

Minisymposia Abstracts

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MS 1. Recent advances in matrix functions

Talk 1. Computational issues related to the geometric mean of structured matrices

In several applications it is required to compute the geometric mean of a set of positive definite matrices. In certain cases, like in the design of radar systems, the matrices are structured, say, they are Toeplitz, and one expects that the mean still keeps the same structure.

Unfortunately, the available definitions of geometric mean, like the Karcher mean, do not generally maintain the structure of the input matrices.

In this talk we introduce a definition of mean which preserves the structure, analyze its properties and present algorithms for its computation.

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Talk 2. Efficient, communication-minimizing algorithms for the symmetric eigenvalue decomposition and the singular value decomposition

We propose algorithms for computing the symmetric eigenvalue decomposition and the singular value decomposition (SVD) that minimize communication in the asymptotic sense while simultaneously having arithmetic operation costs within a factor 3 of that for the most efficient existing algorithms. The essential cost for the algorithms is in performing QR factorizations, of which we require no more than six for the symmetric eigenproblem and twelve for the SVD. We establish backward stability under mild assumptions, and numerical experiments indicate that our algorithms tend to yield decompositions with considerably smaller backward error and eigen/singular vectors closer to orthogonal than existing algorithms.

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Talk 3. The Padé approximation and the matrix sign function

In the talk we focus on the properties of the Padé approximants of a certain hypergeometric function on which the Padé families of iterations for computing the matrix sign and sector functions are based. We have determined location of poles of the Padé approximants and we have proved that all coefficients of the power series expansions of the reciprocals of the denominators of the Padé approximants and of the power series expansions of the Padé approximants are positive. These properties are crucial in the proof of the conjecture – stated by Laszkiewicz and Ziętak, and extending the result of Kenney and Laub – on a region of convergence of these Padé families of iterations. The talk is based on the paper by O. Gomitko, F. Greco, K. Ziętak and the paper by O. Gomitko, D.B. Karp, M. Lin, K. Ziętak. In the talk we also consider a certain different kind of rational approximation to the sign function.

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Talk 4. A recursive blocked schur algorithm for computing the matrix square root

The Schur algorithm for computing a matrix square root reduces the matrix to the Schur triangular form and then computes a square root of the triangular matrix. In this talk I will describe a recursive blocking technique in which the computation of the square root of the triangular matrix can be made rich in matrix multiplication. Numerical experiments making appropriate use of level 3 BLAS show significant speedups over the point algorithm, both in the square root phase and in the algorithm as a whole. The excellent numerical stability of the point algorithm is shown to be preserved by recursive blocking. Recursive blocking is also shown to be effective for multiplying triangular matrices.

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MS 2. Methods for Toeplitz matrices and their application

Talk 1. Toeplitz operators with matrix-valued symbols and some (unexpected) applications

We discuss the eigenvalue distribution in the Weyl sense of general matrix-sequences associated to a symbol. As a specific case we consider Toeplitz sequences generated by matrix-valued (non Hermitian) bounded functions. We show that the canonical distribution can be proved under mild assumptions on the spectral range of the given symbol. Finally some applications are introduced and discussed.

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Talk 2. Fast approximation to the Toeplitz matrix exponential

The shift-invert Lanczos (or Arnoldi) method is employed to generate an orthonormal basis from the Krylov subspace corresponding to the real Toeplitz matrix and an initial vector. The vectors and recurrence coefficients produced by this method are exploited to approximate the Toeplitz matrix exponential. Toeplitz matrix inversion formula and rapid Toeplitz matrix-vector multiplications are utilized to lower the computational costs. For convergence analysis, a sufficient condition is established to guarantee that the error bound is independent of the norm of the matrix. Numerical results and applications to the computational finance are given to demonstrate the efficiency of the method.

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Talk 3. Matrix algebras sequences can be spectrally equivalent with ill-conditioned Toeplitz ones

The construction of fast and efficient iterative procedure or effective multigrid schemes, requires the study of the spectrum of the matrix sequences $\{A_n\}_n$, where $\{A_n\}_n = \{P_n^{-1}(f)T_n(f)\}_n$. In this talk, we focus on the case where $T_n(f)$ is a Toeplitz matrix generated by a nonnegative real function f , and $P_n(f)$ denotes matrices belonging to tau or circulant algebras. Assuming that the symbol f has discrete roots of non integer order, we will show that under suitable assumptions the spectrum of the matrix sequence $\{A_n\}_n$ is bounded by constants far away from zero and infinity. Using the developed theory, we propose effective preconditioners and we give hints for optimal multigrid schemes.

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Talk 4. Aggregation-based multigrid methods for Toeplitz matrices

Aggregation and smoothed aggregation based multigrid methods can be analyzed in the context of the convergence theory for Toeplitz and circulant matrices. As in the aggregation-based multigrid methods, for generating symbols with a single isolated zero at the origin aggregates are formed. The interpolation can then be improved by applying an additional operator. This improvement can be interpreted as the smoothing step in the original smoothed aggregation method. Depending on the original generating symbol, several smoothing steps can be necessary. Numerical examples show the efficiency of the aggregation based approach in the case of Toeplitz and circulant matrices.

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MS 3. Matrix factorizations and applications

Talk 1. Classes of matrices with bidiagonal factorization

Matrices with a bidiagonal decomposition satisfying some sign restrictions are analyzed. They include all nonsingular totally positive matrices, their matrices opposite in sign and their inverses, as well as tridiagonal nonsingular H -matrices. Properties of these matrices are presented and the bidiagonal factorization can be used to perform computations with high relative accuracy.

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Talk 2. Cholesky factorization for singular matrices

Direct and iterative solution methods for linear least-squares problems have been studied in Numerical Linear Algebra. Part of the difficulty for solving least-squares problems is the fact that many methods solve the system by implicitly solving the normal equations $A^T A x = A^T b$ with $A \in \mathbb{R}^{n \times m}$ and $b \in \mathbb{R}^n$. In this talk we consider this problem when A is a rank deficient matrix. Then, $A^T A$ is a positive semidefinite matrix and its Cholesky factorization is not unique. So, we introduce a full rank Cholesky decomposition LL^T of the normal equations matrix without the need to form the normal matrix itself. We present two algorithms to compute the entries of L by rows (or by columns) with the corresponding error analysis. Numerical experiments illustrating the proposed algorithms are given.

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Talk 3. Applications of the singular value decomposition to perturbation theory of eigenvalues of matrix polynomials

In this talk, motivated by a problem posed by Wilkinson, we study the coefficient perturbations of a $n \times n$ matrix polynomial to $n \times n$ matrix polynomials which have a prescribed eigenvalue of specified algebraic multiplicity and index of annihilation. For an $n \times n$ matrix polynomial $P(\lambda)$ and a given scalar $\mu \in \mathbb{C}$, we introduce two weighted spectral norm distances, $\mathcal{E}_r(\mu)$ and $\mathcal{E}_{r,k}(\mu)$, from $P(\lambda)$ to the $n \times n$ matrix polynomials that have μ as an eigenvalue of algebraic multiplicity at least r and to those that have μ as an eigenvalue of algebraic multiplicity at least r and maximum Jordan chain length exactly k , respectively. Then we obtain a singular value characterization of $\mathcal{E}_{r,1}(\mu)$, and derive a lower bound for $\mathcal{E}_{r,k}(\mu)$ and an upper bound for $\mathcal{E}_r(\mu)$, constructing associated perturbations of $P(\lambda)$.

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Talk 4. On reduced rank nonnegative matrix factorization for symmetric nonnegative matrices

For a nonnegative matrix $V \in \mathbb{R}^{m,n}$, the *nonnegative matrix factorization* (NNMF) problem consists of finding nonnegative matrix factors $W \in \mathbb{R}^{m,r}$ and $H \in \mathbb{R}^{r,n}$ such that $V \approx WH$. We consider the algorithm provided by Lee and Seung which finds nonnegative W and H such that $\|V - WH\|_F$ is minimized. For the case $m = n$ and in which V is symmetric, we present results concerning when the best approximate

factorization results in the product WH being symmetric and on cases in which the best approximation cannot be a symmetric matrix. Results regarding other special cases as well as applications are also discussed.

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MS 4. Algorithms on manifolds of low-rank matrices and tensors

Talk 1. Low rank dynamics for computing extremal points of real and complex pseudospectra

We consider the real ε -pseudospectrum of a square matrix, which is the set of eigenvalues of all real matrices that are ε -close to the given matrix, where closeness is measured in either the 2-norm or the Frobenius norm.

We characterize extremal points and compare the situation with that for the unstructured ε -pseudospectrum. We present differential equations for low rank (1 and 2) matrices for the computation of the extremal points of the pseudospectrum. Discretizations of the differential equations yield algorithms that are fast and well suited for sparse large matrices. Based on these low-rank differential equations, we further obtain an algorithm for drawing boundary sections of the structured pseudospectrum with respect to both considered norms.

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Talk 2. Parametric model order reduction using stabilized consistent interpolation on matrix manifolds

A robust method for interpolating reduced-order linear operators on their matrix manifolds is presented. Robustness is achieved by enforcing consistency between the different sets of generalized coordinates underlying different instances of parametric reduced-order models (ROMs), and explicitly stabilizing the final outcome of the interpolation process. Consistency is achieved by transforming the ROMs before interpolation using a rotation operator obtained from the solution of a generalized orthogonal Procrustes problem. Stabilization is achieved using a novel real-time algorithm based on semidefinite programming. The overall method is illustrated with its on-line application to the parametric fluid-structure analysis of a wing-store configuration.

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Talk 3. Treatment of high-dimensional problems by low-rank manifolds of tensors

Many problems in e.g. natural sciences, data mining and statistics are naturally posed as high-dimensional problems. Tensor product representations parametrize these problem on approximation manifolds, often fixed by a given maximal rank for the tensor approximation. A relatively new format is the HT/TT format as developed by Hackbusch (Leipzig) and Oseledets/Tyrtshnikov (Moscow), which overcomes the shortcomings of older formats and gives a stable and often sparse opportunity to represent high-dimensional quantities, so that the treatment of e.g. high-dimensional partial differential equations is on the verge of realization. In this talk, a general framework to realize such tasks in data-sparse tensor formats is presented. For the HT/TT format, we present some theoretical as well as algorithmic results for the treatment of high-dimensional optimization tasks and high-dimensional evolution equations.

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Talk 4. Local convergence of alternating optimization of multivariate functions in the presence of scaling indeterminacies

An easy and widely used approach to minimize functions with respect to certain tensor formats (such as CP, Tucker, TT or HT) is the alternating optimization algorithm, also called nonlinear Gauss-Seidel method. A prominent example is the PARAFAC-ALS algorithm. Due to the usual non-uniqueness of tensor representations, standard convergence results for nonlinear Gauss-Seidel are usually not directly applicable. In this talk we present a quite general approach to prove local convergence, based on a geometric viewpoint, which regards tensors of fixed rank as orbits of a Lie group generating equivalent representations.

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MS 5. Advances in algebraic multigrid - New approaches and applications

Talk 1. Algebraic collocation coarse approximation multigrid

Most algebraic multigrid (AMG) methods define the coarse operators by applying the (Petrov-)Galerkin coarse approximation where the sparsity pattern and operator complexity of the multigrid hierarchy is dictated by the multigrid prolongation and restriction. Therefore, AMG algorithms usually must settle on some compromise between the quality of these operators and the aggressiveness of the coarsening, which affects their rate of convergence and operator complexity. In this paper we propose an algebraic generalization

of the *collocation coarse approximation* (CCA) approach of Wienands and Yavneh, where the choice of the sparsity pattern of the coarse operators is independent of the choice of the high-quality transfer operators. The new algorithm is based on the aggregation framework (smoothed and non-smoothed). Using a small set of low-energy eigenvectors, it computes the coarse grid operator by a weighted least squares process. Numerical experiments for two dimensional diffusion problems with sharply varying coefficients demonstrate the efficacy and potential of this multigrid algorithm.

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Talk 2. **Energy-minimization interpolation for adaptive algebraic multigrid**

Adaptive algebraic multigrid (AMG) methods automatically detect the algebraically smooth error for a linear system and as such, are robust black box approaches for solving difficult problems. However, the two main families of methods, Bootstrap AMG (BAMG) and adaptive smoothed aggregation (α SA), suffer from drawbacks, such as noisy candidate vectors (BAMG) and potentially high operator complexity, especially for scalar problems, (α SA). This work is intended to address some of these drawbacks by combining elements of BAMG and α SA through an energy-minimization interpolation framework. While the approach is general, the challenging, motivating problem is a biquadratic discretization of anisotropic diffusion.

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Talk 3. **Algebraic multigrid (AMG) for complex network calculations**

Clustering, ranking, or measuring distance for vertices on scale-free graphs are all computational task of interest. Such calculations may be obtained by solving eigensystems or linear systems involving matrices whose sparsity structure is related to an underlying scale-free graph. For many large systems of interest, classical iterative solvers (such as conjugate gradient and Lanczos) converge with prohibitively slow rates, due to ill-conditioned matrices and small spectral gap ratios. Efficiently preconditioning these systems with multilevel methods is difficult due to the scale-free topology. For some large model problems and real-world networks, we investigate the performance of a few AMG-related coarsening approaches.

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Talk 4. **The polynomial of best uniform approximation to $1/x$ as smoother in two grid methods**

We discuss a simple convergence analysis of two level methods where the relaxation on the fine grid uses the polynomial of best approximation in the uniform norm to $1/x$ on a finite interval with positive endpoints. The construction of the latter polynomial is of interest by itself, and we have included a derivation of a three-term recurrence relation for computing this polynomial. We have also derived several inequalities related to the error of best approximation, monotonicity of the polynomial sequence, and positivity which we applied in the analysis of two-level methods.

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MS 6. Recent advances in fast iterative solvers - Part I of II

Talk 1. **Challenges in analysis of Krylov subspace methods**

The current state-of-the art of iterative solvers is the outcome of the tremendous algorithmic development over the last few decades and of investigations of *how* to solve given problems. In this contribution we focus on Krylov subspace methods and more on the dual question *why* things do or do not work. In particular, we will pose and discuss open questions such as what the spectral information tells us about the behaviour of Krylov subspace methods, to which extent we can relax the accuracy of local operations in inexact Krylov subspace methods without causing an unwanted delay, how important is considering of rounding errors in various algorithmic techniques, whether it is useful to view Krylov subspace methods as *matching moment model reduction*, and how the algebraic error can be included into locally efficient and fully computable a-posteriori error bounds for adaptive PDE solvers.

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Talk 2. **Updating preconditioners for parameterized systems**

Parameterized linear systems arise in a range of applications, such as model reduction, acoustics, and inverse problems based on parametric level sets. Computing new preconditioners for

many small changes in parameter(s) would be very expensive. However, using one or only a few preconditioners for all systems leads to an excessive total number of iterations. We show strategies to efficiently compute effective multiplicative updates to preconditioners. This has the advantage that, for a slight increase in overhead, the update is more or less independent of the original preconditioner used.

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Talk 3. **Efficient preconditioning techniques for two-phase flow simulations**

In this talk we present efficient preconditioning strategies, suitable for the iterative solution of algebraic systems, arising in numerical simulations of two-phase flow problems, modelled by the Cahn-Hilliard equation.

In this work, we decompose the original Cahn-Hilliard equation, which is nonlinear and of fourth-order, into a system of two second-order equations for the so-called 'concentration' and 'chemical potential'. The so-obtained nonlinear system is discretized using the finite element method and solved by two variants of the inexact Newton method. The major focus of the work is to construct a preconditioner for the corresponding Jacobian, which is of block two-by-two form. The proposed preconditioning techniques are based on approximate factorization of the discrete Jacobian and utilise to a full extent the properties of the underlying matrices.

We propose a preconditioning method that reduces the problem of solving the non-symmetric discrete Cahn-Hilliard system to the problem of solving systems with symmetric positive definite matrices, where off-the-shelf multilevel and multigrid algorithms are directly applicable. The resulting iterative method exhibits optimal convergence and computational complexity properties. The efficiency of the resulting preconditioning method is illustrated via various numerical experiments, including large scale examples of both 2D and 3D problems.

The preconditioning techniques are more generally applicable for any algebraic system of the same structure as, e.g., when solving complex symmetric linear systems.

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Talk 4. **Preconditioners in liquid crystal modelling**

Liquid crystal displays are ubiquitous in modern life, being used extensively in monitors, televisions, gaming devices, watches, telephones etc. Appropriate models feature characteristic length and time scales varying by many orders of magnitude, which provides difficult numerical challenges to those trying to simulate real-life dynamic industrial situations. The efficient solution of the resulting linear algebra sub-problems is of crucial importance for the overall effectiveness of the algorithms used. In this talk we will present some examples of saddle-point systems which arise in liquid crystal modelling and discuss their efficient solution using appropriate preconditioned iterative methods.

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MS 7. Application of statistics to numerical linear algebra algorithms - Part I of II

Talk 1. **Fast linear system solvers based on randomization techniques**

We illustrate how dense linear algebra calculations can be enhanced by randomizing general or symmetric indefinite systems. This approach, based on a multiplicative preconditioning of the initial matrix, revisits the work from [Parker, 1995]. It enables us to avoid pivoting and then to reduce significantly the amount of communication. This can be performed at a very affordable computational price while providing a satisfying accuracy. We describe solvers based on randomization that take advantage of the latest generation of multicore or hybrid multicore/GPU machines and we compare their Gflop/s performance with solvers from standard parallel libraries.

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Talk 2. **Numerical issues in randomized algorithms**

Randomized algorithms are starting to find their way into a wide variety of applications that give rise to massive data sets. These algorithms downsize the enormous matrices by picking and

choosing only particular columns or rows, thereby producing potentially huge savings in storage and computing speed. Although randomized algorithms can be fast and efficient, not much is known about their numerical properties. We will discuss the numerical sensitivity and stability of randomized algorithms, as well as the error due to randomization, and the effect of the coherence of the matrix. Algorithms under consideration include matrix multiplication, least squares solvers, and low-rank approximations.

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Talk 3. **Near-optimal column based matrix reconstruction**

We consider low-rank reconstruction of a matrix using a subset of its columns and we present asymptotically optimal algorithms for both spectral norm and Frobenius norm reconstruction. The main tools we introduce to obtain our results are: (i) the use of fast approximate SVD-like decompositions for column-based matrix reconstruction, and (ii) two deterministic algorithms for selecting rows from matrices with orthonormal columns, building upon the sparse representation theorem for decompositions of the identity that appeared in [Batson, Spielman, Srivastava, 2011].

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Talk 4. **Numerical experiments with statistical condition estimation**

In this talk we present the results of some numerical experiments illustrating the use of statistical condition estimation (SCE). After a brief review of SCE, the use of the technique is demonstrated on a few topics of general interest including the estimation of the condition of large sparse linear systems.

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MS 8. Rational Krylov methods: analysis and applications - Part I of II

Talk 1. **Solving Sylvester equations through rational Galerkin projections**

Recently (B. Beckermann, An error analysis for rational Galerkin projection applied to the Sylvester equation, SIAM J. Num. Anal. 49 (2012), 2430-2450), we suggested a new error analysis for the residual of Galerkin projection onto rational Krylov spaces applied to a Sylvester equation with a rank 1 right-hand side. In this talk we will consider more generally small rank right-hand sides, where block Krylov methods and tangential interpolation problems play an important role.

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Talk 2. **Stability-corrected spectral Lanczos decomposition algorithm for wave propagation in unbounded domains**

Applying Krylov subspace methods to exterior wave field problems has become an active topic of recent research. In this paper, we introduce a new Lanczos-based solution method via stability-corrected operator exponents, allowing us to construct structure-preserving reduced-order models (ROMs) respecting the delicate spectral properties of the original scattering problem. The ROMs are unconditionally stable and are based on a renormalized Lanczos algorithm, which enables us to efficiently compute the solution in the frequency and time domain. We illustrate the performance of our method through a number of numerical examples in which we simulate 2D electromagnetic wave propagation in unbounded domains.

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Talk 3. **Generalized rational Krylov decompositions**

The notion of an orthogonal rational Arnoldi decomposition, as introduced by Axel Ruhe, is a natural generalization of the well-known (polynomial) Arnoldi decomposition. Generalized rational Krylov decompositions are obtained by removing the orthogonality assumption. Such decompositions are interesting linear algebra objects by themselves and we will study some of their algebraic properties, as well as the rational Krylov methods that can be associated with them.

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Talk 4. **Interpolatory model reduction strategies for nonlinear parametric inversion**

We will show how reduced order models can significantly reduce the cost of general inverse problems approached through parametric level set methods. Our method drastically reduces the solution of forward problems in diffuse optical tomography (DOT) by using interpolatory, i.e. rational Krylov based, parametric model reduction. In the DOT setting, these surrogate models can approximate both the cost functional and associated Jacobian with little loss of accuracy and significantly reduced cost.

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MS 9. New trends in tridiagonal matrices - Part I of II

Talk 1. Direct and inverse problems on pseudo-Jacobi matrices

A theorem of Friedland and Melkman states the unique recovery of a non-negative Jacobi matrix from the spectra of its upper and lower principal submatrices obtained by deleting the k th row and column. Here this result is revisited and generalized. Other related problems are also investigated, including existence and uniqueness theorems.

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Talk 2. Schwarz's matrices and generalized Hurwitz polynomials

We present solutions of direct and inverse spectral problems for a kind of Schwarz's matrices (tridiagonal matrices with only one nonzero main-diagonal entry). We study dependence of spectra of such matrices on the signs of their off-main-diagonal entries. We show that for certain distributions of those signs, the characteristic polynomial of the correspondent Schwarz's matrix is a generalized Hurwitz polynomial. Recall that a real polynomial $p(z) = p_0(z^2) + zp_1(z^2)$, where p_0 and p_1 are the even and odd parts of p , respectively, is generalized Hurwitz if and only if the zeroes of p_0 and p_1 are real, simple and interlacing.

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Talk 3. On the Moore-Penrose inverse of singular, symmetric and periodic Jacobi M-matrices

We aim here at determining the Moore-Penrose inverse, J^\dagger of any singular, symmetric and periodic Jacobi M -matrix J , both throughout direct computations or considering it as a perturbation of a singular, symmetric and nonperiodic Jacobi M -matrix. We tackle the problem by applying methods from the operator theory on finite networks, since the off-diagonal entries of J can be identified with the conductance function of a weighted n -cycle. Then, J appears as a positive-semidefinite

Schrödinger operator on the cycle and hence, J^\dagger is nothing else than the corresponding Green operator.

We also consider the problem of characterizing when J^\dagger is itself an M -matrix.

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Talk 4. The commutant of the tridiagonal pattern

We consider patterns that allow real commutativity with an irreducible tridiagonal n -by- n pattern. All are combinatorially symmetric. All also allow a complex symmetric commuting pair, but only some allow a real symmetric commuting pair. We also show that any matrix that commutes with an irreducible tridiagonal matrix satisfies certain ratio equations. Generalizations to matrices with tree patterns are also considered.

