that they compute estimates of a leading size k submatrix from a cheap update of the estimates for the leading size $k-1$ submatrix. We show that a clever combination of both techniques and information on the inverse triangular factors lead to a significantly more accurate estimator.

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PP1

A New Regularization Method for Computational Color Constancy

Computational color constancy is an image processing problem that consists of correcting for colors in digital images distorted by noise and illuminants. The color constancy is an ill-posed problem, therefore regularization methods need to be applied. In this work, we propose a new regularization method for computational color constancy and show its performance in several natural images.

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PP1

Design and Analysis of a Low-Memory Multigrid Algorithm

We develop an efficient multigrid solver with low memory complexity, in the spirit of A. Brandt, M. Adams, and others. The algorithm avoids storing the entire finest grid. We introduce new ideas on how to apply τ-corrections in a full-approximation scheme to preserve the accuracy of a standard full multigrid solver while keeping the computation costs low. We use Fourier analysis to study the error components at different stages of the algorithm.

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PP1

Anderson Acceleration of the Alternating Projections Method for Computing the Nearest Correlation Matrix

In a wide range of applications an approximate correlation matrix arises that is symmetric but indefinite and it is required to compute the nearest correlation matrix in the Frobenius norm. The alternating projections method is widely used for this purpose, but has (at best) a linear rate of convergence and can require many iterations. We show that Anderson acceleration, a technique for accelerating the convergence of fixed-point iterations, can successfully be applied to the alternating projections method, bringing a significant reduction in both the number of iterations and the computation time. We also show that Anderson acceleration remains effective when certain elements of the approximate correlation matrix are required to remain fixed.

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PP1

Block Preconditioning for Time-Dependent Coupled Fluid Flow Problems

Many important engineering and scientific systems require the solution of incompressible flow models or extensions to these models such as coupling to other processes or incorporating additional nonlinear effects. Finite element methods and other numerical techniques provide effective discretizations of these systems, and the generation of the resulting algebraic systems may be automated by high-level software tools such those in the Sundance project, but the efficient solution of these algebraic equations remains an important challenge. In addition, many important applications require time-dependent calculations. We examine block preconditioners for time-dependent incompressible Navier-Stokes problems and some related coupled problems. In some time-dependent problems, explicit time stepping methods can require much smaller time steps for stability than are needed for reasonable accuracy. This leads to taking many more time steps than would otherwise be needed. With implicit time stepping methods, we can take larger steps, but at the price of needing to solve large linear systems at each time step. We consider implicit Runge-Kutta (IRK) methods. Suppose our PDE has been linearized and discretized with N degrees of freedom. Using an s-stage IRK method leads to an $sN \times sN$ linear system that must be solved at each time step. These linear systems are block $s \times s$ systems, where each block is $N \times N$. We investigate preconditioners for such systems, where we take advantage of the fact that each subblock is related to a linear system from the (coupled) fluid flow equations.

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PP1

Structured Computations of Block Matrices with Application in Quantum Monte Carlo Simulation

A block matrix can be regarded as a reshaped fourth-order tensor. A properly structured computation of the block matrix provides insight into the tensor and vice versa. We will present a fast sketching algorithm for computing the inversion of a block p-cyclic matrix, and our synergistic effort in developing stable and high-performance implementation of the algorithm for the applications of the fourth-order tensor computations arising from quantum Monte-Carlo simulation.

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PP1

MHD Stagnation Point over a Stretching Cylinder with Variable Thermal Conductivity

This article addresses the behavior of viscous fluid near stagnation point over a stretching cylinder with variable thermal conductivity. The effects of heat generation/absorption are also encountered. Thermal conductivity is considered as a linear function of temperature. Comparison between solutions through HAM and Numerical is presented. The effect of different parameters on velocity and temperature fields are shown graphically..

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PP1

On Simple Algorithm Approximating Arbitrary Real Powers A^α of a Matrix from Number Representation System

In this paper we present new algorithm for approximating arbitrary real powers A^α of a matrix $A \in \mathbb{C}^{n\times n}$ only using matrix standard operation and matrix square root algorithms. Furthermore, although a real matrix with non-positive eigenvalues is given, we get *real* solution without complex arithmetic. Its accuracy is only depend on a condition number of A and that of matrix roots. Since the new algorithm works for arbitrary real α and is independent on singularity and defectiveness against Padé-approximation and Schur-Parllet algorithm respectively, it seems the only way to get a good approximation of arbitrary real power without any handling when a given matrix has such conditions. To addition this algorithm is also well suited in parallel computation because it can be implemented only by standard matrix operations.