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MS 10. Numerical algorithms for switching systems: from theory to applications

Talk 1. Observer design for hybrid systems

The state estimation problem has been the subject of intensive study for many years by both the computer science community in the discrete domain and the control community in the continuous domain, but only scantily investigated in the hybrid system domain.

In this talk, we present a design methodology for dynamical observers of hybrid systems with linear continuous-time dynamics, which reconstruct the complete state from the knowledge of the inputs and outputs of a hybrid plant. We demonstrate the methodology by building a hybrid observer for an industrial automotive control problem: on-line identification of the actual engaged gear.

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Talk 2. About polynomial instability for linear switched systems

In this talk we present recent results on the characterization of marginal instability for linear switched systems. Our main contribution consists in pointing out a resonance phenomenon associated with marginal instability. In particular we derive an upper bound of the norm of the state at time t , which is polynomial in t and whose degree is computed from the resonance structure of the system. We also derive analogous results for discrete-time linear switched systems.

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Talk 3. Stability and stabilization of positive switched systems: state of the art and open problems

A positive switched system (PSS) consists of a family of positive state-space models and a switching law, specifying when and how the switching among the various models takes place. This class of systems has some interesting practical applications: PSS's have been adopted for describing networks employing TCP and other congestion control applications, for modeling consensus and synchronization problems, and, quite recently, for describing the viral mutation dynamics under drug treatment. In the talk we will provide a comprehensive picture of the conditions for stability and for stabilizability, and we will point out some open problems.

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Talk 4. The joint spectral radius for semigroups generated by switched differential algebraic equations

We introduce the joint spectral radius for matrix semigroups that are generated by switched linear ordinary differential equations with jumps. The jumps are modeled by projectors which are assumed to commute with the generators of the flow. This setup covers switched differential algebraic equations. It is shown that an exponential growth rate can only be defined if the discrete semigroup generated by the projections is product bounded. Assuming this is true we show that Barabanov norms may be defined in the irreducible case and that a converse Lyapunov theorem holds. Some further properties of the exponential growth rate are discussed.

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MS 11. Recent advances in fast iterative solvers - Part II of II

Talk 1. Combination preconditioning of saddle-point systems for positive definiteness

There are by now many preconditioning techniques for saddle-point systems but also a growing number of applications where such are required. In this talks we will discuss preconditioners which preserve self-adjointness in non-standard inner products and the combination of such preconditioners as introduced by Martin Stoll and the first author in 2008. Here we will show how two preconditioners which ensure self-adjointness in different inner products, but which are both indefinite may be combined to yield a positive definite self-adjoint preconditioned system in a third inner product which thus allows robust application of the Hestenes Steifel Conjugate Gradient method in that inner product.

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Talk 2. Preconditioned iterative methods for nonsymmetric matrices and nonstandard inner products

The convergence of a minimum residual method applied to a linear system with a nonnormal coefficient matrix is not well understood in general. This can make choosing an effective preconditioner difficult. In this talk we present a new GMRES convergence bound. We also show that the convergence of a nonstandard minimum residual method, applied to a preconditioned system, is bounded by a term that depends primarily on the eigenvalues of the preconditioned coefficient matrix, provided the preconditioner and coefficient matrix are self-adjoint with respect to nearby Hermitian sesquilinear forms. We relate this result to the convergence of standard methods.

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Talk 3. Multi-preconditioned GMRES

Standard Krylov subspace methods only allow the user to choose a single preconditioner. In many situations, however, there is no 'best' choice, but a number of possible candidates. In this talk we describe an extension of GMRES, multi-preconditioned GMRES, which allows the use of more than one preconditioner, and combines their properties in an optimal way. As well as describing some theoretical properties of the new algorithm we will present numerical results which highlight the utility of the approach.

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Talk 4. **Bounds on the eigenvalues of indefinite matrices arising from interior-point methods**

Interior-point methods feature prominently in the solution of constrained optimization problems, and involve the need to solve a sequence of 3×3 block indefinite matrices that become increasingly ill-conditioned throughout the iteration. Most solution approaches are based on reducing the system size using a block Gaussian elimination procedure. In this talk we use energy estimates to obtain bounds on the eigenvalues of the original, augmented matrix, which indicate that the spectral structure of this matrix may be favorable compared to matrices obtained by performing a partial elimination of variables before solving the system.

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MS 12. **Application of statistics to numerical linear algebra algorithms - Part II of II**

Talk 1. **Spectral graph theory, sampling matrix sums, and near-optimal SDD solvers**

We present a near-optimal solver for Symmetric Diagonally Dominant (SDD) linear systems. The solver is a great example of the power of statistical methods in linear algebra and in particular of sampling sums of positive semi-definite matrices. Crucial to the speed of the solver is the ability to perform fast sampling. In turn, key to fast sampling are low-stretch spanning trees, a central notion in spectral graph theory and combinatorial preconditioning. We will see that a low-stretch tree is essentially a ‘spectral spine’ of a graph Laplacian, allowing us to create a hierarchy of spectrally similar graphs which lends itself to the very fast multilevel solver.

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Talk 2. **Implementation of a randomization algorithm for dense linear algebra libraries**

Randomization algorithms are an alternative to pivoting for factoring dense matrices to solve systems of linear equations. These techniques are more suitable to parallel architectures

when compared to pivoting, requiring a reduced amount of communication and no synchronization during the factorization. The core kernel requires the multiplication of sparse matrices with a specific structure. The main issue in implementing such algorithms resides in the data dependency patterns, especially for the symmetric case. An implementation for the PLASMA library is described and traces are presented, together with performance data.

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Talk 3. **Implementing randomized matrix algorithms in large-scale parallel environments**

Recent work from theoretical computer science on developing randomized matrix algorithms has recently led to the development of high-quality numerical implementations. Here, we describe our parallel iterative least-squares solver LSRN. The parallelizable normal random projection in the preconditioning phase leads to a very well-conditioned system. Hence, the number of iterations is fully predictable if we apply LSQR or the Chebyshev semi-iterative method to the preconditioned system. The latter method is particularly efficient for solving large-scale problems on clusters with high communication cost, e.g., on Amazon Elastic Compute Cloud clusters, that are increasingly common in large-scale data applications.

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Talk 4. **Random sampling preconditioners**

In the talk we study the use of preconditioners based on random sampling of rows for accelerating the solution of linear systems. We argue that the fusion of randomization with preconditioning is what enables fast and reliable algorithms.

We will discuss both dense and sparse matrices. For dense matrices, we will describe Blendenpik, a least-square solver for dense highly overdetermined systems that outperforms LAPACK by large factors, and scales significantly better than any QR-based solver. For sparse matrices, we relate random sampling preconditioners to fast SDD solvers, and generalize some of the techniques to finite element matrices.

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MS 13. **Rational Krylov methods: analysis and applications - Part II of II**

Talk 1. **Rational Krylov methods for nonlinear matrix problems**

This talk is about the solution of non-linear eigenvalue problems and linear systems with a nonlinear parameter. Krylov and Rational Krylov methods are known to be efficient and reliable for the solution of such matrix problems with a linear parameter. The nonlinear function can be approximated by a polynomial. In earlier work, we suggested the use of Taylor expansions of the nonlinear function with an a priori undetermined degree. This led to the Taylor Arnoldi method that is an Arnoldi method applied to an infinite dimensional Companion linearization. When an interpolating polynomial is used instead of Taylor series, there is a similar connection with the rational Krylov subspace method applied on a linearization. The Krylov subspaces enjoy similar properties as the linear case such as moment matching and the convergence looks similar to convergence for a linear problem. We present several choices of polynomials and also discuss ideas for future work.

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Talk 2. **Block Gauss and anti-Gauss quadrature rules with application to networks**

The symmetric and nonsymmetric block Lanczos processes can be applied to compute Gauss quadrature rules for functionals with matrix-valued measures. We show that estimates of upper and lower bounds for these functionals can be computed inexpensively by evaluating pairs of block Gauss and anti-Gauss rules. An application to network analysis is described.

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Talk 3. **On optimality of rational Krylov based low-rank approximations of large-scale matrix equations**

In this talk, we will discuss projection-based approximations for the solution of Lyapunov equations of the form

$$AXE^T + EXA^T + BB^T = 0,$$

with $A = A^T, E = E^T \in \mathbb{R}^{n \times n}$ and $B \in \mathbb{R}^{n \times m}$. Recently, a relation between minimizing the objective function

$$f : \mathcal{M} \rightarrow \mathbb{R}, X \mapsto \text{tr}(XAXE + BB^T)$$

on the manifold \mathcal{M} of symmetric positive semi-definite matrices of rank k and the \mathcal{L} -norm defined by the operator

$$\mathcal{L} := -E \otimes A - A \otimes E$$

together with the inner product $\langle u, v \rangle_{\mathcal{L}} = \langle u, \mathcal{L}v \rangle$ has been shown. While so far this minimization problem was solved by

means of a Riemannian optimization approach, here we will discuss an interpolation-based method which leads to the same results but relies on projecting the original Lyapunov equation onto a rational Krylov subspace. It will turn out that this can be achieved by the iterative rational Krylov algorithm (IRKA). Besides a generalization for the case of $A \neq A^T$, we will also discuss an extension for more general equations of the form

$$AXE + FXB + CD = 0,$$

with $A, F \in \mathbb{R}^{n \times n}$, $B, E \in \mathbb{R}^{m \times m}$, $C \in \mathbb{R}^{n \times p}$ and $D \in \mathbb{R}^{p \times m}$.

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Talk 4. **Inverse problems for large-scale dynamical systems in the H2-optimal model reduction framework**

In this work we investigate the Rational Krylov subspace (RKS) projection method with application to the inverse problems. We derive a representation for the reduced Jacobian as the product of a time-dependent and a stationary part. Then we show that the RKS satisfying the Meier-Luenberger necessary H_2 optimality condition not only minimizes the approximation error but completely annuls its influence on the inversion result (even if the subspace is not optimal globally). More precisely, the approximation error belongs to the (left) null-space of the reduced Jacobian. We compare inversion on such subspaces using other nearly optimal RKS's based on Zolotarev problem and adaptive pole selection algorithm.

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MS 14. **New trends in tridiagonal matrices - Part II of II**

Talk 1. **On generalized Jacobi matrices which are symmetric in Krein spaces**

I will give some motivations to introduce generalized Jacobi matrices of a special type. Then, some direct and inverse problems for these matrices will be presented.

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Talk 2. **On the characteristic function for Jacobi matrices**

For a certain class of infinite Jacobi matrices with a discrete spectrum it is introduced a characteristic function as an analytic

function on a suitable complex domain. It is shown that the zero set of the characteristic function actually coincides with the point spectrum. As an illustration several explicitly solvable examples are discussed.

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Talk 3. **Tridiagonal matrices in comb filters**

In the present talk we use some known and new results on tridiagonal matrices to compute the minimum mean square error for a decision feedback equalizer when the filter is a comb filter. We also apply those mathematical results on tridiagonal matrices to a problem in linear estimation with comb filters.

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Talk 4. **The nullity theorem: forecasting structures in the inverses of sparse matrices**

The Nullity Theorem for matrices was formulated by Markham and Fiedler in 1986. At first sight, this theorem and its five-line proof appear trivial. Examples show, however, that it is powerful tool in computations with sparse and structured rank matrices. It is, e.g., a straightforward consequence of this theorem that the inverse of a tridiagonal is semiseparable, the inverse of a band matrix is higher order semiseparable, without even posing constraints of irreducibility.

We will reconsider the nullity theorem and extend it to predicting structures in LU and QR -factorizations.

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MS 15. Application of compressed sensing in Bio-Medicine

Talk 1. **Evaluation of compressed sensing impact in cardiac signals processing and transmission**

Sensor networks are a field which benefits significantly from compressed sensing (CS), as, for instance, quality of service, or battery lifetime are directly improved by the subsequent reduction of traffic. Networks transmitting biomedical data, and within those, cardiac data, have particular advantages. ECG and PPG are the most studied 1D signals in the biomedical field, and where CS implementation has been more studied. One study scenario is using the sparsity of wavelet decomposition of these signals, and Iterative Shrinkage/Thresholding algorithms. Focus is given in accuracy and computation overhead, the most critical constraints of cardiac data processing. Networking implications are quantified, for different types of real network models, as well as the impact in signals quality, and on the extracted information

(heart rate, oxygen saturation, pulse wave velocity).

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Talk 2. **Compressive sensing in drug discovery**

The design of new drugs is often based on certain interactions between a small molecule (the drug) and a protein. Often a high affinity between the small molecule and the protein is desirable. The affinity can be estimated by using statistical thermodynamics. In order to provide statistical data, high-performance computing machines are used to explore the conformational space of the molecular system. The corresponding algorithms are based on simplified physical models (force fields) for the interaction between the drug molecule and the protein. These models mostly do not take quantum effects into account. The talk will present new ideas to better include quantum chemical information, it will provide some important application areas of molecular simulation in drug discovery, and it gives some hints about using compressive sensing in this field.

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Talk 3. **Reconstruction of bacterial communities using sparse representation**

Determining the identities and frequencies of species present in a sample is a central problem in metagenomics, with scientific, environmental and clinical implications. A popular approach to the problem is sequencing the Ribosomal 16s RNA gene in the sample using universal primers, and using variation in the gene's sequence between different species to identify the species present in the sample. We present a novel framework for community reconstruction, based on sparse representation; while millions of microorganisms are present on earth, with known 16s sequences stored in a database, only a small minority (typically a few hundreds) are likely to be present in any given sample. We discuss the statistical framework, algorithms used and results in terms of accuracy and species resolution.

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Talk 4. **Sensing genome via factorization**

Since the last decade the matrix factorization and dimension reduction methods have been used for mining in genomics and proteomics. Also most recently the norm one optimization is emerging as a useful approach for this purpose. We propose a hybrid algorithm which uses the utility of SVD along with efficiency and robustness of norm one minimization for overcoming the shortcomings of each of these mentioned approaches.

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MS 16. Preconditioning of non-normal linear systems arising in scattering problems

Talk 1. **Approximate deflation preconditioning methods for penetrable scattering problems**

In this talk I consider the Lippmann-Schwinger (LS) integral equation for inhomogeneous acoustic scattering. I demonstrate

that spectral properties of the LS equations suggest that deflation based preconditioning might be effective in accelerating the convergence of a restarted GMRES method. Much of the convergence results on deflation based preconditioning are based on using exact invariant subspaces. I will present an analytical framework for convergence theory of general approximate deflation that is widely applicable. Furthermore, numerical illustrations of the spectral properties also reveal that a significant portion of the spectrum is approximated well on coarse grids. To exploit this, I develop a novel restarted GMRES method with adaptive preconditioning based on spectral approximations on multiple grids.

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Talk 2. **Direct approximate factoring of the inverse**

To precondition a large and sparse linear system, two direct methods for approximate factoring of the inverse are devised. The algorithms are fully parallelizable and appear to be more robust than the iterative methods suggested for the task. A method to compute one of the matrix subspaces optimally is derived. These approaches generalize the approximate inverse preconditioning techniques in several natural ways.

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Talk 3. **Regularization of singular integral operators as a preconditioning strategy**

In this talk we consider the singular integral equation arising in electromagnetic scattering on inhomogeneous objects in free space. To understand the apparent poor convergence of iterative methods, such as GMRES, we analyze the spectrum of both the integral operator and the system matrix. It turns out that the convergence is slowed down by dense spectral clusters, whose origin and location may be traced to the nontrivial essential spectrum of the integral operator. We propose a multiplicative regularizer which reduces the extent of these clusters and in conjunction with the deflation of largest-magnitude eigenvalues makes for a good preconditioner.

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Talk 4. **High-order shifted Laplace preconditioners for wave equations**

Shifted Laplace preconditioners techniques have been introduced by Erlangga, Vuik and Oosterlee (Applied Numerical Mathematics, 2004) for solving PDEs problems related to wave-like equations. The aim of this talk is to propose a

generalization of shifted Laplace preconditioning methods by using operator representation combined with complex Padé approximants. We will show that the resulting high-order shifted Laplace preconditioners are highly efficient and robust for two- and three-dimensional scattering problems that exhibit complex geometrical features (e.g. resonant structures). Furthermore, the convergence is proved to be weakly frequency dependent.

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MS 17. Markov Chains

Talk 1. **Markov Chain properties in terms of column sums of the transition matrix**

Questions are posed regarding the influence that the column sums of the transition probabilities of a stochastic matrix (with row sums all one) have on the stationary distribution, the mean first passage times and the Kemeny constant of the associated irreducible discrete time Markov chain. Some new relationships, including some inequalities, and partial answers to the questions, are given using a special generalized matrix inverse that has not previously been considered in the literature on Markov chains.

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Talk 2. **Hamiltonian cycle problem and Markov chains**

We consider the famous Hamiltonian cycle problem (HCP) embedded in a Markov decision process (MDP). More specifically, we consider the HCP as an optimization problem over the space of either stationary policies, or of occupational measures induced by these stationary policies. This approach has led to a number of alternative formulations and algorithmic approaches involving researchers from a number of countries. These formulations exploit properties of a range of matrices that usually accompany investigations of Markov chains. It will be shown that when these matrices are induced by the given graph some of the graph's underlying structures can be detected in their matrix analytic properties.

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Talk 3. **Inequalities for functions of transition matrices**

Consider an irreducible finite-state Markov chain on N states. It is known that the N by N matrix vanishing on the diagonal and which is equal to the mean first passage matrix elsewhere, is invertible. We prove that if N is greater than two, the diagonal entries of the inverse are negative, and obtain some related inequalities. Analogous results for a closely related matrix are derived as well. Joint with Michael Neumann and Olga Pryporova.

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Talk 4. **Compartmental systems and computation of their stationary probability vectors**

To compute stationary probability vectors of Markov chains whose transition matrices are cyclic of index p may be a difficult task if p becomes large. A class of iterative aggregation/disaggregation methods (IAD) is proposed to overcome the difficulty. It is shown that the rate of convergence of the proposed IAD processes is governed by the maximal modulus of the eigenvalues laying out of the peripheral spectrum of the smoothing matrix. The examined generators of Markov chains come from compartmental systems and cause that the transition matrices under consideration may depend upon the appropriate stationary probability vectors. The nonlinearity represents further difficulties in computation.

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MS 18. Preconditioning for PDE-constrained optimization - Part I of II

Talk 1. **Structural spectral properties of symmetric saddle point problems**

Symmetric and indefinite block structured matrices often arise after the discretization of a large variety of application problems, where the block form stems from the presence of more than one partial differential equation (PDE) in the problem, or from the imposition of some constraints, usually associated with PDEs. Structure-aware preconditioning strategies have emerged as winning devices for efficiently and optimally solving the associated large linear systems. In some relevant applications, the coefficient matrix shows a particular spectral symmetry around the origin, which should be taken into account when selecting both the iterative system solver and the most appropriate preconditioner. In this talk we analyze in detail this symmetry, and discuss its consequences in the solution of three model problems in optimal control, distributed time-harmonic parabolic control and distributed time-harmonic Stokes control.

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Talk 2. **Preconditioned iterative methods for Stokes and Navier-Stokes control problems**

The development of iterative solvers for PDE-constrained optimization problems is a subject of considerable recent interest in numerical analysis. In this talk, we consider the numerical solution of two such problems, namely those of Stokes control and Navier-Stokes control. We describe the role of saddle point theory, mass matrix and Schur complement approximation,

multigrid routines, and commutator arguments, in the construction of solvers for these problems. We also discuss issues involved with regularization terms, and, in the case of Navier-Stokes control, the outer iteration employed. We display numerical results that demonstrate the effectiveness of our solvers.

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Talk 3. **Preconditioners for elliptic optimal control problems with inequality constraints**

In this talk we consider optimal control problems with an elliptic boundary value problem as state equation. Based on recent results for distributed elliptic optimal control problems without inequality constraints we present and discuss preconditioners for the optimality system in the presence of additional control constraints or state constraints. The focus is on the performance of these preconditioners within a Krylov subspace method with respect to model and discretization parameters.

A possible extension of the presented approach to optimal control problems with other state equations, like the steady-state Stokes equations, is discussed.

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Talk 4. **Nearly optimal block preconditioners for block two-by-two linear systems**

For a class of block two-by-two systems of linear equations, we construct block preconditioning matrices and discuss the eigen-properties of the corresponding preconditioned matrices. The block preconditioners can be employed to accelerate the convergence rates of Krylov subspace iteration methods such as MINRES and GMRES. Numerical experiments show that the block preconditioners are feasible and effective when used in solving the block two-by-two linear systems arising from the finite-element discretizations of a class of PDE-constrained optimization problems.

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MS 19. Matrices and graphs - Part I of II

Talk 1. **(0,1) matrices and the analysis of social networks**

In the sociology literature, an $m \times n$ $(0, 1)$ matrix is called an actor–event matrix. In many examples, the matrix A is uniquely determined by AA^T , $A^T A$, and the fact that A is $(0, 1)$. In this talk, we present a result on pairs of actor–event matrices that are distinct but ‘close’, and yield the same AA^T and $A^T A$.

Specifically, using techniques from combinatorial matrix theory, we characterise all pairs of $(0, 1)$ matrices A_1, A_2 such that $A_1 A_1^T = A_2 A_2^T$, $A_1^T A_1 = A_2^T A_2$, and the $(0, 1, -1)$ matrix $A_1 - A_2$ has at most one 1 and one -1 in each row and column.

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Talk 2. Necessary and sufficient conditions for a Hamiltonian graph

A graph is singular if the zero eigenvalue is in the spectrum of its 0-1 adjacency matrix \mathbf{A} . If an eigenvector belonging to the zero eigenspace of \mathbf{A} has no zero entries, then the singular graph is said to be a core graph. A (κ, τ) -regular set is a subset of the vertices inducing a κ -regular subgraph such that every vertex not in the subset has τ neighbours in it. We consider the case when $\kappa = \tau$ which relates to the eigenvalue zero under certain conditions. We show that if a regular graph has a (κ, κ) -regular set, then it is a core graph. By considering the walk matrix, we develop an algorithm to extract (κ, κ) -regular sets and formulate a necessary and sufficient condition for a graph to be Hamiltonian.

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Talk 3. On the eigenvalues of symmetric matrices associated with graphs

Let G be a weighted graph of order n . It is known that $\lambda_1 \geq d_1$ and $\lambda_2 \geq d_3$ where λ_i and d_i are the i^{th} largest Laplacian eigenvalue and degree of G , respectively. For λ_3 and smaller eigenvalues we show that it is possible to construct a weighted graph G of any order n such that $\lambda_j < d_n$.

To obtain these results we show that for every $k \geq 2$ and $n \geq k + 1$ there exists a weighted graph of order n whose adjacency matrix has exactly k negative eigenvalues. This is done by obtaining some beautiful properties of the Schur complements of the adjacency matrix.

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Talk 4. An extension of the polytope of doubly stochastic matrices

We consider a class of matrices whose row and column sum vectors are majorized by given vectors b and c , and whose entries lie in the interval $[0, 1]$. This class generalizes the class of doubly stochastic matrices. We investigate the corresponding polytope $\Omega(b|c)$ of such matrices. Main results include a generalization of the Birkhoff - von Neumann theorem and a characterization of the faces, including edges, of $\Omega(b|c)$.

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MS 20. Tensor based methods for high dimensional problems in scientific computing - Part I of II

Talk 1. Optimal a priori Tensor Decomposition for the Solution of High Dimensional Problems

Tensor-based methods are receiving a growing attention for their use in high dimensional applications in scientific computing where functions of multiple parameters have to be approximated. These methods are based on the construction of tensor decompositions that provide approximate representations of functions on adapted low dimensional reduced bases. Here, we propose algorithms that are able to directly construct an approximation of optimal tensor decompositions with respect to a desired metric, without a priori information on the solution. Connections with optimal model reduction will be discussed.

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Talk 2. Application of the Proper Generalized Decomposition (PGD) to 3D cracked plates and estimation of the discretization error

We present a new numerical approach to solve cracked plates in an efficient way by obtaining a single solution in which the Poisson's ratio ν and the plate thickness B are non-fixed parameters. With a single analysis, it is possible to obtain a numerical solution for a cracked plate problem that can be particularized for any ν and B by simple post-processing, thus providing an efficient tool for the numerical analysis of these problems. The method makes use of the Proper Generalized Decomposition (PGD). In this method, the sought displacement field $\mathbf{u}(x, y, z, \nu, B)$ is written as a series expansion of function products. The formulation proposed here uses a 2D discretization for the plane XY and a 1D discretization in the Z -direction. In addition, independent functions of ν and B are included in the tentative solution to be converged. An iterative process is then carried out by which the necessary terms of the series expansion are added in order to attain the required accuracy. We have also implemented a recovery type error estimator to evaluate the discretization error in energy norm both in the XY plane (2D problem) and along the Z -direction (1D problem). The combination of both errors provides the local error distribution that can be used to drive the h -adaptive refinement.

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Talk 3. A tensor calculus approach for Bézier shape deformation

The goal of our research is to obtain a computationally efficient deformation of a parametric curve. This research is applied to engineering applications as, for example, mobile robotics and liquid composite moulding. A new technique was developed to modify a Bézier curve by minimizing the changes of its shape. This shape modification is computed through a field of vectors, applying them on particular points of the Bézier curve (Bézier Shape Deformation, BSD). In these kinds of applications the computational cost is a critical issue because the parametric curve must be modified in real time. Therefore, the original BSD algorithm has been reformulated using algebra of tensors to reduce the computational time (Tensor-Bézier Shape Deformation, T-BSD). While BSD grows exponentially, T-BSD grows linearly. As a consequence, the Bézier curve is modified with the lowest computational cost.

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Talk 4. Tensor approximation methods for parameter identification

In this talk we present methods for parameter identification—here the coefficient fields of partial differential equations—based on Bayesian procedures. As is well known, Bayes's theorem for random variables (RVs) of finite variance is an orthogonal projection onto a space of functions generated by the observations. Both the quantity to be identified as well as the space to project onto are described as functions of known RVs. All this takes place in high-dimensional tensor product spaces. To limit the numerical effort, we use low-rank tensor approximations for the forward as well as the inverse problem.

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MS 21. Reducing communication in linear algebra - Part I of II

Talk 1. Communication-optimal parallel algorithm for Strassen's matrix multiplication

Parallel matrix multiplication is one of the most studied fundamental problems in distributed and high performance computing. We obtain a new parallel algorithm that is based on Strassen's fast matrix multiplication and minimizes communication. The algorithm outperforms all other parallel matrix multiplication algorithms, classical and Strassen-based, both asymptotically and in practice.

A critical bottleneck in parallelization of Strassen's algorithm is the communication between the processors. Ballard, Demmel, Holtz, and Schwartz (SPAA'11) provide lower bounds on these communication costs, using expansion properties of the underlying computation graph. Our algorithm matches these lower bounds, and so is communication-optimal. It has perfect strong scaling within the maximum possible range. Our parallelization approach generalizes to other fast matrix multiplication algorithms.

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Talk 2. A communication-avoiding symmetric-indefinite factorization

We describe a communication-avoiding symmetric indefinite factorization. The factorization works in two phases. In the first phase, we factor $A = LTL^T$ where L is unit lower triangular and T is banded with bandwidth $\Theta(\sqrt{M})$ where M is the size of the cache. This phase uses a block version of Aasen's algorithm. In the second phase, we factor T ; this can be done efficiently using Kaufman's retraction algorithm, or LU with partial pivoting, or successive band reduction. We show that the algorithm is asymptotically optimal in terms of communication, is work efficient ($n^3/3 + o(n^3)$ flops), and is backward stable.

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Talk 3. **LU factorisation with panel rank revealing pivoting and its communication avoiding version**

We present the LU decomposition with panel rank revealing pivoting (LU_PRRP), an LU factorization algorithm based on strong rank revealing QR panel factorization. LU_PRRP is more stable than Gaussian elimination with partial pivoting (GEPP). Our extensive numerical experiments show that the new factorization scheme is as numerically stable as GEPP in practice, but it is more resistant to pathological cases and easily solves the Wilkinson matrix and the Foster matrix. We also present CALU_PRRP, a communication avoiding version of LU_PRRP that minimizes communication. CALU_PRRP is more stable than CALU, the communication avoiding version of GEPP.

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Talk 4. **2.5D algorithms for parallel dense linear algebra**

We give a ‘2.5D’ parallelization scheme for dense linear algebra computations. Our scheme exploits any extra available memory adaptively. The scheme generalizes previous work on 2D and 3D algorithms in matrix multiplication. Further, we extend 2.5D algorithms to LU, Cholesky, and Cholesky-QR factorizations, triangular solve, and the all-pairs-shortest-path problem. These new algorithms perform asymptotically less communication than any previous counterparts. 2.5D algorithms are also practical and map well to torus networks. We benchmark 2.5D matrix multiplication and LU factorization on 65,536 cores of a Blue Gene/P supercomputer. Our results demonstrate that memory replication improves strong scalability and overall efficiency significantly.

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MS 22. **Linear algebra for inverse problems - Part I of II**

Talk 1. **Block-extrapolation methods for linear matrix ill-posed problems**

In this talk, we consider large-scale linear discrete ill-posed problems where the right-hand side contains noise. In many applications such as in image restoration the coefficient matrix is given as a sum of Kronecker products of matrices and then Tikhonov regularization problem leads to a generalized linear matrix equation. We define some block extrapolation methods and show how they could be used in combination with the singular value decomposition (SVD) to solve these problems. In particular, the proposed methods will be applied in image restoration. Some theoretical results and numerical tests in image restoration are also given.

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Talk 2. **Convergence properties of GMRES and RRGMES method for ill posed problems**

Range restricted iterative methods (RRGMRES) based on the Arnoldi process are attractive for the solution of large nonsymmetric linear discrete ill-posed problems with error-contaminated data (right-hand side).

GMRES is one of the most widely used iterative methods for the solution of linear system of equations, with a large real or complex nonsingular matrix. Convergence properties of GMRES are discussed by many authors.

We present some theoretical results for GMRES and RRGMES and we give some numerical tests.

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Talk 3. **Inverse problems for regularization matrices**

Discrete ill-posed problems are difficult to solve, because their solution is very sensitive to errors in the data and to round-off errors introduced during the solution process. Tikhonov regularization replaces the given discrete ill-posed problem by a nearby penalized least-squares problem whose solution is less sensitive to perturbations. The penalization term is defined by a regularization matrix, whose choice may affect the quality of the computed solution significantly. We describe several inverse matrix problems whose solution yields regularization matrices adapted to the desired solution. Numerical examples illustrate the performance of the regularization matrices determined.

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Talk 4. **Meshless regularization for the numerical**

computation of the solution of steady Burgers-type equations

In this talk, we introduce a meshless method approximation for the numerical solution of the Burgers-type steady equations. The numerical approximation to the exact solution is obtained from the exact values of the analytical solution on a finite set of scattered data points in the interior of the domain. The exact values are in fact unknown and contaminated by a noise. Regularization techniques are needed to obtain the numerical approximation as the smoothing thin plate splines. This strategy leads to a nonlinear system which may be solved by using the Tikhonov regularization method. The estimation of the regularization parameter is obtained by using the classical GCV or the L-curve criteria. We present some theoretical results and we give some numerical tests.

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MS 23. Modern matrix methods for large scale data and networks

Talk 1. Nonlinear eigenproblems in data analysis and graph partitioning

It turns out that many problems in data analysis and beyond have natural formulations as nonlinear eigenproblems. In this talk I present our recent line of research in this area. This includes the efficient computation of nonlinear eigenvectors via a generalization of the inverse power method and a general result showing that a certain class of NP-hard combinatorial problems such as balanced graph cuts or the (constrained) maximum density subgraph have tight relaxations as nonlinear eigenproblems.

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Talk 2. LSRN: a parallel iterative solver for strongly over- or under-determined systems

We develop a parallel iterative least squares solver named LSRN that is based on random normal projection. It computes the unique minimum-length solution to $\min_{x \in \mathbb{R}^n} \|Ax - b\|_2$, where $A \in \mathbb{R}^{m \times n}$ can be rank-deficient with $m \gg n$ or $m \ll n$. A can be a dense matrix, a sparse matrix, or a linear operator, and LSRN speeds up automatically on sparse matrices and fast operators. The preconditioning phase consists of a random normal projection, which is embarrassingly parallel, and a singular value decomposition of size $\lceil \gamma \min(m, n) \rceil \times \min(m, n)$, where γ is moderately larger than 1, e.g., $\gamma = 2$. We show that the preconditioned system is well-conditioned with a strong concentration result on the

extreme singular values. Hence the number of iterations is fully predictable if we apply LSQR or the Chebyshev semi-iterative method to the preconditioned system. The latter method is particularly efficient for solving large-scale problems on clusters with high communication cost. LSRN is also capable of handling certain types of Tikhonov regularization. Numerical results show that LSRN outperforms LAPACK's DGELSD on large-scale dense problems and MATLAB's backslash (SuiteSparseQR) on sparse problems on a shared memory machine, and LSRN scales well on Amazon Elastic Compute Cloud (EC2) clusters.

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Talk 3. Solving large dense linear systems with covariance matrices

Gaussian processes are a fundamental tool in spatial/temporal statistics, and they have broad applications to fields such as nuclear engineering and climate science. The maximum likelihood approach for fitting a Gaussian model requires the manipulation of the covariance matrix through inversion, logarithmic action and trace computation, all of which pose significant challenges for large dense matrices. We consider a reformulation of the maximum likelihood through a stochastic approximation framework, which narrows down the several linear algebra challenges to solving a linear system with the covariance matrix for multiple right-hand sides. In this talk I will present an iterative technique integrating the designs of the solver, the preconditioner and the matrix-vector multiplications, which lead to a scalable method for solving the maximum likelihood problem in data analysis.

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Talk 4. Fast coordinate descent methods with variable selection for non-negative matrix factorization

Non-negative Matrix Factorization (NMF) is a dimension reduction method for non-negative matrices, and has proven to be useful in many areas, such as text mining, bioinformatics and image processing. In this talk, I will present a new coordinate descent algorithm for solving the least squares NMF problem. The algorithm uses a variable selection scheme that employs the gradient of the objective function. This new method is considerably faster in practice, especially when the solution is sparse, as is often the case in real applications. In these cases, our method benefits by selecting important variables to update more often, thus resulting in higher speed. As an example, on a text dataset RCV1, our method is 7 times faster than FastHals, which is a cyclic coordinate descent algorithm, and more than 15 times faster when the sparsity is increased by adding an L1 penalty. We also develop new coordinate descent methods when error in NMF is measured by KL-divergence by applying the Newton method to solve the one-variable sub-problems.

Experiments indicate that our algorithm for minimizing the KL-divergence is faster than the Lee & Seung multiplicative rule by a factor of 10 on the CBCL image dataset.

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MS 24. Novel and synergetic algorithms for multicore and multinode architecture

Talk 1. Novel and synergetic linear algebra algorithms on multicore and multinode architecture

The advent of parallel computers from multiple CPUs to, more recently, multiple processor cores within a single CPU has continued to spur innovative linear algebra algorithms. This minisymposium aims to present a number of works that not only exhibit new algorithmic ideas suitable for these modern computer architectures, but also present interesting synergies among themselves in several levels. This talk gives an overview on how a set of such algorithms work together and sets the stage for the details to follow in each of the subsequent presentations.

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Talk 2. Towards hybrid factorization methods for solving large sparse systems

The availability of large-scale computing platforms comprised of thousands of multicore processors motivates the need for highly scalable sparse linear system solvers. In this talk I will review some recent work by researchers at Purdue University, University of Lugano, and Intel Corporation on the combined use of direct and iterative methods for solving very large linear systems of equations. We will present recent progress in the area of parallel direct solvers and present a new parallel solver that combines the desirable characteristics of direct methods (robustness) and iterative solvers (computational efficiency), while alleviating their drawbacks (high memory requirements, lack of robustness).

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Talk 3. Eigensolver-based reordering and parallel traceMIN

The eigenvector corresponding to the second smallest eigenvalue of the Laplacian of a graph, known as the Fiedler vector, has a number of applications in areas that include matrix reordering, graph partitioning, protein analysis, data mining, machine learning, and web search. The computation of the Fiedler vector has been regarded as an expensive process as it involves solving a large eigenvalue problem. We present an efficient parallel algorithm for computing the Fiedler vector of large graphs based on the Trace Minimization algorithm. We compare the parallel performance of our method against one of the best implementations of a sequential multilevel scheme, designed

specifically for computing the Fiedler vector – routine MC73 of the Harwell Subroutine Library (HSL). In addition, we present results showing how such reordering: (i) enhances data locality for sparse matrix-vector multiplication on parallel architectures, as well as (ii) helps in extracting effective and scalable preconditioners.

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Talk 4. FEAST a density matrix based eigensolver

The FEAST algorithm takes its inspiration from the density matrix representation and contour integration technique in quantum mechanics. It combines simplicity and efficiency and offers many important capabilities for achieving high performance, robustness, accuracy, and scalability for solving large sparse eigenvalue problems on parallel architectures. Starting from a random set of vectors, FEAST's main computational tasks consist of solving a few complex-valued independent linear systems with multiple right-hand sides, and one reduced eigenvalue problem orders of magnitude smaller than the original one. Accuracy can be systematically improved through an iterative process that usually converges in two to three iterations. In this talk, FEAST will first be presented as an outer-layer interface to any linear system solvers either shared-memory or distributed such as PSPIKE. In addition, it will be shown that a single FEAST iteration provides the best suitable eigen-subspace which can be used for initiating the TraceMIN algorithm.

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MS 25. Direction preserving and filtering methods for solving sparse linear systems

Talk 1. Algebraic two-level domain decomposition methods

We consider the solving of linear systems arising from porous media flow simulations with high heterogeneities. The parallel solver is a Schwarz domain decomposition method. The unknowns are partitioned with a criterion based on the entries of the input matrix. This leads to substantial gains compared to a partition based only on the adjacency graph of the matrix. From the information generated during the solving of the first linear system, it is possible to build a coarse space for a two-level domain decomposition algorithm. We compare two coarse spaces: a classical approach and a new one adapted to parallel implementation.

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Talk 2. **Filtering solvers**

In this talk, we give an overview on filtering solvers. This comprises frequency filtering and the smoothing correction scheme, the tangential frequency filtering (TFFD) by Wagner, the two frequency decomposition by Buzdin et al. We then discuss the adaptive filtering method. The adaptive test vector iterative method allows the combination of the tangential frequency decomposition and other iterative methods such as multi-grid. We further discuss the Filtering Algebraic Multigrid (FAMG) method. Interface problems as well as problems with stochastically distributed properties are considered. Realistic numerical experiments confirm the efficiency of the presented algorithms.

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Talk 3. **Bootstrap algebraic multigrid**

By the time of its development Algebraic Multigrid (AMG) was thought of as a black box solver for systems of linear equations. Yet, the classical formulation of AMG turned out to lack the robustness to overcome challenges encountered in many of today's computational simulations which lead to the development of adaptive techniques in AMG methods.

We present in this talk a Bootstrap approach to adaptive AMG introducing the so-called "Least Squares Interpolation" (LSI) which allows to define interpolation operators solely based on prototypes of algebraically smooth error. Furthermore, we introduce a "Bootstrap Setup" which enables us to compute accurate LSI operators using a multigrid approach in the setup to efficiently compute the required prototypes of algebraically smooth error.

We demonstrate the potential of the Bootstrap AMG approach in the application to a variety of problems, each illustrating a certain aspect of the method.

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Talk 4. **Block filtering decomposition**

We describe a preconditioning technique that is suitable for matrices arising from the discretization of a system of PDEs on unstructured grids. The preconditioner satisfies a filtering property, which ensures that the input matrix is identical with the preconditioner on a given filtering vector. This vector is chosen to alleviate the effect of low frequency modes on convergence.

We present a general approach that allows to ensure that the filtering condition is satisfied in a matrix decomposition. The input matrix can have an arbitrary sparse structure, and can be reordered using nested dissection to allow a parallel implementation.

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MS 26. Advances in Krylov subspace methods

Talk 1. **The new challenges to Krylov subspace methods**

Solution methods based on preconditioned Krylov subspace methods have reached a certain level of maturity and research in this area is now mostly concerned with issues related to preconditioning. This state of equilibrium is currently being challenged by the emerging computational architectures. For example, general purpose GPUs put a high cost on inner products on which Krylov methods rely heavily. At the same time the many-core environment will make standard Krylov method unreliable due to the potentially high number of possible hardware failures when tens or hundreds of thousands of cores are deployed. In this talk we will explore these challenges and see what options are available to face them.

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Talk 2. **Random shadow vectors in IDR(s): an explanation of its GMRES-like convergence**

The IDR(s) method [Sonneveld and van Gijzen, SISC 31, 1035-1062 (2008)], is a family of short-term recurrent Krylov subspace solvers for large sparse, not necessarily symmetric linear systems. For increasing s , the convergence behaviour shows an increasing similarity with full GMRES. The residuals of IDR(s) are, roughly speaking, orthogonalized with respect to s shadow vectors. Usually these are randomly chosen. Each iteration step can be related to a Galerkin approximation in a corresponding Krylov subspace. In this talk we describe why the quality of this Galerkin approximation comes close to the optimal (GMRES), if s is large enough.

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Talk 3. **Truncated and inexact Krylov subspace methods for parabolic control problems**

We study the use of inexact and truncated Krylov subspace methods for the solution of linear systems arising in the discretized solution of optimal control of a parabolic partial differential equation. An all-at-once temporal discretization and a reduced Hessian approach are used. The solutions of the two linear systems involved in this reduced Hessian can be approximated, and in fact they can be less and less exact as the

iterations progress. The option we propose is the use of the parareal-in-time algorithm for approximating the solution of these two linear systems. Truncated methods can be used without much delay in convergence, but with important savings in storage. Spectral bounds are provided and numerical experiments are presented, illustrating the potential of the proposed methods.

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Talk 4. **Convergence of iterative solution algorithms for least-squares problems**

We consider the iterative solution of linear least-squares problems. We ask the following questions: which quantities should be used to monitor convergence, and how can these quantities be estimated at every iteration of commonly used algorithms? We argue that the backward error, appropriately scaled, is an excellent measure of convergence. We show how certain projections of the residual vector can be used to bound or estimate it. We present theoretical results and numerical experiments on the convergence of the backward error and its estimates in the algorithms LSQR of Paige and Saunders and LSMR of Fong and Saunders.

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MS 27. **Preconditioning for PDE-constrained optimization - Part II of II**

Talk 1. **On linear systems arising in Trust-region methods**
Trust-region methods are widely used for the numerical solution of nonlinear constrained and unconstrained optimization problems. Similar as line-search methods, they take turns in minimizing local models of the objective. In contrast to line-search methods, however, trust-region approaches do not require nor promote the positive definiteness of the local Hessian approximations.

In this presentation, we address issues arising in the context of the preconditioned approximate solution of these local models. The talk will highlight connections between algorithmic optimization and linear algebra.

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Talk 2. **Preconditioning for PDE-constrained optimization using proper orthogonal decomposition**

The main effort of solving a PDE constrained optimization problem is devoted to solving the corresponding large scale linear system, which is usually sparse and ill conditioned. As a result, a suitable Krylov subspace solver is favourable, if a proper preconditioner is embedded. Other than the commonly used block preconditioners, we exploit knowledge of proper orthogonal decomposition (POD) for preconditioning and achieve some interesting features. Numerical results on nonlinear test problems are proposed.

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Talk 3. **Preconditioning for Allen-Cahn variational inequalities with non-local constraints**

The solution of Allen-Cahn variational inequalities with mass constraints is of interest in many applications. This problem can be solved in its scalar and vector-valued form as a PDE-constrained optimization problem. At the heart of this method lies the solution of linear systems in saddle point form. In this talk we propose the use of Krylov-subspace solvers and suitable preconditioners for the saddle point systems. Numerical results illustrate the competitiveness of this approach.

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Talk 4. **A one-shot approach to time-dependent PDE control**

In this talk, we motivate, derive and test effective preconditioners to be used with the MINRES algorithm for solving a number of saddle point systems, which arise in PDE constrained optimization problems. We consider the distributed control and boundary control problems subject to partial differential equations such as the heat equation or Stokes equations. Crucial to the effectiveness of our preconditioners in each case is an effective approximation of the Schur complement of the matrix system. In each case, we state the problem being solved, propose the preconditioning approach, and provide numerical results which demonstrate that our solvers are effective for a wide range of regularization parameter values, as well as mesh sizes and time-steps.

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MS 28. Matrices and graphs - Part II of II

Talk 1. Parameters related to maximum nullity, zero forcing number, and tree-width of a graph

Tree-width, and variants that restrict the allowable tree decompositions, play an important role in the study of graph algorithms and have application to computer science. The zero forcing number is used to study the maximum nullity/minimum rank of the family of symmetric matrices described by a graph. Relationships between these parameters and several Colin de Verdière type parameters, and numerous variations (including the minor monotone floors and ceilings of some of these parameters) are discussed.

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Talk 2. Colin de Verdière numbers of chordal and split graphs

I will discuss the Colin de Verdière number of a chordal graph, showing that it always takes one of two possible values. For the important subcase of split graphs, I will present a complete distinction between the two cases. Finally, I will show how to deduce from the result on chordal graphs an improvement of factor 2 to Colin de Verdière's well-known tree-width upper

bound for the eponymous number. This work was done while the author was at Technion.