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PP1

Cycles of Linear and Semilinear Mappings

A mapping $\mathcal{A}$ from a complex vector space U to a complex vector space V is *semilinear* if

$$\mathcal{A}(u+u') = \mathcal{A}u + \mathcal{A}u', \qquad \mathcal{A}(\alpha u) = \bar{\alpha}\mathcal{A}u$$

for all $u, u' \in U$ and $\alpha \in C$. We give a canonical form of matrices of a cycle of linear or semilinear mapping

$$V_1 \longrightarrow V_2 \longrightarrow \cdots \longrightarrow V_{t-1} \longrightarrow V_t \longrightarrow V_1$$

in which all V_i are complex vector spaces, each line is an arrow $\longrightarrow$ or $\longleftarrow$, and each arrow denotes a linear or semilinear mapping. The talk is based on the article [Linear Algebra Appl. 438 (2013) 3442–3453].

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PP1

Regularization of the Kernel Matrix via Covariance Matrix Shrinkage Estimation

The kernel trick concept, formulated as an inner product in a feature space, facilitates powerful extensions to many well-known algorithms. While the kernel matrix involves inner products in the feature space, the sample covariance matrix of the data requires outer products. Therefore, their spectral properties are tightly connected. This allows us to examine the kernel matrix through the sample covariance matrix in the feature space and vice versa. The use of kernels often involve a large number of features, compared to the number of observations. In this scenario, the sample covariance matrix is not well-conditioned nor is it necessarily invertible, mandating a solution to the problem of estimating high-dimensional covariance matrices under small sample size conditions. We tackle this problem through the use of a shrinkage estimator that offers a compromise between the sample covariance matrix and a well-conditioned matrix (also known as the "target") with the aim of minimizing the mean-squared error (MSE). We propose a distribution-free kernel matrix regularization approach that is tuned directly from the kernel matrix, avoiding the need to explicitly address the feature space. Numerical simulations demonstrate that the proposed regularization is effective in classification tasks.

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PP1

Computationally Enhanced Projection Methods for Symmetric Lyapunov Matrix Equations

In the numerical treatment of large-scale Lyapunov equations, projection methods require solving a reduced Lyapunov problem to check convergence. As the approximation space expands, this solution takes an increasing portion of the overall computational efforts. When data are symmetric, we show that convergence can be monitored at significantly lower cost, with no reduced problem solution. Numerical experiments illustrate the effectiveness of this strategy for standard and extended Krylov methods.

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PP1

Fast Interior Point Solvers for PDE-Constrained Optimization

We present a fast interior point method for solving quadratic programming problems arising from a number of PDE-constrained optimization models with bound constraints on the state and control variables. Particular emphasis is given to the development of preconditioned iterative methods for the large and sparse saddle point systems arising at each Newton step. Having motivated and derived our recommended preconditioners, we present numerical results demonstrating the potency of our solvers.

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PP1

An Optimal Solver for Linear Systems Arising from

Stochastic FEM Approximation of Diffusion Equations with Random Coefficients

Stochastic Galerkin approximation of elliptic PDE problems with correlated random data often results in huge symmetric positive definite linear systems. The novel feature of our preconditioned MINRES solver involves incorporation of error control in the natural "energy' norm together with an effective a posteriori estimator for the PDE approximation error leading to a robust and optimally efficient stopping criterion: the iteration terminates when the algebraic error becomes insignificant compared to the approximation error.

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PP1

Approximation of the Scattering Amplitude Using Nonsymmetric Saddle Point Matrices

This poster presents iterative methods for solving the forward and adjoint systems where the matrix is large, sparse, and nonysmmetric, such as those used to approximate the scattering amplitude. We use a conjugate gradient-like iteration for a nonsymmetric saddle point matrix that has a real positive spectrum and a full set of eigenvectors that are, in some sense, orthogonal. Numerical experiments demonstrate the effectiveness of this approach compared to other iterative methods for nonsymmetric systems.

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PP1

Generalizing Block Lu Factorization:A Lower-Upper-Lower Block Triangular Decomposition with Minimal Off-Diagonal Ranks

We propose a factorization that decomposes a 2×2-blocked non-singular matrix into a product of three matrices that are respectively lower block-unitriangular, upper block-triangular, and lower block-unitriangular. In addition, we make this factorization "as block-diagonal as possible' by minimizing the ranks of the off-diagonal blocks. We present sharp lower bounds for these ranks and an algorithm to compute an optimal solution. One application of this factorization is the design of optimal logic circuits for streaming permutations.

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PP1

Existence and Uniqueness for the Inverse Problem for Linear and Linear-in-parameters Dynamical Systems

Certain experiments are non-repeatable, because they result in the destruction or alteration of the system under study, and thus provide data consisting of at most a single trajectory in state space. Before proceeding with parameter estimation for models of such systems, it is important to know if the model parameters can be uniquely determined, or identified, from idealized (error free) single trajectory data. For linear models and a class of nonlinear systems that are linear in parameters, I will present several characterizations of identifiability. I will establish necessary and sufficient conditions, solely based on the geometric structure of an observed trajectory, for these forms of identifiability to arise. I will extend the analysis to consider collections of discrete data points, where, due to properties of the fundamental matrix solution, we can recover the parameters explicitly in certain cases. I will then examine the role of measurement error in the data and determine regions in the data space which correspond to parameter sets with desired properties, such as identifiability, model equilibrium stability, and sign structure.