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Talk 3. Kochen-Specker sets and the rank-1 quantum chromatic number

The quantum chromatic number of a graph G is sandwiched between its chromatic number and its clique number, which are well known NP-hard quantities. We restrict our attention to the rank-1 quantum chromatic number $\chi_q^{(1)}(G)$, which upper bounds the quantum chromatic number, but is defined under stronger constraints. We study its relation with the chromatic number $\chi(G)$ and the minimum dimension of orthogonal representations $\xi(G)$. It is known that $\xi(G) \leq \chi_q^{(1)}(G) \leq \chi(G)$. We answer three open questions about these relations: we give a necessary and sufficient condition to have $\xi(G) = \chi_q^{(1)}(G)$, we exhibit a class of graphs such that $\xi(G) < \chi_q^{(1)}(G)$, and we give a necessary and sufficient condition to have $\chi_q^{(1)}(G) < \chi(G)$. Our main tools are Kochen-Specker sets, collections of vectors with a traditionally important role in the study of noncontextuality of physical theories, and more recently in the quantification of quantum zero-error capacities. Finally, as a corollary of our results and a result by Avis, Hasegawa, Kikuchi, and Sasaki on the quantum chromatic number, we give a family of Kochen-Specker sets of growing dimension.

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Talk 4. On the null vectors of graphs

Eigenvalues and eigenvectors associated with graphs have been important areas of research for many years. My plan for this talk is to revisit a basic, yet important, result by Fiedler on the inertia of acyclic matrices and discuss its impact on some previous related work and highlight some interesting new implications on certain null vectors associated with a graph.

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MS 29. Tensor based methods for high dimensional problems in scientific computing - Part II of II

Talk 1. A greedy algorithm for the convergence of a Laplacian operators in the blind deconvolution problem

In this talk we present new results on the a greedy algorithm to study the convergence of the Fractional Blind Deconvolution in a Hilbert Space. We will show the theoretical results and the application to the artistic Restoration.

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Talk 2. Algorithms for approximate inverse of operators for preconditioning systems of equations in tensor format

We here propose and analyze greedy algorithms for the approximation of the inverse of an operator in tensor format. Algorithms are based on successive best approximations with respect to non usual norms that makes possible the decomposition of the inverse operator without any a priori information. This approximate inverse is then used for preconditioning iterative solvers and PGD algorithms for the solution of high dimensional PDEs in tensor format. The efficiency of the proposed preconditioner is illustrated on numerical examples, where it is compared to other preconditioners.

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Talk 3. Geometric structures in tensor representations

In this talk we discuss about the geometric structures associated with tensor representations based in subspaces. We introduce a generalization of the hierarchical Tucker format. Then we give a Banach manifold structure to the set of tensors in generalized hierarchical Tucker format with fixed hierarchical rank. It allows to extend the dynamical low-rank tensor approximation framework to tensor Banach spaces.

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MS 30. Reducing communication in linear algebra - Part II of II

Talk 1. Communication-avoiding sparse matrix-matrix multiplication

Sparse matrix-matrix multiplication is a key primitive for many high performance graph algorithms as well as some linear solvers, such as algebraic multigrid. There is a significant gap between communication costs of existing algorithms and known lower bounds. We present new 1D and 2.5D algorithms that perform less communication than existing algorithms. These algorithms have different memory requirements, and they scale

differently with increasing matrix density and processor count. We also report on our performance results on large-scale experiments and our recent progress in obtaining tighter lower bounds.

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Talk 2. Improving the stability of communication-avoiding Krylov subspace methods

Krylov Subspace Methods (KSMs) are commonly used for solving linear systems, eigenvalue problems, and singular value problems. Standard KSMs are communication-bound on modern computer architectures, due to required sparse matrix-vector multiplication and projection operations in each iteration. This motivated s -step KSMs, which can use blocking strategies to increase temporal locality, allowing an $O(s)$ reduction in communication cost. Despite attractive performance benefits, these variants are often considered impractical, as increased error in finite precision can negatively affect stability. We discuss practical techniques for alleviating these problems in s -step methods while still achieving an asymptotic reduction in communication cost.

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Talk 3. Hiding global synchronization latencies in Krylov methods for systems of linear equations

In Krylov methods, global synchronization due to reduction operations for dot-products is becoming a bottleneck on parallel machines. We adapt GMRES and CG such that this global communication latency is completely overlapped by other local work. This requires the global communication to be performed in a non-blocking or asynchronous way. To maintain stability even at the strong scaling limit, different Krylov bases, like Newton and Chebychev bases, can be used. Our performance model predicts large benefits for future exascale machines as well as for current-scale applications such as solving the coarsest level of a multigrid hierarchy in parallel.

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Talk 4. **Avoiding communication with hierarchical matrices**

We show how to reorganize the construction of a Krylov basis $[x, Ax, \dots, A^s x]$ to asymptotically reduce data movement, when A is a hierarchical matrix. Our approach extends the blocking covers algorithm of Leiserson, Rao, and Toledo, and requires that off-diagonal blocks of A are low-rank. This approach enables communication-avoiding s -step Krylov subspace methods with hierarchical preconditioners. We also discuss extensions to multigrid and fast multipole methods.

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MS 31. Linear algebra for inverse problems - Part II of II

Talk 1. **Implicit filtering methods for inverse problems**

In this talk we consider a nonlinear least squares framework to solve separable nonlinear ill-posed inverse problems. It is shown that with proper constraints and well chosen regularization parameters, it is possible to obtain an objective function that is fairly well behaved. Although uncertainties in the data and inaccuracies of linear solvers make it unlikely to obtain a smooth and convex objective function, it is shown that implicit filtering optimization methods can be used to avoid becoming trapped in local minima. An application to blind deconvolution is used for illustration.

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Talk 2. **Iterative reconstruction methods for adaptive optics**

The image quality of large ground based astronomical telescopes suffers from turbulences in the atmosphere. Adaptive Optics is a hardware-based technique that corrects the influence of the turbulence. To this end, wavefront measurements from the incoming wavefront of several guide stars are used for the reconstruction of the turbulent layers in the atmosphere. The reconstructed atmosphere is then used to compute the surface of several deformable mirrors such that, in the reflected light, the

influence of the turbulence is removed. The reconstruction of the turbulence in the atmosphere is related to a limited angle tomography problem and therefore severely ill posed. For the new class of extremely large telescopes, the numerical task is to invert a linear system with a dimension of approximately 60.000×10.000 every millisecond.

We present iterative methods, based on Kaczmarz and cg, for the reconstruction of the layers. The methods will be evaluated in different function spaces. In particular, we will include the modeling of specific effects that are related to the use of laser guide stars. We will also demonstrate that our method are able to compute the correcting shape of the deformable mirrors within the available time frame.

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Talk 3. **Approximated nonstationary iterated Tikhonov with application to image deblurring**

In this talk we present new iterative regularization methods, based on the approximation of nonstationary iterated Tikhonov. In particular we investigate the image deblurring problem, where the blurring matrix is not easily invertible with a low computational cost, while an approximation with such property is available. This is for instance the case of block Toeplitz matrices with Toeplitz blocks that can be well approximated by block circulant matrices with circulant blocks matrices which can be diagonalized by two dimensional fast Fourier transforms. Matrices arising from the imposition of other boundary conditions can be considered as well.

A detailed analysis is proposed in the stationary case and we discuss relations with preconditioned Landweber method and other known methods. A large numerical experimentation with different boundary conditions, blurring phenomena and noise level is presented.

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Talk 4. **On the Richardson-Lucy method for image restoration**

Image deconvolution problems with a symmetric point-spread function arise in many areas of science and engineering. These problems often are solved by the Richardson-Lucy method, a nonlinear iterative method. In this talk we first show a convergence result for the Richardson-Lucy method. The proof sheds light on why the method may converge slowly. Subsequently, we describe an iterative active set method that imposes the same constraints on the computed solution as the Richardson-Lucy method. Computed examples show the latter method to yield better restorations than the Richardson-Lucy method with less computational effort.

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MS 32. Orderings in sparse matrix computation

Talk 1. Orderings and solvers for “non-uniform sparse matrices”

Sparse matrices from non-PDE problems come in rich varieties. We specifically address sparse matrices that have a non-uniform distribution of nonzeros per row (power-law graphs are a popular example that lead to these), which may be called “non-uniform sparse matrices.” We examine the appropriateness of traditional orderings to solve various problems for these types of matrices. For example, instead of RCM reordering for $ILU(k)$, it is natural and indeed better to use an ordering by increasing degree. By studying why such orderings are effective, we are lead to “incomplete” versions of minimum degree ordering, i.e., the ordering operates like minimum degree, but the maximum degree is capped by a parameter, just as fill-in level in $ILU(k)$ is capped. Lee, Raghavan, and Ng proposed such a technique for pivoting in 2006. In our studies, tie-breaking and the complementary strategies of reducing the number of fill-ins and the aggregate size of fill-ins are important issues. Sparse matrices from PDEs have well-defined model problems; to further study non-uniform sparse matrices, we propose models (structure and values) derived from realistic applications.

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Talk 2. On hypergraph partitioning based ordering methods for sparse matrix factorization

We discuss the use of hypergraph-based methods for orderings of sparse matrices in Cholesky, LU and QR factorizations. For the Cholesky factorization case, we investigate a recent result on pattern-wise decomposition of sparse matrices, generalize the result and develop effective ordering algorithms. The generalized results help us formulate the ordering problem in LU as we do in the Cholesky case, without ever symmetrizing the given matrix. For the QR factorization case, the use of hypergraph models is fairly standard; the method does not symmetrize the given matrix. We present comparisons with the most common alternatives in all three cases.

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Talk 3. Orderings governed by numerical factorization

We study the solution of sparse least-squares problems using an augmented system approach:

$$\begin{pmatrix} I & A \\ A^T & 0 \end{pmatrix} \begin{pmatrix} r \\ x \end{pmatrix} = \begin{pmatrix} b \\ 0 \end{pmatrix}$$

If the null space approach for constrained optimization is used, a crucial aspect is the selection of the basis rows from the overdetermined matrix A . We discuss the effect of this showing that the concept of condition number and conditioning needs to be rethought in this case. We illustrate our discussion with runs using a basis selection routine from HSL that involves a sparse factorization with rook pivoting and a subsequent solution of the augmented system using iterative methods.

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Talk 4. Reordering sparse Cholesky factorization: minimum fill vs. minimum FLOP count

Given a sparse positive definite matrix A , we discuss the problem of finding a permutation matrix P such that the number of floating point operations for computing the Cholesky factorization $PAP^T = LL^T$ is minimum. Two theoretical results are presented: First, we outline a reduction from MAXCUT in order to give an NP-hardness result. Second, we discuss the relationship of minimizing FLOPs and the minimum fill problem. Using an explicit construction we show that orderings which minimize the operation count may be non-optimal in terms of the fill and vice versa.

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MS 33. Moving from multicore to manycore in applied linear algebra

Talk 1. Parallel preconditioners and multigrid methods for sparse systems on GPUs

Large-scale numerical simulation relies on both efficient parallel solution schemes and platform-optimized parallel implementations. Due to the paradigm shift towards multicore and manycore technologies, both aspects have become more intricate. In this talk we address fine-grained parallel preconditioning techniques and multigrid solvers that are compliant with SIMD-like parallelism of graphics processing units. By means of multi-coloring reordering combined with the power(q)-pattern method for incomplete LU decompositions with fill-ins we show how scalable parallelism can be introduced to the triangular solution phase of smoothers and preconditioners. Performance results demonstrate efficiency and

scalability of our approach on recent GPUs and on multicore-CPUs.

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Talk 2. Towards a GPU-accelerated direct sparse solver

We present a detailed study about the acceleration of a direct method to solve sparse linear systems using GPU-based computing. Particularly, we describe a variant for the factorization stage of the multifrontal method which combines CPU and GPU computations. Additionally, the developed routine is included in the CSparse library to cover the whole solver. We evaluate the proposal and compare it with an ad-hoc multicore implementation and the implementation included in MUMPS library (combined with Goto BLAS) The results obtained show that this is a promising research line to accelerate this kind of sparse matrix solvers on cheap hardware platforms.

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Talk 3. Exploiting the flexibility of libflame for novel multi-core and many-core architectures

The libflame library is a modern, high-performance dense linear algebra library that is extensible, easy to use, and available under an open source license, and offers competitive (and in many cases superior) real-world performance when compared to traditional libraries like LAPACK. It can optionally exploit multiple cores by casting an algorithm as an algorithm-by-blocks which can generate a directed acyclic graph (DAG) that is then scheduled to cores via a runtime system called SuperMatrix. In this talk we demonstrate its flexibility for running efficiently dense linear algebra codes on general-purpose architectures, including single core, multi-core and GPU-based architectures. In addition, we adapt our runtime to support a novel, highly efficient HPC architecture: the Texas Instrument's C6678 multi-core DSP.

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Talk 4. High-performance genome studies

In the context of the genome-wide association study (GWAS), one has to solve long sequences of generalized least-squares

problems; such a problem presents two limiting factors: execution time –often in the range of days or weeks– and data management –in the order of Terabytes–. We present algorithms that obviate both issues. By taking advantage of domain-specific knowledge, exploiting parallelism provided by multicores and GPU, and handling data efficiently, our algorithms attain unequalled high performance. When compared to GenABEL, one of the most widely used libraries for GWAS, we obtain speedups up to a factor of 50.

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MS 34. Least squares methods and applications

Talk 1. Block Gram–Schmidt algorithms with reorthogonalization

The talk discusses reorthogonalized block classical Gram–Schmidt algorithms for factoring a matrix A into $A = QR$ where Q is left orthogonal (has orthonormal columns) and R is upper triangular. These algorithms are useful in developing BLAS-3 versions of orthogonal factorization in the implementation of Krylov space methods and in modifying an existing orthogonal decomposition.

In previous work, we have made assumptions about the diagonal blocks of R to insure that a block classical Gram–Schmidt algorithm with reorthogonalization will produce a backward stable decomposition with a near left orthogonal Q . The context of this talk is where these diagonal blocks violate those assumptions and are allowed to be singular or very ill-conditioned. A strategy for using rank-revealing decompositions to deal with that contingency is given that insures a similar result to the case where the assumptions about the blocks of R hold. The algorithm is considered in the context of block downdating.

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Talk 2. A numerical method for a mixed discrete bilinear least squares problem

For CPU utilization control in distributed real-time embedded systems, we recently proposed a new scheme to make synchronous rate and frequency adjustment to enforce the utilization set point. In this scheme, we need to solve a mixed discrete bilinear least squares problem, in which one unknown vector is subject to a box constraint and the other unknown vector's each entry has to be taken from a discrete set of numbers. In this talk we propose an alternating iterative method to solve this problem.

This is joint work with Xi Chen and Xue Liu.

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Talk 3. On condition numbers for constrained linear least squares problems

Condition numbers are important in numerical linear algebra, which can tell us the posterior error bounds for the computed solution. Classical condition numbers are normwise, but they ignore the input data sparsity and/or scaling. Componentwise analysis have been introduced, which gives a powerful tool to study the perturbations on input and output data regarding the sparsity and scaling. In this paper under componentwise perturbation analysis we will study the condition numbers for constrained linear least squares problems. The obtained expressions of the condition numbers avoid the explicit forming of Kronecker products, which can be estimated by power methods efficiently. Numerical examples show that our condition numbers can give better error bounds.

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Talk 4. SOR inner-iteration GMRES for underdetermined least squares problems

Successive over-relaxation (SOR) inner iterations are proposed for preconditioning the generalized minimal residual method (GMRES) for underdetermined least squares problems. The right-preconditioned GMRES (AB-GMRES) may fail to converge for inconsistent problems. Instead, the left-preconditioned GMRES method (BA-GMRES) works since we can transform an inconsistent system to a consistent one. Numerical experiments show that BA-GMRES with SOR for the normal equation works efficiently. Moreover, we show conditions under which BA-GMRES determines a minimum-norm least squares solution without breakdown and present numerical results.

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MS 35. Nonlinear eigenvalue problems

Talk 1. Computable error bounds for nonlinear eigenvalue problems allowing for a minimax characterization

For a nonlinear eigenvalue problem

$$T(\lambda)x = 0$$

allowing for a variational characterization of its eigenvalues we discuss computable error bounds of Krylov–Bogoliubov and of Kato–Temple type.

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Talk 2. A restarting technique for the infinite Arnoldi method

Different adaptations of the Arnoldi method are often used to compute partial Schur factorizations. We propose here a technique to compute a partial Schur factorization of a nonlinear eigenvalue problem (NEP). The technique is inspired by the algorithm in [E. Jarlebring, K. Meerbergen, W. Michiels, *A linear eigenvalue algorithm for the nonlinear eigenvalue problem, 2012*], now called the *infinite Arnoldi method*, for which we design an appropriate restarting technique. The technique is based on a characterization of the invariant pairs of the NEP, which turn out to be equivalent to the invariant pairs of an operator. We characterize the structure of the invariant pairs of the operator and show how one can carry out a modification of the infinite Arnoldi method by respecting this structure. This also allows us to naturally add the feature known as locking. We nest this algorithm with an outer iteration, where the infinite Arnoldi method for a particular type of structured functions is appropriately restarted. The restarting exploits the structure and is inspired by the well-known implicitly restarted Arnoldi method for standard eigenvalue problems.

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Talk 3. Robust successive computation of eigenpairs for nonlinear eigenvalue problems

The successive computation of several eigenpairs of a nonlinear eigenvalue problem requires a means to prevent our algorithm from repeatedly converging to the same eigenpair. For linear eigenproblems, this is usually accomplished by restricting the problem to the subspace orthogonal to all previously computed eigenvectors. In the nonlinear case, though, this strategy is harmful as it may cause eigenpairs to be missed due to possible linear dependencies among the eigenvectors. In this talk, we present a modified orthogonalization scheme based on the concept of minimal invariant pairs, which does not bear this danger.

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Talk 4. **Triangularization of matrix polynomials**

Using similarity transformations that preserve the structure of the companion matrix, we show that any matrix polynomial $P(\lambda)$ over the complex numbers can be triangularized in the sense that there always exists a triangular matrix polynomial $T(\lambda)$ having the same degree and elementary divisors (finite and infinite) as $P(\lambda)$. Although the result is theoretical the approach is constructive and hints on possible numerical algorithms.

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MS 36. Hybrid solvers for sparse linear equations

Talk 1. **The augmented block-Cimmino distributed method**

In row projection methods, such as Block-Cimmino, near linear dependency between partitions implies small eigenvalues in the spectrum of the iteration matrix. In this work we try to break this near linear dependency by augmenting the matrix to enforce orthogonality between partitions. We formulate a linear system in a super-space, where the extra equations that are introduced for consistency are obtained by projections and can be handled implicitly. In the ideal case the resulting iteration matrix has all eigenvalues almost equal to one. We investigate the numerical components of this approach and ways to reduce the number of super-space variables.

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Talk 2. **On a parallel hierarchical algebraic domain decomposition method for a large scale sparse linear solver**

The emerging petaflop computers have processing nodes based on multi-/many-core chips. To fully utilize such parallel architectures, a natural approach is to exploit medium-grain parallelism through multi-threading within a node and coarse-grain parallelism using message-passing (MPI) between nodes. For a hybrid direct/iterative solver, this can be implemented by using a parallel sparse direct solver within a node on local subproblems. The available multi-threaded sparse direct solvers can be used to take advantage of the multicore architecture of the nodes. The MPI paradigm is then used to implement the iterative scheme for the interfaces between the

subproblems. In this talk, we will present such a parallel implementation and illustrate its performance scalability on a set of academic and industrial test problems. In addition, we will propose a model to compute the subsequent computational and memory costs, depending on the ratio of computation performed in the direct solver. We apply this model to several classes of problems and illustrate the possible trade-offs in terms of computational and memory complexity.

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Talk 3. **A two-level Schwarz method for systems with high contrasts**

Two-level Schwarz methods are popular domain decomposition methods. They are based on direct solves in each subdomain as well as in a specified coarse space. Used as a preconditioner for the Conjugate Gradient algorithm they lead to efficient hybrid solvers.

Heterogeneous coefficients in the PDEs are a known challenge for robustness in domain decomposition, specially if the heterogeneities are across interfaces. We introduce a new coarse space for which the Schwarz method is robust even in this case. It relies on solving local generalized eigenvalue problems in the overlaps between subdomains which isolate exactly the terms responsible for slow convergence.

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Talk 4. **A 3-level parallel hybrid preconditioner for sparse linear systems**

We describe ShyLU, a hybrid direct-iterative preconditioner and solver for general sparse linear systems. We use a Schur complement approach where subproblems are solved using a direct solver while the Schur complement is solved iteratively.

We employ a block decomposition, which is formed in a fully automatic way using state-of-the-art partitioning and ordering algorithms in the Zoltan and Scotch software packages. The method can be viewed as a two-level scheme. We show results that demonstrate the robustness and effectiveness of ShyLU for problems from a variety of applications. We have found it is particularly effective on circuit simulation problems where many iterative methods fail. We also show results from a hybrid MPI + threads version of ShyLU. The Schur complement strategy in ShyLU works well for moderate amount of parallelism. For very large problems on very large parallel systems, we introduce a third level based on domain decomposition to improve scalability. We study how ShyLU behaves as a subdomain solver. This strategy looks promising for peta- and exa-scale systems, which usually have a hierarchical structure.

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MS 37. Optimization methods for tensor decomposition

Talk 1. Efficient algorithms for tensor decompositions

The canonical polyadic and rank- $(L_r, L_r, 1)$ block term decomposition (CPD and BTD, respectively) are two closely related tensor decompositions. The CPD is an important tool in psychometrics, chemometrics, neuroscience and data mining, while the rank- $(L_r, L_r, 1)$ BTD is an emerging decomposition in signal processing and, recently, blind source separation. We present a decomposition that generalizes these two and develop algorithms for its computation. Among these algorithms are alternating least squares schemes, several general unconstrained optimization techniques, as well as matrix-free nonlinear least squares methods. In the latter we exploit the structure of the Jacobian's Gramian by means of efficient expressions for its matrix-vector product. Combined with an effective preconditioner, numerical experiments confirm that these methods are among the most efficient and robust currently available for computing the CPD, rank- $(L_r, L_r, 1)$ BTD and their generalized decomposition.

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Talk 2. Symmetric tensor decomposition via a power method for the generalized tensor eigenproblem

We present an approach for approximate (least-squares) decomposition of a symmetric positive-definite tensor of

dimension n into a given number p of symmetric rank-1 terms. This is accomplished in two parts. The first part is to transform the decomposition problem into a "generalized tensor eigenproblem" (GTEP) for tensors of dimension np . The GTEP is of independent interest and, for example, subsumes the previously defined Z -eigenpairs and H -eigenpairs. The second part is to extend a previously developed power method for Z -eigenpairs to solve the GTEP. We discuss the concepts underlying these techniques and provide numerical examples.

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Talk 3. All-at-once optimization for coupled matrix and tensor factorizations

Joint analysis of data from multiple sources can enhance knowledge discovery. The task of fusing data, however, is challenging since data may be incomplete and heterogeneous, i.e., data consists of matrices and higher-order tensors. We formulate this problem as a coupled matrix and tensor factorization problem where heterogeneous data are modeled by fitting outer-product models to higher-order tensors and matrices in a coupled manner. Unlike traditional approaches using alternating algorithms, we use a gradient-based all-at-once optimization approach. Using numerical experiments, we demonstrate that the all-at-once approach is often more accurate than the alternating approach and discuss the advantages of coupled analysis in terms of missing data recovery.

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Talk 4. An algebraic multigrid optimization method for low-rank canonical tensor decomposition

A new algorithm based on algebraic multigrid is presented for computing the rank- R canonical decomposition of a tensor for small R . Standard alternating least squares (ALS) is used as the relaxation method. Transfer operators and coarse-level tensors are constructed in an adaptive setup phase that combines multiplicative correction and bootstrap algebraic multigrid. An accurate solution is computed by an additive solve phase based on the full approximation scheme. Numerical tests show that for certain test problems, our multilevel method significantly outperforms standalone ALS when a high level of accuracy is required.

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MS 38. Generalized inverses and applications - Part I

of II

Talk 1. The group inverse of additively modified matrices

Let $A \in \mathbb{C}^{n \times n}$. We recall that the group inverse of A , is the unique matrix $A^\# \in \mathbb{C}^{n \times n}$, if it exists, which satisfies the equations: $A^\# A A^\# = A^\#$; $A A^\# A = A$; $A A^\# = A^\# A$. If A is nonsingular then $A^\# = A^{-1}$. It is well known that the group inverse of A exists if $\text{rank}(A) = \text{rank}(A^2)$. Alternatively, $A^\#$ exists if $A + I - A A^-$ is nonsingular, independently of the choice of A^- , where A^- denotes an inner inverse of A , i.e. $A A^- A = A$. Let $B \in \mathbb{C}^{n \times r}$, $C \in \mathbb{C}^{r \times n}$, and $r < n$. If A and $I - C A^{-1} B$ are nonsingular, then to adapt the inverse of the modified matrix $A - B C$ we can apply the Sherman-Morrison-Woodbury formula: $(A - B C)^{-1} = A^{-1} + A^{-1} B (I - C A^{-1} B)^{-1} C A^{-1}$; and, hence, we need to compute the inverse of $I - C A^{-1} B$, which has size $r < n$. This talk will be focused on the group inverse of additively modified matrices, $(A - B C)^\#$, when it exists. Extensions of the previous formula will be considered. An application to the perturbation of the group inverse of $A = I - T$, where T is the transition matrix of a Markov chain will be given. The research is partially supported by Project MTM2010-18057, "Ministerio de Ciencia e Innovación" of Spain.

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Talk 2. The Moore-Penrose inverse of a linear combination of commuting generalized and hypergeneralized projectors

We present new results concerning the representation of the Moore-Penrose inverse of a linear combination of generalized and hypergeneralized projectors and give the form for the Moore-Penrose inverse, i.e., the group inverse of $c_1 A + c_2 B$, where A, B are two commuting generalized or hypergeneralized projectors and $c_1, c_2 \in \mathbb{C} \setminus \{0\}$ and $c_1^3 + c_2^3 \neq 0$. Furthermore, we show that under that conditions the invertibility of $c_1 A + c_2 B$ is independent of the choice of the scalars c_1, c_2 . Also, we present some results relating different matrix partial orderings and the invertibility of a linear combination of EP matrices.

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Talk 3. Generalized inverses of operators on Hilbert C^* -modules

We present new results on the theory and applications of generalized inverses of operators between Hilbert C^* -modules.

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Talk 4. Some results on the reverse order law

We presented some necessary and sufficient conditions concerning the reverse order laws for the group inverses of elements in rings and rings with involution. In particular, assuming that a and b are Moore-Penrose invertible or group invertible elements, we study equivalent conditions which are related to the reverse order law for the group inverse of the product ab . Also, some equivalent condition which ensure that

the product ab is EP element are consider too. Several conditions for $(ab)^\# = b^\# (a^\# a b b^\#)^\# a^\#$ to hold in rings are investigate. We extend the recent results to more general settings, giving some new conditions and providing simpler proofs to already existing conditions.

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MS 39. Challenges for the solution and preconditioning of multiple linear systems - Part I of II

Talk 1. Preconditioners for sequences of shifted linear systems

Sequences of shifted linear systems with the same right-hand side can be solved with multi-shift Krylov methods at almost the same cost as for solving the unshifted system. This is possible due to the fact that the Krylov subspaces for the shifted and the unshifted problems are the same. The main drawback of multi-shift Krylov methods is that they cannot be combined with an arbitrary preconditioner since in general the Krylov subspaces for the preconditioned shifted problems will be different. In the talk we will discuss this problem in detail and also explain how to construct preconditioners that can be combined with multi-shift Krylov methods.

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Talk 2. Solving sequences of linear systems with application to model reduction

To obtain efficient solutions for sequences of linear systems arising in interpolatory model order reduction (both parametric and nonparametric), we recycle Krylov subspaces from one system (or pair of systems) in a sequence to the next. We first introduce a generalization of BiCG. Here we show that even for non-Hermitian matrices one can build bi-orthogonal bases (for the associated two Krylov subspaces) using a short-term recurrence. We then adapt and apply Recycling BiCG and Recycling BiCGSTAB to model reduction algorithms. For a model reduction problem we demonstrate that solving the problem without recycling leads to (about) a 50% increase in runtime.

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Talk 3. Krylov subspace recycling for families of shifted linear systems

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

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

where L_i is the number of shifts at step i . We propose a new method which solves the base system using GMRES with subspace recycling while constructing approximate corrections to the solutions of the shifted systems. At convergence of the base system solution, GMRES with subspace recycling is applied to further improve the solutions of the shifted systems to tolerance. We present analysis of this method and numerical results involving systems arising in lattice quantum chromodynamics.

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Talk 4. Krylov subspace recycling for faster model reduction algorithms

The numerical solution of shifted linear system with multiple right-hand sides is a recurring task in many computational problems related to model reduction. Shifts and right-hand sides may be known in advance or may become available only after the previous linear system has been solved. We will survey some model reduction algorithms where these tasks occur and will demonstrate that Krylov subspace recycling may significantly accelerate the computation of reduced-order models in these situations.

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MS 40. Different perspectives on conditioning and numerical stability - Part I of II

Talk 1. Highly accurate numerical linear algebra via rank revealing decompositions

High accuracy algorithms are those that produce relative forward errors of order the unit roundoff of the computer even for matrices that are very ill-conditioned in a traditional sense. This type of algorithms only exist for certain structured matrices. A wide class of these matrices are the matrices for which it is possible to compute accurate rank revealing decompositions (RRDs), i.e., factorizations XDY where D is diagonal and non-singular, and X and Y are well conditioned. This class comprise many important structured matrices, like

Vandermonde, Cauchy, graded matrices and many others.

Originally, high accuracy algorithms acting on the factors of RRDs (instead of acting directly on the matrix) were designed for computing Singular Value Decompositions (1999), then for computing eigenvalues/eigenvectors of symmetric matrices (2003, 2009), and very recently for computing solutions of linear systems (2011) and least square problems (2012). The purpose of this talk is to present a unified description of all these algorithms and to pose some open problems in this area.

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Talk 2. Stability of numerical algorithms with quasiseparable matrices

Quasiseparable matrices are encountered in PDEs, computations with polynomials (interpolation, root finding etc.), design of digital filters and other areas of applied mathematics. There have been major interest in fast algorithms with quasiseparable matrices in the last decade. Many linear complexity algorithms have been developed including QR factorization, system solver, QR iterations and others. However, their numerical stability has not received equal attention of the scientific community. In our talk we will present first results of error analysis of QR decomposition and system solvers. We will also present a generalization of Parlett's dqds algorithm and discuss perspectives of using quasiseparable matrices for stable evaluation of polynomials' roots.

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Talk 3. Gram-Schmidt orthogonalization with standard and non-standard inner product: rounding error analysis

In this contribution we consider the most important schemes used for orthogonalization with respect to the standard and non-standard inner product and review the main results on their behavior in finite precision arithmetic. Although all the schemes are mathematically equivalent, their numerical behavior can be significantly different. We treat separately the particular case of the standard inner product and show that similar results hold also for the case when the inner product is induced by a positive diagonal matrix. We will show that in the case of general inner product the orthogonality between computed vectors besides the linear independence of initial vectors depends also on the condition number of the matrix that induces the non-standard inner product. Finally we discuss the extension of this theory to some bilinear forms used in the context of various structure-preserving transformations.

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Talk 4. **Backward stability of iterations for computing the polar decomposition**

Among the many iterations available for computing the polar decomposition the most practically useful are the scaled Newton iteration and the recently proposed dynamically weighted Halley iteration. Effective ways to scale these and other iterations are known, but their numerical stability is much less well understood. In this work we show that a general iteration $X_{k+1} = f(X_k)$ for computing the unitary polar factor is backward stable under two conditions. The first condition requires that the iteration is implemented in a mixed backward–forward stable manner and the second requires that the mapping f does not significantly decrease the size of any singular value relative to the largest singular value. Using this result we show that the dynamically weighted Halley iteration is backward stable when it is implemented using Householder QR factorization with column pivoting and either row pivoting or row sorting. We also prove the backward stability of the scaled Newton iteration under the assumption that matrix inverses are computed in a mixed backward–forward stable fashion; our proof is much shorter than a previous one of Kielbasiński and Ziętak. We also use our analysis to explain the instability of the inverse Newton iteration and to show that the Newton–Schulz iteration is only conditionally stable. This work shows that by carefully blending perturbation analysis with rounding error analysis it is possible to produce a general result that can prove the backward stability or predict or explain the instability (as the case may be) of a wide range of practically interesting iterations for the polar decomposition.

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MS 41. Recent advances in model reduction - Part I of II

Talk 1. **The Loewner framework in data-driven model reduction**

In this talk we will survey recent advances in model reduction concentrating on the method of model reduction directly from data using the Loewner framework. In addition we will show how the Loewner framework can be extended to handle reduction of systems depending on parameters.

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Talk 2. **Robust computational approaches to \mathcal{H}_2 -optimal**

model reduction

We present an approach to model reduction for MIMO linear dynamical systems that is numerically stable, nonintrusive, and computationally tractable even for very large order systems. Our strategy is a hybrid of the Iterative Rational Krylov Algorithm (IRKA) and a trust-region method with logarithmic barrier that guarantees stability. The method produces a monotonically improving (with respect to \mathcal{H}_2 error) sequence of stable reduced order models that is rapidly and globally convergent. The effectiveness of the algorithm is illustrated through numerical examples drawn from a variety of challenging dynamical systems that arise in practical settings.

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Talk 3. **Reduced order modeling via frames**

In this talk we present a new concept that arises in the discretization of PDEs. Instead of using bases (like hierarchical finite elements) to represent the solution in a certain function space, we use frames, which consist of a set of standard basis functions enriched by specific functions that allow to address specific solution behavior like singularities, boundary layers or small amplitude, high frequency oscillations. We then determined sparse solutions represented in these frames, by solving the under-determined problems to compute sparse solutions. We show that by doing this in a multilevel approach we can achieve much smaller models than with classical adaptive FEM.

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Talk 4. **Semidefinite Hankel-type model reduction based on frequency response matching**

In this talk a model reduction method for linear time-invariant systems is discussed. It is based on frequency response matching and semidefinite programming techniques. The method is related to Hankel model reduction. It can be claimed that the presented method is a scalable approach to Hankel model reduction. Numerical simulations show that the accuracy of the method is comparable to the well-known techniques, such as balanced truncation and Hankel model reduction. The developed method can be applied to various problems. In this talk we are going to briefly discuss two: parameterized model reduction and reduction in the nu-gap metric.

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MS 42. Structured solution of nonlinear matrix equations and applications - Part I of II

Talk 1. Structured solution of large-scale algebraic Riccati and nonlinear matrix equations

We consider the solution of large-scale algebraic Riccati and nonlinear matrix equations (AREs, NMEs). For discrete-time AREs, the structure-preserving doubling algorithm will be adapted for the corresponding sparsity and low-ranked structures. For continuous-time AREs, the Cayley transform is applied before doubling. Similar methodology is applied to large-scale nonsymmetric AREs and NMEs. With n being the dimension of the equations, the resulting algorithms are of $O(n)$ complexity. Numerical results will be presented. As an example, a DARE with 3.19 billion unknowns was solved using MATLAB on a MacBook Pro to machine accuracy within 1,100 seconds.

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Talk 2. Accurate solutions of nonlinear matrix equations in queueing models

In this talk, we discuss numerical issues arising in finite precision implementations of iterative methods for solving nonlinear matrix equations arising in queueing models. Exploring the structure of the problem, we shall present some numerically more stable implementations. A rounding error analysis together with numerical examples are given to demonstrate the higher accuracy achieved by the refined implementations.

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Talk 3. A numerical approach for solving nonlinear matrix equations in economic dynamics

Modern economic theory views the economy as a dynamical system. The dynamics includes changes over time of market behavior such as consumption, investment, labor supply, and technology innovation. To make analytical analysis, the naive approach is to set up the Euler equation and subsequently solve it by finding the policy functions. Indeed, this is a process of solving the nonlinear matrix equation. In this work, we propose a Newton iterative scheme on approximating the unknown policy functions. Applications to the neoclassical growth model with leisure choice are used to demonstrate the working of the idea.

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Talk 4. A structure-preserving doubling algorithm for quadratic eigenvalue problems arising from time-delay systems

We propose a structure-preserving doubling algorithm for a quadratic eigenvalue problem arising from the stability analysis of time-delay systems. We are particularly interested in the eigenvalues on the unit circle, which are difficult to estimate. The convergence and backward error of the algorithm are analyzed and three numerical examples are presented. Our experience shows that our algorithm is efficient in comparison to the few existing approaches for small to medium size problem.

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MS 43. Challenges for the solution and preconditioning of multiple linear systems - Part II of II

Talk 1. Low-rank techniques for parameter-dependent linear systems and eigenvalue problems

Motivated by the need for quantifying the impact of uncertainties in engineering applications, recently a number of new approaches for solving parameter-dependent and stochastic PDEs have been developed. In particular, this includes sparse grid Galerkin and collocation methods, as well as low-rank techniques. Depending on the regularity of the parameter dependence, these methods are able to deal with potentially many parameters. The aim of this talk to provide a survey of recent work on low-rank techniques for solving linear systems arising from the spatial discretization of parameter-dependent PDEs. The extension of these techniques to general parameter-dependent eigenvalue problems is nontrivial and will also be briefly discussed.

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Talk 2. Recycling Krylov subspace information in sequences of linear systems

Many problems in numerical simulations in physics require the solution of long sequences of slowly changing linear systems. One problem that is of interest to us arises in Lattice QCD simulations, e.g., while computing masses of elementary particles. In each time step, we have to solve a linear system with a Dirac operator which changes slightly from time step to time step. Based on the work of M. Parks, E. de Sturler et al. (Recycling Krylov subspaces for sequences of linear systems, SIAM J. on Scientific Computing, 28(2006), 1651 – 1674) we will show how the cost of solving subsequent systems is reduced by recycling selected subspaces generated for previous systems. Furthermore, we have investigated how the algorithm behaves when we use the solution of the previous system as an initial guess and also, when we use different kinds of extrapolations of the previous solutions as an initial guess. We will show these results and the effectiveness of the algorithm in comparison to the algorithm that solves each system separately.

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Talk 3. Efficiently updating preconditioners in quantum Monte Carlo simulations

In the quantum Monte Carlo method for computing properties of materials, we need to solve a very long sequence of linear systems arising from importance sampling. Each system in the sequence is a so-called Slater matrix, and the matrices change by one row (or a few rows) at a time corresponding to small moves by particles. We will combine a method for incremental matrix reordering with multilevel preconditioning to develop effective preconditioners that can be recycled efficiently.

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Talk 4. A domain decomposition preconditioned recycling GMRES for stochastic parabolic PDE

We discuss an implicit space-time approach for solving stochastic parabolic PDEs. We first decouple the space-time discretized stochastic equation into some uncoupled deterministic systems by using a Karhunen-Loeve expansion and double orthogonal polynomials. And then a domain decomposition method is combined with recycling GMRES to solve the large number of systems with similar structures. We report experiments obtained on a parallel computer with a large number of processors. This is a joint work with Cui Cong.

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MS 44. Different perspectives on conditioning and numerical stability - Part II of II

Talk 1. Accuracy and sensitivity of Monte Carlo matrix multiplication algorithms

Randomized matrix multiplication algorithms were designed to approximate very large matrix products for which a deterministic algorithm is prohibitively expensive. For an algorithm introduced by Drineas, Kannan, and Mahoney, we analyze the error resulting from randomization and derive a bound that improves existing results. In addition, we formulate a measure for the sensitivity of the algorithm to perturbations in the input and present a bound for this measure. We also compare the sensitivity of the randomized algorithm to the sensitivity of the deterministic algorithm.

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Talk 2. Hyperdeterminant and the condition number of a multilinear system

The condition number of a problem is the reciprocal of its normalized distance to the nearest ill-posed instance in that class of problems. We shall see that in solving a system of multilinear equations, the set of ill-posed problems is given by the set of coefficient tensors with vanishing hyperdeterminant. The parallel with matrices goes further: the hyperdeterminant of a tensor is zero iff it has a zero singular value; and in the case of a symmetric tensor, iff it has a zero eigenvalue. Moreover, the criterion is invariant under Gaussian elimination or Householder/Givens transformations applied to ‘all k sides’ of the tensor viewed as a k -dimensional hypermatrix.

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Talk 3. Condition numbers and backward errors in functional setting

In this talk we present a functional perturbation results, i.e., a functional normwise backward error, for the PDE eigenvalue problems. Inspired by the work of Arioli et al. for linear systems arising from the finite element discretization of boundary value problems we extend the ideas of the functional *Compatibility Theorem* and condition numbers to eigenvalue problems in their variational formulation. Moreover, we discuss a new *spacewise backward error* for PDEs using the componentwise error analysis, i.e., by performing the error analysis using the so-called hypernorms of order k .

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Talk 4. Orthogonality and stability in large-sparse-matrix iterative algorithms

Many iterative algorithms for large sparse matrix problems are based on orthogonality, but this can rapidly be lost using vector orthogonalization (subtracting multiples of earlier vectors from the latest vector to produce the next orthogonal vector). Yet these are among the best algorithms we have, and include the Lanczos process, CG, Golub and Kahan bidiagonalization, and MGS-GMRES.

Here we describe a form of orthogonal matrix that arises from any sequence of supposedly orthogonal vectors. We illustrate some of its properties, including a beautiful measure of orthogonality of the original set of vectors. We will show how this leads to new concepts of conditioning and stability for these algorithms.

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MS 45. Recent advances in model reduction - Part II of II

Talk 1. Automating DEIM for nonlinear model reduction

The discrete empirical interpolation method (DEIM) can provide spectacular dimension and complexity reduction for challenging systems large scale nonlinear ordinary differential equations. The DEIM replaces orthogonal projection of POD with an interpolatory projection of the nonlinear term that only requires the evaluation of a few selected components. However, the implementation at present is intrusive in the sense that a user must provide a scheme for evaluating the selected components of the nonlinear terms in order to integrate the reduced order system. We have utilized some of the techniques of automatic differentiation to fully automate this process. In particular, this approach will automatically generate a new code derived directly from the original C-code for the right hand side of a first order ODE.

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Talk 2. Model reduction for optimal control problems in field-flow fractionation

We discuss the application of model order reduction to optimal control problems governed by coupled systems of the Stokes-Brinkmann and advection diffusion equations. Such problems arise in field-flow fractionation processes for the efficient and fast separation of particles of different size in microfluidic flows. Our approach is based on a combination of balanced truncation and tangential interpolation for model reduction of the semidiscretized optimality system. Numerical results demonstrate the properties of this approach.

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Talk 3. Numerical implementation of the iterative rational Krylov algorithm for optimal \mathcal{H}_2 model order reduction

The Iterative Rational Krylov (IRKA) algorithm for model order reduction (Gugercin, Antoulas, Beattie 2008.) has recently attracted attention because of its effectiveness in real world applications, as well as because of its mathematical elegance. Our current work is focused on the development of efficient and numerically reliable mathematical software that implements the IRKA algorithm. The first step is, necessarily, a theoretical study of the algorithm. We analyze the convergence of fixed point iterations that run in the background of IRKA, in particular the morphology of the mapping $\sigma^{(k+1)} = \phi(\sigma^{(k)})$ (fixed points, periodic points and their classification). Other theoretical issues include perturbation theory to analyze stability of the shifts, revealing relevant condition numbers, Cauchy-like structure of certain key matrices, connection of the fixed point iterations and pole placement, proper stopping criterion that translates into a backward stability relation, etc.

Besides rich theory, IRKA also offers many numerical challenges. How to implement the algorithm efficiently using direct or iterative solvers for

$\mathbf{V}(\sigma) = ((\sigma_1 \mathbf{I} - \mathbf{A})^{-1} \mathbf{b}, \dots, (\sigma_r \mathbf{I} - \mathbf{A})^{-1} \mathbf{b})$,
 $\mathbf{W}(\sigma) = ((\sigma_1 \mathbf{I} - \mathbf{A}^T)^{-1} \mathbf{c}, \dots, (\sigma_r \mathbf{I} - \mathbf{A}^T)^{-1} \mathbf{c})$, and how to deal with numerical rank deficiency? How to adapt iterative solvers in an inner loop that communicates with the outer fixed point iterations loop? When to stop? This requires estimates in the \mathcal{H}_2 space, and we show to combine them together with the usual stopping scheme for fixed point iterations. All these and many other questions (e.g. implementations on modern parallel architectures such as CPU/GPU) are analyzed during software development. We will give some answers and illustrate the performances of the software package.

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Talk 4. Low rank deflative/iterative solutions of Lur'e equations

The bottleneck of model reduction by passivity-preserving balanced truncation is the numerical solution of Lur'e equations. A typical approach is an a priori perturbation leading to an algebraic Riccati equation. This is however, from an analytical point of view, insufficiently understood and, from a numerical point of view, leads to an ill-conditioned problem. Hence we are following an alternative approach that is basically consisting of two steps:

- a) 'Filter out' the 'critical part' of the Lur'e equations: This will lead us to an eigenproblem of moderate complexity, the outcome is an algebraic Riccati equation on some subspace.

b) Solve algebraic Riccati equation on the subspace.

We show that this method provides low rank approximative solutions of the Lur'e equations. Especially this makes the presented method feasible for large-scale model order reduction problems.