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PP1

Is Numerical Stability an Important Issue in Iterative Computations?

Although the answer seems obvious, the practice might be not. Full numerical stability analysis might be intriguing or our of reach. This contribution examines several situations where the presentation and analysis of iterative numerical algorithms assumes exact arithmetic. Such approach can be well justified in some cases and it can severely limit application of the obtained results in others.

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PP1

Computing Geodesic Rotations

An element of a *flag manifold* is a frame—a decomposition of Euclidean space into orthogonal components—and a geodesic path on a flag manifold provides a "direct" rotation from one frame to another. Furthermore, a geodesic path corresponds to a decomposition of unitary matrices that generalizes the CS decomposition. We develop efficient methods for numerical computation on a flag manifold, including the location of geodesic paths, and consider a question of uniqueness.

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PP1

On the Numerical Behavior of Quadrature-based Bounds for the A-Norm of the Error in CG

The A-norm of the error in the conjugate gradient (CG) method can be estimated using quadrature-based bounds. Our numerical experiments predict that some numerical difficulties may arise when computing upper bounds based on modified quadrature rules like Gauss-Radau, regardless whether we use the CGQL algorithm or our new CGQ algorithm for their computation. In this presentation we

analyze this phenomenon and try to explain when possible numerical difficulties can appear.

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PP1

Tensor Notation: What Would Hamlet Say?

It is hard to spread the word about tensor computations. Summations, transpositions, and symmetries are described through vectors of subscripts and vectors of superscripts. Is there a magic notation for handling that stuff? Einstein notation and Dirac notation are noble efforts. Other worthy notations flow from traditional "SIAM style" matrix computations. I will suggest with examples how the research community might navigate among these schemes. Shakespeare points the way: "There is nothing either good or bad [about any given tensor notation] but thinking makes it so". Hamlet II,II,250.

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PP1

Best Rank-1 Approximations Without Orthogonal Invariance for the 1-norm and Frobenius 1-norm

We consider finding the best rank-1 approximations to a matrix A where the error is measured as the operator induced 1-norm (maximum column 1-norm) or Frobenius 1-norm (sum of absolute values over the matrix). Neither of these norms are unitarily invariant and the typical SVD procedure is insufficient. For the case of a 2×2 matrix A, there is a simple solution procedure and the resulting approximation bound for the Frobenius 1-norm is the $\frac{|\det(A)|}{\max_{ij}|A_{ij}|}$. We present some thoughts on how to extend the arguments to larger matrices.

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PP1

Pseudospectra Computation Via Rank-Revealing QR Factorization

The pseudospectrum of a matrix is a way to visualize the non-normality of a matrix and the sensitivity of its eigenvalues. In this paper, we propose an equivalent definition of pseudospectra of matrices using Rank-Revealing QR (RRQR) factorization. We give the proof of the equivalency between this definition and classical ones. And, we propose some generalizations of eigenvalue theorems to pseudospectra theorems based on the equivalent definition. Also, an algorithm of pesudospectra computation via RRQR is given. Numerical experiments and comparisons are given to illustrate the efficiency of the results in this paper.

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PP1

Linear Response and the Estimation of Absorption Spectrum in Time-Dependent Density Functional Theory

The absorption spectrum of a molecular system can be estimated from the dynamic dipole polarizability associated with the linear response of a molecular system (at its ground state) to an external perturbation. Although an accurate description of the absorption spectrum requires the diagonalization of the so-called Casida Hamiltonian, there are more efficient ways to obtain a good approximation to the general profile of the absorption spectrum without computing eigenvalues and eigenvectors. We will describe these methods that only require multipling the Casida Hamiltonian with a number of vectors. When highly accurate oscillator strength is required for a few selected excitation energies, we can use a special iterative method to obtain the eigenvalues and eigenvectors associated with these energies efficiently.

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PP1

A Set of Fortran 90 and Python Routines for Solving Linear Equations with IDR(s)

We present Fortran 90 and Python implementations of [Van Gijzen and Sonneveld, Algorithm 913: An Elegant IDR(s) Variant that Efficiently Exploits Bi-orthogonality Properties. ACM TOMS, Vol. 38, No. 1, pp. 5:1-5:19, 2011]. Features of the new software include: (1) the capability of solving general linear matrix equations, including systems with multiple right-hand-sides, (2) the possibility to extract spectral information, and (3) subspace recycling.

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