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MS 46. Structured solution of nonlinear matrix equations and applications - Part II of II

Talk 1. Inertia and rank characterizations of the expressions $A - BXB^* - CYC^*$ and $A - BXC^* \pm CX^*B^*$

In this talk we consider the admissible inertias and ranks of the expressions $A - BXB^* - CYC^*$ and $A - BXC^* \pm CX^*B^*$ with unknowns X and Y in the four cases when these expressions are: (i) complex self-adjoint, (ii) complex skew-adjoint, (iii) real symmetric, (iv) real skew symmetric. We also provide a construction for X and Y to achieve the desired inertia/rank, that uses only unitary/orthogonal transformation thus leading to a numerically reliable construction. Consequently, necessary and sufficient solvability conditions for matrix equations

$$A - BXB^* - CYC^* = 0;$$

and

$$A - BXC^* \pm CX^*B^* = 0$$

are provided.

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Talk 2. Structure-preserving Arnoldi-type algorithm for solving eigenvalue problems in leaky surface wave propagation

We study the generalized eigenvalue problems (GEP) arising from modeling leaky surface waves propagation in a acoustic resonator with infinitely many periodically arranged interdigital transducers. The constitution equations are discretized by finite element method with mesh refinement along the electrode interface and corners. The associated GEP is then transformed to a T-palindromic quadratic eigenvalue problem so that the eigenpairs can be accurately and efficiently computed by using structure-preserving algorithm with a generalized T-skew-Hamiltonian implicitly-restarted Arnoldi method. Our numerical results show that the eigenpairs produced by the proposed structure-preserving method not only preserve the reciprocal property but also possess high efficiency and accuracy.

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Talk 3. Structure-preserving curve for symplectic pairs

We study the stabilizing solution of the equation $X + A^*X^{-1}A = Q$, where Q is Hermitian positive definite. We construct a smooth curve, parameterized by $t \geq 1$, of symplectic pairs with a special structure, in which the curve passes through all iteration points generated by the known numerical methods, including the fixed-point iteration, structured preserving doubling algorithm and Newton's method, under specified conditions. We give a necessary and sufficient condition for the existence of this structured symplectic pairs and characterize the behavior of this curve. We also use this curve to measure the convergence rates of these numerical methods. Some numerical results are presented.

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Talk 4. A doubling algorithm with shift for solving a nonsymmetric algebraic Riccati equation

In this talk, we analyze a special instance of nonsymmetric algebraic matrix Riccati equation (NARE) arising from transport theory. Traditional approaches for finding the minimal nonnegative solution of NARE are based on the fixed point iteration and the speed of the convergence is linear. Recently, a structure-preserving doubling algorithm (SDA) with quadratic convergence is designed for improving the speed of convergence. Our contribution is to show that applied with a shifted technique, the SDA is guaranteed to converge quadratically with no breakdown. Also, we modify the conventional simple iteration algorithm to dramatically improve the speed of convergence.

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MS 47. Generalized inverses and applications - Part II of II

Talk 1. On a partial order defined on certain matrices

For a given matrix $A \in \mathbb{C}^{m \times n}$, we recall that the weighted Moore-Penrose inverse with respect to two Hermitian positive definite matrices $M \in \mathbb{C}^{m \times m}$ and $N \in \mathbb{C}^{n \times n}$ is the unique solution $X \in \mathbb{C}^{n \times m}$ satisfying the equations: $AXA = A$, $XAX = X$, $(MAX)^* = MAX$, $(NXA)^* = NXA$. This matrix will be used to define a partial order on certain class of complex matrices. Some properties on predecessors and successors of a given matrix in that class will be established.

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Talk 2. Generalized inverses and path products

Let $M = [a_{ij}]$ be a lower triangular matrix over an arbitrary ring with unity 1, and set $a_i := a_{ii}$. We may split M as $M = D + N$, where $D = \text{diag}(a_1, \dots, a_n)$ and $N = M - D$. The latter is strictly lower triangular and hence nilpotent. Associated with the matrix M , we will consider the weighted digraph $G = (V, E)$ where $V = \{S_i\}$ is a set of nodes (or sites) and $E = \{(S_i, S_j)\} \in V \times V$ is a collection of arcs such that $(S_i, S_j) \in E$ if $a_{ij} \neq 0$. We add a loop at site S_i if $a_i \neq 0$. We will relate the existence of the generalized inverse, namely von Neumann, group and the Moore-Penrose inverse, of a lower triangular matrix again gives a matrix of the same type by means of path products obtained in the graph associated to the matrix.

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Talk 3. On structured condition numbers for a linear functional of Tikhonov regularized solution

A structured componentwise and normwise perturbation analysis of Tikhonov regularization problems are presented. The structured matrices we consider include: Toeplitz, Hankel, Vandermonde, and Cauchy matrices. Structured normwise, mixed and componentwise condition numbers for these Tikhonov regularization problems are introduced and their expressions are derived. Such expressions for many other classes of matrices can be similarly derived. By means of the power method, the fast condition estimated algorithms are proposed. The condition numbers and perturbation bounds are examined on some numerical examples and compared with unstructured normwise, mixed and componentwise condition numbers. The numerical examples show that the structured mixed condition numbers give better perturbation bounds than others.

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Talk 4. Explicit characterization of the Drazin index

Let $\mathbb{B}(X)$ be the set of bounded linear operators on a Banach space X , and $A \in \mathbb{B}(X)$ be Drazin invertible. An element

$B \in \mathbb{B}(X)$ is said to be a stable perturbation of A if B is Drazin invertible and $I - A^\pi - B^\pi$ is invertible, where I is the identity operator on X , A^π and B^π are the spectral projectors of A and B respectively. Under the condition that B is a stable perturbation of A , a formula for the Drazin inverse B^D is derived. Based on this formula, a new approach is provided to the computation of the explicit Drazin indices of certain 2×2 operator matrices

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MS 48. Parallelization of efficient algorithms

Talk 1. A highly scalable error-controlled fast multipole method

We present a linear scaling, error-controlled FMM implementation for long-range interactions of particle systems with open, 1D, 2D and 3D periodic boundary conditions. Similarly to other fast summation algorithms the FMM allows to reduce the total runtime significantly. This runtime advantage however comes with considerably increased memory requirements posing constraints to the overall particle system size. In this talk we focus on the reduced memory footprint as well as the communication pattern for trillions of particles. The current code is designed to lower the memory consumption to only 45Byte/particle already including a small 16.2% parallel overhead for 300k MPI ranks.

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Talk 2. A parallel fast Coulomb solver based on nonequispaced Fourier transforms

The fast calculation of long-range Coulomb interactions is a computational demanding problem in particle simulation. Therefore, several fast approximate algorithms have been developed, which reduce the quadratic arithmetic complexity of the plain summation to linear complexity (up to a logarithmic factor). This talk focuses on Fourier based methods with special attention to the application of the nonequispaced fast Fourier transform and its parallelization.

We present a massively parallel Coulomb solver software library for distributed memory architectures. The underlying fast algorithms for periodic and non-periodic boundary conditions will be explained and extensive performance evaluations will be presented.

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Talk 3. Generalized fast Fourier transforms via CUDA

The fast Fourier transform (FFT) belongs to the algorithms with large impact on science and engineering. By appropriate approximations, this scheme has been generalized for arbitrary spatial sampling points. We discuss the computational costs in detail for this so called nonequispaced FFT and its variations.

Because of the evolution of programmable graphic processor units into highly parallel, multithreaded, manycore processors with enormous computational capacity and very high memory bandwidth, we parallelized the nonequispaced FFT by means of the so called Compute Unified Device Architecture (CUDA) using the CUDA FFT library and a dedicated parallelization of the approximation scheme.

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Talk 4. **Efficient regularization and parallelization for sparse grid regression**

Regression, (high-dimensional) function reconstruction from scattered data, is a common problem in data-driven tasks. Typically, meshfree methods are employed to circumvent the curse of dimensionality. To deal with regression by discretizing the feature space, sparse grids can be employed. Due to their primarily data-independent approach, sparse grids enable one to deal with massive amounts of data. Adaptive refinement then allows to adapt to the peculiarities of the problem at hand. To be able to deal with large, noisy datasets, efficient algorithms and parallelizations have to be employed, and the full potential of modern hardware architectures has to be exploited. This can be complicated having to deal with hierarchical basis functions on multiple levels. We present the special challenges posed to hierarchical and recursive sparse grid algorithms and discuss efficient solutions for regularization and parallelization.

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MS 49. Analysis and computation on matrix manifold

Talk 1. **Best low multilinear rank approximation of symmetric tensors by Jacobi rotations**

We consider third-order symmetric tensors and seek their best low multilinear rank approximations. The proposed algorithm is based on Jacobi rotations and symmetry is preserved at each iteration. Examples are provided that illustrate the need of such algorithms. Our algorithm converges to stationary points of the objective function. The proof of convergence can be considered as an advantage of the algorithm over existing symmetry-preserving algorithms in the literature.

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Talk 2. **Differential geometry for tensors with fixed hierarchical Tucker rank**

A number of authors have recently proposed several geometries for rank-structured matrix and tensor spaces, namely for matrices or tensors with fixed matrix, Tucker, and TT rank. In this talk we present a unifying approach for establishing a smooth, differential structure on the set of tensors with fixed hierarchical Tucker rank. Our approach describes this set as a smooth submanifold, globally embedded in the space of real tensors. The previous spaces are shown to be specific instances of a particular hierarchical Tucker tree (possibly with additional constraints on the frames). As numerical example we show how this geometry can be used to dynamically update a time-varying tensor. This approach compares favorably to point-wise SVD-based computations.

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Talk 3. **Deterministic approaches to the Karcher mean of positive definite matrices**

We propose a deterministic approach to the Karcher mean of positive definite matrices via geometric power means. For a matrix geometric mean G , we construct one-parameter group G_t of geometric means varying continuously over $t \in [-1, 1] \setminus \{0\}$ and approaching the Karcher mean as $t \rightarrow 0$. Each of these means arises as unique positive definite solution of a non-linear matrix equation and has the distance less $\leq \sqrt{t/2}$ to the Karcher mean. This provides not only a structured and deterministic sequence of matrix means converging to the Karcher mean, but also a simple proof of the monotonicity of the Karcher mean, conjectured by Bhatia and Holbrook, and other new properties, which have recently been established by Lawson and Lim and also Bhatia and Karandikar using probabilistic methods on the metric structure of positive definite matrices equipped with the trace metric.

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Talk 4. **The Karcher mean: first and second order optimization techniques on matrix manifolds**

In this talk, we present a collection of implementations for the Karcher mean, which is a specific instance of the matrix geometric mean. The Karcher mean is defined as the solution to an optimization problem on the manifold of positive definite matrices, where it exhibits an appealing analogy with the arithmetic mean. Generalization of classical optimization schemes results in Riemannian optimization, where the intrinsic properties of the manifold are maintained and exploited throughout the algorithm. We examine several optimization techniques, such as SD, CG, Trust Region, and BFGS, and compare the results with the ALM, BMP and CHEAP mean algorithms.

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MS 50. Advanced methods for large eigenvalue problems and their applications

Talk 1. DQDS with aggressive early deflation for computing singular values

The DQDS algorithm is the standard method for computing all the singular values of a bidiagonal matrix with high relative accuracy. Its efficient implementation is now available as a LAPACK subroutine DLASQ. In order to reduce the DQDS runtime, we incorporate into DQDS a technique called aggressive early deflation, which has been applied successfully to the Hessenberg QR algorithm. In addition, a shift-free version of our algorithm has a potential to be parallelized in a pipelined fashion. Our mixed forward-backward stability analysis proves that with our proposed deflation strategy, DQDS computes all the singular values to high relative accuracy.

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Talk 2. A scalable parallel method for large-scale nonlinear eigenvalue problems

In this presentation, we present parallel software for nonlinear eigenvalue problems that has interfaces for PETSc. The software implements an eigensolver based on contour integral. It finds a partial set of eigenpairs of large sparse nonlinear eigenvalue problems and has high scalability. We demonstrate parallel performance of the implemented method through numerical experiments arising from several practical applications.

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Talk 3. Application of the Sakurai-Sugiura method in the field of density functional theory on highly parallel systems

Density Functional Theory (DFT) is one of the most important methods in computational material science. Despite the steadily

increasing computational power, computation time is still the limiting factor for many systems of interest. In many cases the most time consuming part is solving a series of generalized eigenvalue problems that emerge inside an iterative loop. In the context of Siesta, a widely spread DFT software, the Sakurai-Sugiura method is a promising approach. This talk will show how, due to its three obvious levels of parallelization, this algorithm scales much better than other widely used libraries (e.g. ScaLAPACK), how it offers possibilities to use many GPUs in parallel, and how it also supports dealing with sparse matrices.

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Talk 4. MERAM for neutron physics applications using YML environment on post petascale heterogeneous architecture

Eigenvalue problem is one of the key elements in neutron physics applications. Studying and designing efficient and scalable eigenvalue solvers is thus necessary for post petascale neutrons physics applications. In this talk, after recalling the principle of multiple explicitly restarted Arnoldi method (MERAM), we will present the design model used for its implementation on distributed heterogeneous architectures. The performance results on CURIE and GRID5000 platforms making use of the software environments KASH (Krylov bAsed Solvers for Hybrid architectures) YML and PETSc/SLEPc for typical neutron physics problems will be presented.

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MS 51. Accurate and verified numerical computations for numerical linear algebra

Talk 1. Product decomposition and its applications

A product decomposition algorithm of a real number on floating point system is proposed. The product decomposition of a real number x is a floating point decomposition defined by

$$x \simeq \tilde{x}_1 (1 + \tilde{x}_2) (1 + \tilde{x}_3) \cdots (1 + \tilde{x}_n),$$

where \tilde{x}_i denote floating point numbers ($1 \leq i \leq n$). \tilde{x}_1 implies an approximation of x and \tilde{x}_i ($2 \leq i \leq n$) involve approximations of relative errors of an approximate value by the decomposition using $\tilde{x}_1, \tilde{x}_2, \dots, \tilde{x}_{i-1}$. This decomposition is used in numerical analysis to calculate the accurate logarithm value and so on. In this talk we present an efficient algorithm to construct the product decomposition and its applications.

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Talk 2. **The MPACK: multiple precision version of BLAS and LAPACK**

We have been developing a multiple precision version of linear algebra package based on BLAS and LAPACK. We translated and reimplemented FORTRAN by C++, and the MPACK supports GMP, MPFR, and QD (DD) multiple precision libraries; users can choose the library on their needs. Currently BLAS part is completed and 100 LAPACK routines are implemented and well tested. Moreover DD version of matrix-matrix multiplication routine has been accelerated using NVIDIA C2050 GPU. Development is ongoing at <http://mplapack.sourceforge.net/>, and available under open source (2-clause BSD) license.

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Talk 3. **On eigenvalue computations of nonderogatory matrices**

In this talk I present some problems and results concerning the eigenvalue problem of nonderogatory matrices. The first group of problems is related to the detection of multiple eigenvalues of unreduced upper Hessenberg matrices and their refinements in multiple floating point arithmetic. The second group of problems is the perturbation of invariant subspaces and its characterizations in terms of the matrix perturbation.

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Talk 4. **Verified solutions of sparse linear systems**

Algorithms for calculating verified solutions of sparse linear systems are proposed. The proposed algorithms are based on standard numerical algorithms for a block LDL^T factorization and error estimates for specified eigenvalues by Lehmann's theorem. Numerical results are presented for illustrating the performance of the proposed algorithms.

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MS 52. Numerical linear algebra libraries for high end computing - Part I of II

Talk 1. **Large-scale eigenvalue computation with PETSc and YML**

In the context of parallel and distributed computation, the currently existing numerical libraries do not allow sequential and parallel code reuse. Besides, they are not able to exploit the multi-level parallelism offered by modern emerging numerical methods.

In this talk, we present a design model for numerical libraries based on a component approach allowing code reuse and problem solving scalability. We present then, an implementation of this design using YML scientific workflow environment jointly with the object oriented library PETSc. Some numerical experiments on GRID5000 platform and NERSC computers validate our approach and show its efficiency.

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Talk 2. **Sparse matrix-matrix operations in PETSc**

Sparse matrix-matrix operations, $A * B$, $A^T * B$ (or $A * B^T$) and $P^T * A * P$ (or $R * A * R^T$), are computational kernels in the PETSc library. Recent addition of a geometric-algebraic multigrid preconditioner requires these matrix operations to be scalable to tens of thousands processors cores, which forces us to take an innovated approach in algorithm design and implementations for these operations, including some relevant data structures. In this talk, we will present our newly developed scalable sparse matrix-matrix algorithms, implementations and performance, along with lessons learned and experiences gained from this work.

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Talk 3. **Hierarchical QR factorization algorithms for multi-core cluster systems**

This paper describes a new QR factorization algorithm which is especially designed for massively parallel platforms combining parallel distributed multi-core nodes. These platforms make the present and the foreseeable future of high-performance computing. Our new QR factorization algorithm falls in the category of the tile algorithms which naturally enables good data locality for the sequential kernels executed by the cores (high sequential performance), low number of messages in a parallel distributed setting (small latency term), and fine granularity (high parallelism).

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Talk 4. **Towards robust numerical algorithms for exascale simulation**

The advent of exascale machines will require the use of parallel resources at an unprecedented scale, leading to a high rate of

hardware faults. High Performance Computing applications that aim at exploiting all these resources will thus need to be resilient, i.e., being able to compute a correct output in presence of faults. Contrary to checkpointing techniques or Algorithm Based Fault Tolerant (ABFT) mechanisms, strategies based on interpolation for recovering lost data do not require extra work or memory when no fault occurs. We apply this latter strategy to Krylov iterative solvers, which are often the most computational intensive kernels in HPC simulation codes. Our main contribution is the proposition and discussion of several variants compared to previous works. For that, we propose a new variant for recovering data, we study the occurrence of multiple faults, we consider the GMRES, CG and BICGSTAB solvers, and we inject faults according to an advanced model of fault distribution. We assess the impact of the recovery method, the fault rate and the number of processors on resilience. Rather than implementing a particular actual parallel code, we assess all our strategies based on sequential Matlab implementations that simulate parallel executions.

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MS 53. Efficient preconditioners for real world applications - Part I of II

Talk 1. A parallel factored preconditioner for non-symmetric linear systems

The efficient solution to non-symmetric linear systems is still an open issue on parallel computers. In this communication we generalize to the non-symmetric case the Block FSAI (BFSAI) preconditioner which has already proved very effective on symmetric problems arising from different applications. BFSAI is a hybrid approach combining an “inner” preconditioner, with the aim of transforming the system in a block diagonal one, with an “outer” one, a block diagonal incomplete decomposition, intended to decrease the conditioning of each block. The proposed algorithm is experimented with in a number of large size problems showing both good robustness and scalability.

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Talk 2. Preconditioning for linear least-squares problems

In this talk we deal with iterative methods for solving large and sparse linear least squares problems. In particular we describe two new preconditioning techniques for the CGLS method. First we consider the strategy which is based on the LU factorization. Our approach includes a new reordering based on a specific weighting transversal problem. Direct preconditioning of the normal equations by the balanced symmetric and positive definite factorization is our second approach. Numerical experiments demonstrate effectiveness of the algorithmic and implementational features of the new approaches.

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Talk 3. Robust and parallel preconditioners for mechanical problems

We consider the simulation of displacements under loading for mechanical problems. Large discontinuities in material properties, lead to ill-conditioned systems of linear equations, which leads to slow convergence of the Preconditioned Conjugate Gradient (PCG) method. This paper considers the Recursively Deflated Preconditioned Conjugate Gradient (RDPCG) method for solving such systems. Our deflation technique uses as deflation space the rigid body modes of sets of elements with homogeneous material properties. We show that in the deflated spectrum the small eigenvalues are mapped to zero and no longer negatively affect the convergence. We justify our approach through mathematical analysis and we show with numerical experiments on both academic and realistic test problems that the convergence of our RDPCG method is independent of discontinuities in the material properties.

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Talk 4. Block factorized forms of SPAI

In this talk we present new results on block versions of sparse approximate inverse preconditioners M for sparse matrix A . We consider the Frobenius norm minimization $\min_M \|AM - I\|_F$. Blocked versions are interesting because often the underlying problem introduces in a natural way a block structure. Furthermore, they allow a more efficient memory access, and

they reduce the number of least squares problems that have to be considered in the construction of the preconditioner M . We are interested in determining appropriate block patterns for a general sparse matrix. Therefore, we want to combine columns of M with similar least squares problems to blocks in order to reduce the number of least squares problems that have to be solved for constructing the preconditioner. Furthermore, given an arbitrary blocking we also have to find the nonzero blocks that we have to include to derive a good preconditioner.

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MS 54. Solving ill-posed systems via signal-processing techniques - Part I of II

Talk 1. Sequential updates for L1 minimization: sparse Kalman filtering, reweighted L1, and more

Sparse signal recovery often involves solving an L1-regularized optimization problem. Most of the existing algorithms focus on the static settings, where the goal is to recover a fixed signal from a fixed system of equations. In this talk, we present a collection of homotopy-based algorithms that dynamically update the solution of the underlying L1 problem as the system changes. The sparse Kalman filter solves an L1-regularized Kalman filter equation for a time-varying signal that follows a linear dynamical system. Our proposed algorithm sequentially updates the solution as the new measurements are added and the old measurements are removed from the system.

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Talk 2. Solving basis pursuit: infeasible-point subgradient algorithm, computational comparison, and improvements

We propose a subgradient algorithm called ISAL1 for the ℓ_1 -minimization (Basis Pursuit) problem which applies approximate projections via a truncated CG scheme. We will also present results of an extensive computational comparison of our method and various state-of-the-art ℓ_1 -solvers on a large testset. It turns out our algorithm compares favorably. Moreover, we show how integrating a new heuristic optimality check called HSE can improve the solution speed and accuracy of several of these solvers.

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Talk 3. Semismooth Newton methods with multi-dimensional filter globalization for l_1 optimization

We present a class of methods for l_1 -regularized optimization problems. They are based on a flexible combination of semismooth Newton steps and globally convergent descent methods. A multidimensional filter framework is used to control the acceptance of semismooth Newton steps. We prove global convergence and transition to fast local convergence for both the convex and the nonconvex case. Numerical results show the efficiency of the method.

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Talk 4. Improved first-order methods: how to handle constraints, non-smoothness, and slow convergence

There are many specialized solvers that solve specific convex programs efficiently, but few algorithms can deal with general complicated constraints and non-smooth functions. To address these difficult problems, we introduce a framework and software package called TFOCS (Becker/Candès/Grant). The method relies on two tricks: dualization and smoothing. This talk describes the framework and also discusses recent splitting methods such as the method by Chambolle and Pock and by Combettes et al. We also cover recent progress in improving the convergence of first-order algorithms by using non-diagonal preconditioners (with J. Fadili).

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MS 55. Max-algebra - Part I of II

Talk 1. Tropical bounds for the eigenvalues of structured matrices

We establish several inequalities of log-majorization type, relating the moduli of the eigenvalues of a complex matrix or matrix polynomial with the tropical eigenvalues of auxiliary matrix polynomials. This provides bounds which can be computed by combinatorial means. We consider in particular structured matrices and obtain bounds depending on the norms of block submatrices and on the pattern (graph structure) of the matrix.

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Talk 2. Sensitivity in extremal systems of linear equations and inequalities

A survey of some recent results concerning the properties of finite systems of linear equations and inequalities in extremal algebra will be presented. Problems connected with sensitivity and parametric analysis of such systems will be discussed. Possible applications of the results for post-optimal analysis of optimization problems, the set of feasible solutions of which is described by the systems of (max, min) and (max, plus) linear systems, will be shown. The objective functions of the optimization problems are expressed as the maximum of finitely many continuous functions, each depending on one variable.

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Talk 3. Multiplicative structure of tropical matrices

I shall report on a programme of research aiming to understand the structure of tropical (max-plus) matrix semigroups. This structure turns out to be intimately connected with the geometry of tropical convexity; indeed, it transpires that almost every algebraic property of the full $n \times n$ tropical matrix semigroup manifests itself in some beautiful geometric phenomenon involving polytopes. Various parts of the programme are joint work with people including Christopher Hollings, Zur Izhakian and Marianne Johnson.

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Talk 4. Transience bounds for matrix powers in max algebra

In this talk we demonstrate how the concept of CSR expansions developed by Schneider and Sergeev helps to unify and compare the bounds on periodicity transient existing in the literature. Unlike in the theory of graph exponents, these bounds are not strongly polynomial. To this end, we also present some max-algebraic extensions of polynomial bounds on graph exponents, due to Wielandt and Schwartz.

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MS 56. Eigenvalue perturbations and pseudospectra - Part I of II

Talk 1. Inclusion theorems for pseudospectra of block triangular matrices

The ϵ -pseudospectrum of $A \in \mathbb{C}^{n \times n}$, denoted by $\sigma_\epsilon(A)$, is the union of the spectra of the matrices $A + E$, where $E \in \mathbb{C}^{n \times n}$ and $\|E\|_2 \leq \epsilon$. In this talk we consider inclusion relations of the form

$$\begin{aligned} \sigma_{f(\epsilon)}(A_{11}) \cup \sigma_{f(\epsilon)}(A_{22}) &\subseteq \sigma_\epsilon \left(\begin{bmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{bmatrix} \right) \\ &\subseteq \sigma_{g(\epsilon)}(A_{11}) \cup \sigma_{g(\epsilon)}(A_{22}). \end{aligned}$$

We derive formulae for $f(\epsilon)$ and $g(\epsilon)$ in terms of $\text{sep}_\lambda(A_{11}, A_{22})$ and $\|R\|_2$, where R is the solution of the Sylvester equation $A_{11}R - RA_{22} = A_{12}$.

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Talk 2. Conjectures on pseudospectra of matrices

We discuss some conjectures concerning coalescence points of connected components of pseudospectra of a square complex matrix A . We call pseudospectrum of A of order j and level ϵ , $\Lambda_{\epsilon,j}(A)$, to the set of eigenvalues of multiplicity $\geq j$ of matrices whose distance to A is $\leq \epsilon$.

- The coalescence points of the components of $\Lambda_{\epsilon,j}(A)$ are points where the pseudospectra $\Lambda_{\epsilon,j+1}(A)$ arise from.
- The coalescence points of the components of $\Lambda_{\epsilon,1}(A)$ are in line segments connecting eigenvalues of A , and analogously for $\Lambda_{\epsilon,j}(A)$.

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Talk 3. Sensitivity of eigenvalues of an unsymmetric tridiagonal matrix

The Wilkinson condition number ignores the tridiagonal form and so can be unduly pessimistic. We propose several *relative* condition numbers that exploit the tridiagonal form. Some of these numbers are derived from different factored forms (or representations) of the (possibly shifted) matrix and so they shed light on which factored forms are best for computation. We show some interesting examples.

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Talk 4. First order structured perturbation theory for eigenvalues of skew-adjoint matrices

The main goal of structured matrix perturbation theory is to identify situations where eigenvalues are much less sensitive to structured perturbations (i.e., those belonging to the same kind of matrices as the unperturbed one) than to unstructured ones. In this talk we analyze one such situation: the relevant structure is skew-adjointness with respect to an indefinite scalar product. Explicit formulas are obtained for both the leading exponent and the leading coefficient of asymptotic perturbation expansions when the perturbations are taken to be also skew-adjoint. Using

the Newton diagram as the main tool, it is shown that the leading coefficient depends on both first (i.e., eigenvectors) and second vectors in the longest Jordan chains associated with the eigenvalue under study.

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MS 57. Numerical linear algebra and optimization in imaging applications - Part I of II

Talk 1. Some numerical linear algebra and optimization problems in spectral imaging

In this talk we overview some of our recent work on numerical algorithms for spectral image analysis. Spectral imaging collects and processes image information from across the electromagnetic spectrum (often represented visually as a cube), and has a wide array of modern applications, for example in remote sensing for ecology and surveillance. Here we describe some of our work on the design and analysis of mathematical techniques for compressive sensing, processing, and analysis of spectral data. Topics considered include: (1) random SVD methods for dimensionality reduction, (2) joint reconstruction and classification of spectral images, and (3) applications of unmixing, clustering and classification methods to target identification. Tests on real data are described.

This represents is joint work with several people, including team members on projects funded by the U.S. Air Force Office of Scientific Research and the National Geospatial-Intelligence Agency.

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Talk 2. Image restoration via constrained optimization: an approach using feasible direction methods

Image restoration is an ill-posed inverse problem which requires regularization. Regularization leads to reformulate the original restoration problem as a constrained optimization problem where the objective function is a regularization term and the constraint imposes fidelity to the data.

In this talk, we present a feasible direction method for obtaining restored images as solutions of the optimization problem. The presented method computes feasible search directions by inexact solving trust region subproblems whose radius is adjusted in order to maintain feasibility of the iterates.

Numerical results are presented to illustrate the effectiveness and efficiency of the proposed method.

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Talk 3. On the solution of linear systems in Newton-type methods for image reconstruction

Some imaging applications are usually modeled as a minimization problem with nonnegative constraints on the solution. For large size problems, projected-Newton methods are very attractive because of their fast convergence. In order to make them computationally competitive, the inner linear system for the search direction computation should be solved efficiently. In this talk we focus on the solution of the linear system when different objective functions are considered. The objective function is related to the application, to the noise affecting the recorded image and to the kind of regularization chosen.

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Talk 4. Alternating direction optimization for convex inverse problems. Application to imaging and hyperspectral unmixing

In this talk I will address a new class of fast of algorithms for solving convex inverse problems where the objective function is a sum of convex terms with possibly convex constraints. Usually, one of terms in the objective function measures the data fidelity, while the others, jointly with the constraints, enforce some type of regularization on the solution. Several particular features of these problems (huge dimensionality, nonsmoothness) preclude the use of off-the-shelf optimization tools and have stimulated a considerable amount of research. In this talk, I will present a new class of algorithms to handle convex inverse problems tailored to image recovery applications and to hyperspectral unmixing. The proposed class of algorithms is an instance of the so-called alternating direction method of multipliers (ADMM), for which convergence sufficient conditions are known. We show that these conditions are satisfied by the proposed algorithms. The effectiveness of the proposed approach is illustrated in a series of imaging inverse problems, including

deconvolution and reconstruction from compressive observations, and hyperspectral unmixing problems, including sparse unmixing and positive matrix factorization.

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MS 58. Parametric eigenvalue problems - Part I of II

Talk 1. Computing double eigenvalues via the two-parameter eigenvalue problem

A task of computing all values of the parameter λ , such that the matrix $A + \lambda B$ has a double eigenvalue, can be interpreted as a singular (quadratic) two-parameter eigenvalue problem. Using a numerical method for the singular two-parameter eigenvalue problem it is possible to obtain all solutions as eigenvalues of a certain generalized eigenvalue problem.

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Talk 2. Lyapunov inverse iteration for identifying Hopf bifurcations in models of incompressible flow

The identification of instability in large-scale dynamical systems caused by Hopf bifurcation is difficult because of the problem of computing the rightmost pair of complex eigenvalues of large sparse generalised eigenvalue problems. A method developed in [Meerbergen & Spence, SIMAX (2010), pp.1982-1999] avoids this computation, instead performing an inverse iteration for a certain set of real eigenvalues that requires the solution of a large-scale Lyapunov equation at each iteration. This talk discusses a refinement of the method of Meerbergen & Spence and tests it on challenging problems arising from fluid dynamics.

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Talk 3. A quadratically convergent algorithm for matrix distance problems

We discuss a method for the computation of the distance of a stable matrix to the unstable matrices with respect to the open

left-half plane. First, we provide a fast algorithm to compute the *complex unstructured stability radius*. Second, based on a formula by Qiu et al. (Automatica, 31 (1995), pp. 879–890) we give a new fast method to compute the *real structured stability radius*. Both algorithms are based on finding Jordan blocks corresponding to a pure imaginary eigenvalue in a parameter-dependent Hamiltonian eigenvalue problem. Numerical results show the performance of both algorithms for several examples.

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Talk 4. A real Jacobi-Davidson algorithm for the 2-real-parameter eigenvalue problem

We consider the nonlinear eigenvalue problem

$$(i\omega M + A + e^{-i\omega\tau} B)u = 0$$

for real matrices $M, A, B \in \mathbb{R}^{n \times n}$ with invertible M . Sought are triples (ω, τ, u) consisting of a complex eigenvector $u \in \mathbb{C}^n$ and two real eigenvalues ω and τ .

Problems of this type appear e.g. in the search for critical delays of linear time invariant delay differential equations (LTI-DDEs)

$$M\dot{x}(t) = -Ax(t) - Bx(t - \tau).$$

In [Meerbergen, Schröder, Voss, 2010, submitted] this problem is discussed for complex M, A, B . Like there we are considering a Jacobi-Davidson-like projection method. The main differences in the real case are that a) the search space is kept real and b) a specialized method for the small projected problem is used. Numerical experiments show the effectiveness of the method.

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MS 59. Structured matrix computations - Part I of II

Talk 1. Factorization of \mathcal{H}^2 -matrices

Hierarchical matrices (\mathcal{H} -matrices) have been shown to be very useful tools for a variety of applications, e.g., the construction of efficient and robust preconditioners for the solution of elliptic partial differential equations and integral equations. Most \mathcal{H} -matrix algorithms are based on a recursive algorithm that approximates the product of two \mathcal{H} -matrices by a new \mathcal{H} -matrix, since this fundamental algorithm can be combined with simple recursive techniques to approximate the inverse or the LR factorization.

Combining \mathcal{H} -matrices with multilevel techniques leads to \mathcal{H}^2 -matrices that can reach significantly higher compression rates, particularly for very large matrices. Although most algorithms can take advantage of the rich multilevel structure to significantly improve efficiency, the construction of \mathcal{H}^2 -matrices poses a challenge since the connections between a large number of blocks have to be taken into account at each step.

The talk presents a new approach to the latter task: by adding a small amount of book-keeping information to the usual

\mathcal{H}^2 -matrix structure, it is possible to develop an algorithm that computes a low-rank update of a submatrix $G|_{t \times s}$ in an \mathcal{H}^2 -matrix in $\mathcal{O}(k^2(\#t + \#s))$ operations, where k is the local rank.

With this new algorithm at our disposal, several important higher-level operations become very simple: Low-rank approximations of submatrices, e.g., computed by popular cross approximation schemes, can easily be merged into an \mathcal{H}^2 -matrix, leading to an algorithm of complexity $\mathcal{O}(nk^2 \log n)$. The multiplication of two \mathcal{H}^2 -matrices can be implemented as a sequence of low-rank updates, the resulting algorithm also has a complexity of $\mathcal{O}(nk^2 \log n)$. Using the matrix multiplication, we can also construct the inverse and the LR factorization in $\mathcal{O}(nk^2 \log n)$ operations.

Similar to \mathcal{H} -matrix techniques, the new algorithm is fully adaptive, e.g., it can reach any given accuracy, and it is able to easily handle matrices resulting from the discretization of two- or three-dimensional geometries. Its main advantages over \mathcal{H} -matrix algorithms are the significantly reduced storage requirements and the higher efficiency for large matrices.

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Talk 2. **The polynomial root finding problems and quasiseparable representations of unitary matrices**

The effective tool to compute all the roots of a polynomial is to determine the eigenvalues of the corresponding companion matrix using the QR iteration method. The companion matrix belongs to the class of upper Hessenberg matrices which are rank one perturbations of unitary matrices. This class is invariant under QR iterations. Moreover it turns out that for every matrix in this class the corresponding unitary matrix has quasiseparable structure. This structure may be used to develop fast algorithms to compute eigenvalues of companion matrices. We discuss implicit fast QR eigenvalue algorithms solving this problem. The obtained algorithm is of complexity $\mathcal{O}(N)$ in contrast to $\mathcal{O}(N^2)$ for non-structured methods.

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Talk 3. **A fast direct solver for structured matrices arising from non-oscillatory integral equations**

We present a fast direct solver for structured dense matrices arising from non-oscillatory integral equations. The solver is based on (1) multilevel matrix compression techniques that exploit a complex hierarchical low-rank block structure, and (2) a sparse matrix embedding that allows fast and robust matrix factorization and inverse application. For boundary integral equations in 2D, the solver has optimal $\mathcal{O}(N)$ complexity, where N is the system size; in 3D, it incurs an $\mathcal{O}(N^{3/2})$ precomputation cost, followed by $\mathcal{O}(N \log N)$ solves. Numerical experiments suggest the utility of our method as both a direct solver and a preconditioner for complex problems.

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Talk 4. **Multivariate orthogonal polynomials and inverse eigenvalue problems**

It is well known that the computation of the recurrence coefficients of orthogonal polynomials with respect to a discrete inner product is related to an inverse eigenvalue problem. In this talk we present an algorithm to compute these recurrence coefficients for multivariate orthogonal polynomials. This algorithm generalizes previous results for the bivariate case and uses Givens transformations to solve the related inverse eigenvalue problem. We give a number of numerical examples using different configurations of points that define the discrete inner product.

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MS 60. Numerical linear algebra libraries for high end computing - Part II of II

Talk 1. **Thick-restart Lanczos methods for**

symmetric-indefinite generalized eigenproblems in SLEPc

In this talk we present results on a Lanczos method for generalized eigenvalue problems $Ax = \lambda Bx$ where both A and B are symmetric matrices but the pair (A, B) is not definite. In this case, eigenvalues are not guaranteed to be real and also an eigenvalue can be defective. The standard B -Lanczos cannot be used, but still the symmetry of the matrices can be exploited to some extent by means of the pseudo-Lanczos process. We show results of a thick-restart variant implemented in the SLEPc library, and compare it with other solvers that totally ignore symmetry.

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Talk 2. **Parametric approach to smart-tuning and auto-tuning of the DOE ACTS collection**

The Advanced Computational Software (ACTS) Collection is a set of computational tools and libraries developed primarily at DOE laboratories. Here we look at deriving parameters to automatically identify, at run-time, the most suitable auto-tuned kernels to load with a given application. Additionally, these parameters can be used in the context of "Smart-Tuning" to select the best algorithmic functionality and arguments to a library's API.

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Talk 3. **Trilinos: foundational libraries that enable next-generation computing**

With the availability and diversity of powerful computational resources, including multi-core CPU and GPU technology, there is significant interest in numerical software libraries that allow a developer to optimize the trade-off between effort and impact. In this talk we will discuss the current and ongoing efforts by which Trilinos is providing enabling technologies for the development of academic and industrial software targeted at next-generation architectures. We will cover a wide variety of Trilinos packages, from the foundational libraries for numerical linear algebra to the solver libraries that can leverage these fundamental capabilities to develop next-generation algorithms.

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Talk 4. **Rethinking distributed dense linear algebra**

It is a commonly held misconception that matrices must be distributed by blocks in order to translate the local computation of classical dense matrix operations into level 3 BLAS operations. In this talk, the performance and programmability implications of element-wise matrix distributions are discussed in the context of a recently introduced implementation, Elemental. In order to be able to effectively convey code samples, both the FLAME methodology and its extension to distributed-memory computation will be briefly introduced.

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MS 61. **Efficient preconditioners for real world applications - Part II of II**

Talk 1. **Relaxed mixed constraint preconditioners for ill-conditioned symmetric saddle point linear systems**

We develop efficient preconditioners for generalized saddle point linear system $\mathcal{A}x = b$, where $\mathcal{A} = \begin{bmatrix} A & B^T \\ B & -C \end{bmatrix}$ and $A > 0$, $C \geq 0$ and B a full-rank rectangular matrix. Given two preconditioners for A (P_A and \tilde{P}_A) and a preconditioner (P_S) for $S = B\tilde{P}_A^{-1}B^T + C$, the Relaxed Mixed Constraint Preconditioners (RMCP) is denoted by $\mathcal{M}^{-1}(\omega)$ where

$$\mathcal{M}(\omega) = \begin{bmatrix} I & 0 \\ BP_A^{-1} & I \end{bmatrix} \begin{bmatrix} P_A & 0 \\ 0 & -\omega P_S \end{bmatrix} \begin{bmatrix} I & P_A^{-1}B^T \\ 0 & I \end{bmatrix}.$$

Eigenanalysis of $\mathcal{M}^{-1}(\omega)\mathcal{A}$ shows that the optimal ω is related to the (cheaply estimated) spectral radius of $P_A^{-1}A$ and $P_S^{-1}S$. Results regarding large linear systems arising from discretizations of geomechanical problems as well as fluid flow in porous media, show that proper choice of ω improves considerably the MCP performance.

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Talk 2. **Chebyshev acceleration of iterative refinement**

Gaussian elimination with partial pivoting followed by iterative refinement can compute approximate solutions of linear systems of equations that are backward stable. In some situations, the number of refinement steps can be large and their cost prohibitive. Limiting the number of steps is particularly important on multicore architectures where the solve phase of a sparse direct solver can represent a bottleneck.

We propose variants of the Chebyshev algorithm that can be used to accelerate the refinement procedure without loss of numerical stability. Numerical experiments on sparse problems from practical applications corroborate the theory and illustrate the potential savings offered by Chebyshev acceleration.

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Talk 3. **Parallel deflated GMRES with the Newton basis**

The GMRES iterative method is widely used as a Krylov subspace accelerator for solving sparse linear systems when the coefficient matrix is nonsymmetric. The Newton basis implementation has been proposed for distributed memory computers as an alternative of the Arnoldi-based approach to avoid low-grained communications. The aim of our work here is to introduce a modification based on deflation techniques. This approach builds an augmented subspace in an adaptive way to accelerate the convergence of the restarted formulation. In our numerical experiments, we show the benefits of using this implementation in the PETSc package with Schwarz preconditioners for solving large CFD linear systems.

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Talk 4. **Rank- k updates of incomplete Sherman-Morrison preconditioners**

Let $B = A + PQ^T$ be a large and sparse matrix where A is a nonsingular matrix and PQ^T is a rank- k matrix. In this work we are interested in solving the updated linear system $Bx = b$ by preconditioned iterations. We study the problem of updating an already existing preconditioner M for the matrix A . In particular we consider how to update the incomplete LU factorization computed by the BIF algorithm (SIAM J. Sci. Comput. Vol. 30(5), pp. 2302-2318, (2008)). The results of the numerical experiments with different types of problems will be presented.

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MS 62. Solving ill-posed systems via signal-processing techniques - Part II of II

Talk 1. Effects of prox parameter selection strategies in exact and inexact first-order methods for compressed sensing and other composite optimization problems

We will discuss theoretical and practical implications of various strategies for choosing the prox parameter in prox gradient methods and related alternating direction methods. We will show extension of existing convergence rates for both accelerated and classical first-order methods. Practical comparison based on a testing environment for L1 optimization will be presented.

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Talk 2. An adaptive inverse scale space method for compressed sensing

In this talk a novel adaptive approach for solving ℓ^1 -minimization problems as frequently arising in compressed sensing is introduced, which is based on the recently introduced inverse scale space method. The scheme allows to efficiently compute minimizers by solving a sequence of low-dimensional nonnegative least-squares problems. Moreover, extensive comparisons between the proposed method and the related orthogonal matching pursuit algorithm are presented.

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Talk 3. CGSO for convex problems with polyhedral constraints

Conjugate Gradient with Subspace Optimization (CGSO) is a variant of conjugate gradient algorithm that achieves the optimal complexity bound of Nemirovski-Yudin's algorithm for the class of strongly convex functions. In this talk we are extending CGSO to constrained problems in which we are minimizing a strictly convex function over a convex polyhedron. We discuss the theoretical properties of CGSO for this class of problems as well as its practical performance.

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Talk 4. Phase-retrieval using explicit low-rank matrix factorization

Recently, Candes et al. proposed a novel methodology for phase retrieval from magnitude information by formulating it as a matrix-completion problem. In this work we develop an algorithm aimed at solving large-scale instances of this problem. We take advantage of the fact that the desired solution is of rank one and use low-rank matrix factorization techniques to attain considerable speed-up over existing approaches. We consider phase recovery in both the noisy and noiseless setting and study how various design choices affect the performance and reliability of the algorithm.

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MS 63. Max-algebra - Part II of II

Talk 1. Three-dimensional convex polyhedra tropically spanned by four points

In this talk we show how a 3-dimensional convex polyhedron T_A is obtained from a 4×4 normal tropically idempotent integer matrix A (i.e., $A = (a_{ij})$, $a_{ij} \in \mathbb{Z}_{\leq 0}$, $a_{ii} = 0$, $A \odot A = A$, with $\oplus = \max$, $\odot = +$).

Which polyhedra arise this way? T_A has 20 vertices and 12 facets, at most. By Euler's formula, the f -vector is $(20, 30, 12)$, at most. Facets have 6 vertices, at most.

We show that a polyhedron T_A combinatorially equivalent to the regular dodecahedron does not occur, for any A , i.e., the polygon-vector of T_A cannot be $(0, 0, 12, 0)$. The polygon-vector of T_A cannot be $(0, 1, 10, 1)$, either, but we have examples where the polygon-vector of T_A is $(0, 2, 8, 2)$. We provide families of matrices with T_A having polygon-vector $(0, 3, 6, 3)$. Finally, certain families of circulant matrices yield T_A with polygon-vector $(0, 4, 4, 4)$ i.e., the facets of T_A are 4 quadrilaterals, 4 pentagons and 4 hexagons. Previous work has been done by Joswig and Kulas, Develin and Sturmfels.

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Talk 2. Algorithmic problems in tropical convexity

We present recent advances in tropical computational geometry, including the fundamental problem of computing the vertices of a tropical polyhedron described as intersection of half-spaces, or inversely. We also discuss the connection of these problems with

hypergraph transversals, directed hypergraphs, and mean payoff games. We finally point out applications of tropical convexity to other fields in computer science, such as formal verification.

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Talk 3. On the weak robustness of interval fuzzy matrices

A fuzzy matrix A (i.e. matrix in a (max, min)-algebra) is called weakly robust if every orbit sequence of A with starting vector x contains no eigenvectors, unless x itself is an eigenvector of A . Weak robustness is extended to interval fuzzy matrices and their properties are studied. A characterization of weakly robust interval fuzzy matrices is described and a quadratic algorithm for checking the weak robustness of a given interval fuzzy matrix is presented.

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Talk 4. Weakly stable matrices

Given a square matrix A and a vector x the sequence $\{A^k \otimes x\}_{k=0}^{\infty}$ in the max-plus algebra is called the orbit of A with starting vector x . For some matrices the orbit never reaches an eigenspace unless it starts in one; such matrices are called weakly stable. We will characterise weakly stable matrices both in the reducible and irreducible case. It turns out that irreducible weakly stable matrices are exactly matrices whose critical graph is a Hamiltonian cycle in the associated graph. This talk is based on joint work with S. Sergeev and H. Schneider.

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MS 64. Eigenvalue perturbations and pseudospectra - Part II of II

Talk 1. Ritz value localization for non-Hermitian matrices

The Ritz values of Hermitian matrices have long been well understood, thanks to the Cauchy Interlacing Theorem. Recent progress has begun to uncover similar properties for Ritz values of non-Hermitian matrices. For example, the “inverse field of values problem” asks whether a set of k points in the field of values can be Ritz values from a k dimensional subspace. We survey results on this problem, describe how majorization can lead to Ritz value containment regions, and provide a detailed analysis for a Jordan block.

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Talk 2. Optimization of eigenvalues of Hermitian matrix functions

This work concerns a Hermitian matrix function depending on its parameters analytically. We introduce a numerical algorithm for the global optimization of a specified eigenvalue of such a Hermitian matrix function. The algorithm is based on constructing piece-wise quadratic under-estimators for the eigenvalue function, and finding global minimizers of these quadratic models. In the multi-dimensional case finding the global minimizers of the quadratic models is equivalent to solving quadratic programs. The algorithm generates sequences converging to global optimizers (linearly in practice). The applications include the H-infinity norm of a linear system, and the distance from a matrix to defectiveness.

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Talk 3. Algorithms for approximating the H_{∞} norm

H_{∞} norm methods are used in control theory to design optimal controllers. The controllers are designed so as to minimize the H_{∞} norm of the $n \times n$ closed-loop transfer matrix where n is the system order. This optimization procedure necessitates efficient methods for the computation of the H_{∞} norm itself. Existing methods compute the H_{∞} norm accurately but the cost is multiple singular value decompositions and eigenvalue decompositions of size n , making them impractical when n is large. We present a novel method which provides a fast computation of the H_{∞} norm for large and sparse matrices, such as the ones arising in the control of PDE's. The method is a nested fixed point iteration, where the outer iteration is a Newton step and the inner iteration is associated with the problem of the computation of the ε -pseudospectral abscissa, i.e. the real part of a rightmost point of the ε -pseudospectrum of a certain linear operator. The fixed points of the iteration are characterized, local linear convergence of the algorithm for small enough ε is given and some applications to the control of PDE's are discussed.

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Talk 4. Reduced basis methods for computing pseudospectral

quantities

Reduced basis methods have been developed to efficiently solve parameter-dependent partial differential equations and, after a spatial discretization, the resulting linear systems. They typically consist of two phases. In an offline phase, the linear system is solved for several parameter samples and a low-dimensional subspace containing these solutions (approximately) is constructed. In an online phase, only the compression of the linear system with respect to this subspace needs to be solved, leading to greatly reduced execution times. The effectivity of reduced basis methods crucially depends on the regularity of the parameter dependence and the chosen sampling strategy. In this talk, we show how an approach inspired by reduced basis methods can be used to compute pseudospectra and associated quantities of a matrix A . Instead of solving a parameter-dependent linear system, one needs to consider the computation of the singular vector(s) belong to the smallest singular value(s) of $A - zI$ for all values of the complex parameter z of interest. While the computation of pseudospectra itself is still under development, we show how these technique can already be used to speed up a recently proposed algorithm by Gulgielmi and Overton for computing the pseudospectral abscissa.

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MS 65. Numerical linear algebra and optimization in imaging applications - Part II of II**Talk 1. A recursion relation for solving L-BFGS systems with diagonal updates**

We investigate a formula to solve limited-memory BFGS quasi-Newton Hessian systems with full-rank diagonal updates. Under some mild conditions, the system can be solved via a recursion that uses only vector inner products. This approach has broad applications in trust region and barrier methods in large-scale optimization.

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Talk 2. Wavefront gradients reconstruction using $l^1 - l^p$ models

Images of objects in outer space acquired by ground-based telescopes are usually blurred by atmospheric turbulence. To improve the quality of these images, the wavefront of the light is utilized to derive the point spread function (PSF). We proposed the $l^1 - l^p$ ($p = 1, 2$) model for reconstructing the wavefront gradients and hence the wavefront itself. The model can give a more accurate PSF and therefore better restored images. Numerical results are given to illustrate the performance of the proposed models.

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Talk 3. Edge-preserving image enhancement via blind deconvolution and upsampling operators

We consider the super-resolution model introduced by S.J. Osher and A. Marquina in J. Sci. Comput., 2008 volume 37, 367382, consisting of the solution of a total-variation based variational problem that solves a linear degradation model involving a convolution operator and a down-sampling operator. In this research work we explore different edge preserving up/down-sampling operators with different orders of spatial accuracy and estimated convolution operators to remove unknown blur from degraded low resolved images to solve this genuine inverse problem. Some numerical examples are provided to show the features of the proposed algorithm.

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Talk 4. A new hybrid-optimization method for large-scale, non-negative, full regularization

We present a new method for solving the *full* regularization problem of computing both the regularization parameter and the corresponding solution of a linear or nonlinear ill-posed problem. The method is based on stochastic and fast, gradient-based optimization techniques, and computes non-negative solutions to l_1 or l_2 regularization problems. We describe the method and present numerical results for large-scale image restoration problems.

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MS 66. Parametric eigenvalue problems - Part II of II**Talk 1. A subspace optimization technique for the generalized minimal maximal eigenvalue problem.**

Consider the Generalized Minimal Maximal Eigenvalue

Problem:

$$\lambda_{\max}^* := \min_x \max_{\lambda, \vec{v}} \lambda$$

$$\text{st : } \begin{cases} \mathbf{K}(x)\vec{v} = \lambda\mathbf{M}(x)\vec{v}, \\ x \in \mathcal{H} \subset \mathbb{R}^p, \\ \vec{v} \in \mathbb{R}^n \end{cases}$$

where the matrices $\mathbf{K}(x)$ and $\mathbf{M}(x)$ are affine matrix functions, creating a symmetric positive definite pencil $(\mathbf{M}(x), \mathbf{K}(x))$ on the hypercube \mathcal{H} . It is a quasi-convex, non-smooth optimization problem.

We present a subspace iteration method for computing the minimal maximal eigenvalue of a large scale eigenvalue problem. The idea is based on Kelley's Classical cutting plane method for convex problems. In each iteration λ_1 and a corresponding eigenvector \vec{v} are computed for a specific x . The eigenvector \vec{v} is then used to expand the subspace and the next iterate x is determined from the minimal maximum eigenvalue of the small scale projected problem. Convergence theory of the method relies on the fact that the maximal Ritz value is a support to the maximal eigenvalue.

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Talk 2. An iterative method for computing pseudospectral abscissa and stability radii for nonlinear eigenvalue problems

We consider the following class of nonlinear eigenvalue problems,

$$\left(\sum_{i=1}^m A_i p_i(\lambda) \right) v = 0,$$

where A_1, \dots, A_m are given $n \times n$ matrices and the functions p_1, \dots, p_m are assumed to be entire. This does not only include polynomial eigenvalue problems but also eigenvalue problems arising from systems of delay differential equations. Our aim is to compute the ϵ -pseudospectral abscissa, i.e. the real part of the rightmost point in the ϵ -pseudospectrum, which is the complex set obtained by joining all solutions of the eigenvalue problem under perturbations $\{\delta A_i\}_{i=1}^m$, of norm at most ϵ , of the matrices $\{A_i\}_{i=1}^m$.

In analogy to the linear eigenvalue problem we prove that it is sufficient to restrict the analysis to rank-1 perturbations of the form $\delta A_i = \beta_i u v^*$ where $u \in \mathbb{C}^n$ and $v \in \mathbb{C}^n$ with $\beta_i \in \mathbb{C}$ for all i . Using this main - and unexpected - result we present new iterative algorithms which only require the computation of the spectral abscissa of a sequence of problems obtained by adding rank one updates to the matrices A_i . These provide lower bounds to the pseudospectral abscissa and in most cases converge to it. A detailed analysis of the convergence of the algorithms is made.

The methods available for the standard eigenvalue problem in the literature provide a robust and reliable computation but at the cost of full eigenvalue decompositions of order $2n$ and singular value decompositions, making them unfeasible for large systems. Moreover, these methods cannot be generalized to

nonlinear eigenvalue problems, as we shall explain. Therefore, the presented method is the first generally applicable method for nonlinear problems. In order to be applied it simply requires a procedure to compute the rightmost eigenvalue and the corresponding left and right eigenvectors. In addition, if the matrices A_i are large and sparse then the computation of the rightmost eigenvalue can for many classes of nonlinear eigenvalue problems be performed in an efficient way by iterative algorithms which only rely on matrix vector multiplication and on solving systems of linear equations, where the structure of the matrices (original sparse matrices plus rank one updates) can be exploited. This feature, as well other properties of the presented numerical methods, are illustrated by means of the delay and polynomial eigenvalue problem.

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Talk 3. Statistical pseudospectrum and eigenvalue robustness to rank-one disturbance

In this talk, we present a new statistical measure of the robustness (or sensitivity) of linear dynamic systems to rank-one random disturbances. The sensitivity assessment is a statistical pseudospectrum: given the probability distribution of the random disturbance magnitude, it measures the expected frequency region where the system eigenvalues are located. We discuss the properties of the robustness and sensitivity measure. We notably stress the existence of an invariant of the measure that consequently shows that under certain conditions, the rate of increase of a rank-one pseudospectrum area is constant as a function of the disturbance magnitude.

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MS 67. Structured matrix computations - Part II of II

Talk 1. Randomized numerical matrix computations with applications

It is long and well known that random matrices tend to be well conditioned, but exploitation of this phenomenon in numerical matrix computations is more recent and there are still various new directions to investigate. Some of them will be covered in this talk. This includes pivoting-free but safe Gaussian elimination, randomized preconditioning of linear systems of equations, computation of a basis for the null space of a singular matrix, approximation by low-rank matrices, and applications to polynomial root-finding.

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Talk 2. Massively parallel structured direct solver for the equations describing time-harmonic seismic waves

We consider the discretization and approximate solutions of equations describing time-harmonic seismic waves in 3D. We discuss scalar qP polarized waves, and multi-component elastic waves in inhomogeneous anisotropic media. The anisotropy comprises general (tilted) TI and orthorhombic symmetries. We are concerned with solving these equations for a large number of different sources on a large domain. We consider variable order finite difference schemes, to accommodate anisotropy on the one hand and allow higher order accuracy – to control sampling rates for relatively high frequencies – on the other hand.

We make use of a nested dissection based domain decomposition, with separators of variable thickness, and introduce an approximate direct (multifrontal) solver by developing a parallel Hierarchically SemiSeparable (HSS) matrix compression, factorization, and solution approach. In particular, we present elements of the following new parallel algorithms and their scalability: The parallel construction of an HSS representation or approximation for a general dense matrix, the parallel ULV factorization of such a matrix, and the parallel solution with multiple right-hand sides. The parallel HSS construction consists of three phases: Parallel rank revealing QR (RRQR) factorization based on a Modified Gram-Schmidt (MGS) method with column pivoting, parallel row compression, and parallel column compression. The parallel HSS factorization involves the use of two children's contexts for a given parent context. The communication patterns are composed of intra-context and inter-context ones. Similar strategies are applied to the HSS solution.

We present various examples illustrating the performance of our algorithm as well as applications in so-called full waveform inversion.

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Talk 3. On the conditioning of incomplete Cholesky factorizations with orthogonal dropping

We consider incomplete Cholesky factorizations based on orthogonal dropping for the iterative solution of symmetric positive definite linear systems. These methods become increasingly popular tools for computing an approximate

factorization of large dense matrices, including update matrices and Schur complements that arise in sparse solvers. For the system preconditioned with these incomplete factorizations we present an upper bound on the condition number which only depends on the accuracy of the individual approximation (dropping) steps. The analysis is illustrated with some existing factorization algorithms in the context of discretized elliptic partial differential equations.

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Talk 4. Randomized direct solvers

We propose some new structured direct solvers for large linear systems, using randomization and other techniques. Our work involves new flexible methods to exploit structures in large matrix computations. Our randomized structured techniques provide both higher efficiency and better applicability than some existing structured methods. New efficient ways are proposed to conveniently perform various complex operations which are difficult in standard rank-structured solvers. Extension of the techniques to least squares problems and eigenvalue problems will also be shown.

We also study the following issues:

1. Develop matrix-free structured solvers.
2. Update a structured factorization when few matrix entries change.
3. Relaxed rank requirements in structured solvers. We show the feasibility of our methods for solving various difficult problems, especially high dimensional ones.
4. Develop effective preconditioners for problems without significant rank structures. We analyze the criterion for compressing off-diagonal blocks so as to achieve nearly optimal effectiveness and efficiency in our preconditioner.

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MS 68. Linear algebra for structured eigenvalue computations arising from (matrix) polynomials

Talk 1. A QR algorithm with generator compression for structured eigenvalue computation

In this talk we present a new structured implicit QR algorithm for fast computation of matrix eigenvalues. The algorithm, which relies on the properties of quasiseparable structure, applies to unitary-plus-rank-one Hessenberg matrices and, in particular, to Frobenius companion matrices. It computes the eigenvalues of an $n \times n$ matrix in $\mathcal{O}(n^2)$ operations with $\mathcal{O}(n)$ memory. The introduction of a generator compression step allows to reduce complexity – without spoiling accuracy – with respect to a previous fast eigensolver for companion matrices ([Bini, Boito, Eidelman, Gemignani, Gohberg, LAA 2010]). Numerical results will be presented for the single- and double shift strategies.

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Talk 2. Quadratic realizability for structured matrix polynomials

Which lists of elementary divisors \mathcal{L} can be realized by some quadratic matrix polynomial $Q(\lambda)$? For regular $Q(\lambda)$ over the field \mathbb{C} , this problem has recently been solved by several researchers. Indeed, if \mathcal{L} can be realized at all by some regular Q over \mathbb{C} , then it can always be realized by some upper triangular Q ; several independent proofs are now known. This talk focuses on the analogous question for structured matrix polynomials. If \mathcal{S} is a class of structured polynomials, which elementary divisor lists \mathcal{L} can be realized by some quadratic $Q(\lambda)$ in \mathcal{S} ? We survey current progress on this problem for various structure classes \mathcal{S} , including palindromic, alternating, and Hermitian matrix polynomials. As time permits we will also consider the quadratic realizability of additional features, such as sign characteristics and minimal indices, for these same structure classes.

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Talk 3. Fast computation of zeros of a polynomial

The usual method for computing the zeros of a polynomial is to

form the companion matrix and compute its eigenvalues. In recent years several methods that do this computation in $\mathcal{O}(n^2)$ time with $\mathcal{O}(n)$ memory by exploiting the structure of the companion matrix have been proposed. We propose a new method of this type that makes use of Fiedler's factorization of a companion matrix into a product of $n - 1$ essentially 2×2 matrices. Our method is a non-unitary variant of Francis's implicitly-shifted QR algorithm that preserves this structure. As a consequence the memory requirement is a very modest $4n$, and the flop count is $\mathcal{O}(n)$ per iteration (and $\mathcal{O}(n^2)$ overall). We will present numerical results and compare our method with other methods.

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Talk 4. Eigenvector recovery of linearizations and the condition number of eigenvalues of matrix polynomials

The standard formula for the condition number of a simple eigenvalue of a matrix polynomial involves the left and right eigenvectors associated with the eigenvalue [F. TISSEUR, *Backward error and condition of polynomial eigenvalue problems*, Linear Algebra Appl., 309 (2000) 339–361]. The usual way to solve polynomial eigenvalue problems is by using linearizations. In the past few years, different families of linearizations have been introduced. In order to compare the condition number for the eigenvalues of these linearizations, we need formulas for the associated eigenvectors. We present in this talk formulas for the eigenvectors of several families of Fiedler-like linearizations. These formulas are introduced using the notion of *eigencolumn*, which allows us to relate the eigenvectors of the linearizations with the eigenvectors of the polynomial. This fact may allow also to compare the condition number of the eigenvalue in the polynomial with the condition number of the eigenvalue in the linearizations. Moreover, the use of eigencolumns allows us to express similar formulas for minimal bases of singular polynomials.

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MS 69. Advances in sparse matrix factorization

Talk 1. A sparse inertia-revealing factorization

We show how to apply Wilkinson's inertia-revealing factorization to sparse matrices in a way that preserves sparsity. No other inertia-revealing factorization is guaranteed to preserve sparsity. The input matrix A is factored row by row, thereby producing the triangular factors of all its leading blocks. The inertia is derived from the number of sign changes in the sequence of determinants (revealed by the factors) of these blocks. We show that the fill in the triangular factors is bounded by the fill in the QR factorization of A . Therefore, symmetrically pre-permuting A to a doubly-bordered form guarantees sparsity in our algorithm.

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Talk 2. Multifrontal factorization on heterogeneous multicore systems

When solving the sparse linear systems that arise in MCAE applications, the multifrontal method is particularly attractive as it transforms the sparse matrix factorization into an elimination tree of dense matrix factorizations. The vast majority of the floating point operations can be performed with calls to highly tuned BLAS3 routines, and near peak throughput is expected. Such computations are performed today on clusters of multicore microprocessors, often accelerated by graphics processing units (GPUs). This talk discusses how concurrency in the multifrontal computation is processed with message passing (MPI), shared memory (OpenMP), and GPU accelerators (CUDA), exploiting the unique strengths of each.

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Talk 3. Towards an optimal parallel approximate sparse factorization algorithm using hierarchically semi-separable structures

Hierarchically semiseparable (HSS) matrix algorithms are emerging techniques in constructing the superfast direct solvers for both dense and sparse linear systems. We present a set of novel parallel algorithms for the key HSS operations that are needed for solving large linear systems, including the parallel rank-revealing QR factorization, the HSS constructions with hierarchical compression, the ULV HSS factorization, and the HSS solutions. We have applied our new parallel HSS-embedded multifrontal solver to the anisotropic Helmholtz equations for seismic imaging, and were able to solve a linear

system with 6.4 billion unknowns using 4096 processors, in about 20 minutes.

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Talk 4. Improving multifrontal methods by means of low-rank approximation techniques

By a careful exploitation of the low-rank property of discretized elliptic PDEs, a substantial reduction of the flops and memory consumption can be achieved for many linear algebra operations. In this talk, we present how low-rank approximations can be used to significantly improve a sparse multifrontal solver. We introduce a blocked, low-rank storage format for compressing frontal matrices and compare it to the HSS storage format. Finally, we present experimental results showing the reduction of flops and memory footprint achieved on the solution of large scale matrices from applications such as the acoustic wave equation and thermo-mechanics.

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MS 70. Accurate algorithms and applications**Talk 1. High-precision and accurate algorithms in Physics and Mathematics**

In this talk we present a survey of recent applications in Physics and Mathematics where high level of numeric precision is required. Such calculations are facilitated, on one hand, by high-precision software packages that include high-level language translation modules to minimize the conversion effort, and on the other hand, by the use of theoretical error bounds and accurate algorithms when available. These applications include supernova simulations, planetary orbit calculations, Coulomb n -body atomic systems, scattering amplitudes of quarks, gluons and bosons, nonlinear oscillator theory, experimental mathematics, evaluation of recurrence relations, numerical integration of ODEs, computation of periodic orbits, studies of the splitting of separatrices, detection of strange non-chaotic

attractors, Ising theory, quantum field theory, and discrete dynamical systems. We conclude that high-precision arithmetic facilities are now an indispensable component of a modern large-scale scientific computing environment.

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Talk 2. Accurate evaluation of 1D and 2D polynomials in Bernstein form

In this talk we present some fast and accurate algorithms to evaluate the 1D and 2D polynomials expressed in the Bernstein form in CAGD. As a well-known and stable algorithm, De Casteljau algorithm may be still less accurate than expected owing to cancelation in some circumstances. Our compensated algorithms, applying error-free transformation, can yield a result as accurate as if computed by the De Casteljau algorithm in twice working precision. Numerical tests illustrate that our algorithms can run significantly faster than the De Casteljau algorithm using double-double library.

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Talk 3. Some issues related to double roundings

Double rounding is a phenomenon that may occur when different floating-point precisions are available on a same system, or when performing scaled operations whose final result is subnormal. Although double rounding is, in general, innocuous, it may change the behavior of some useful small floating-point algorithms. We analyze the potential influence of double roundings on the Fast2Sum and 2Sum algorithms, on some summation algorithms, and Veltkamp's splitting. We also show how to handle possible double roundings when performing scaled Newton-Raphson division iterations (to avoid possible underflow problems).

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Talk 4. Error bounds for floating-point summation and dot product

The sum and dot product of vectors of floating-point numbers are ubiquitous in numerical calculations. Since four decades the error is bounded by the classical Wilkinson estimates. However, those contain some nasty denominator covering higher order terms. In this talk we show that the latter can be omitted. A key to the (mostly) simple proofs is our ufp-concept denoting the "unit in the first place". In contrast to the well-known ulp (unit in the last place) it is defined for real numbers and allows sharp, simple and nice error estimates for floating-point operations. The practical relevance of the new estimates is limited; however, they are aesthetically pleasing and confirm that it is true what one may (hope or) expect.

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MS 71. Theoretical and applied aspects of graph Laplacians

Talk 1. Potential theory for perturbed Laplacian of finite networks

Given a symmetric and irreducible M -matrix M , the off-diagonal entries of M can be identified with the conductance function of a connected network Γ . In particular the matrix obtained by choosing $d_i = \sum_{j=1, j \neq i}^n c_{ij}$, where n is the order of the network, is nothing but the combinatorial Laplacian of the network. Therefore, any matrix with off-diagonal values given by $-c_{ij}$ can be considered as a perturbed Laplacian of Γ . From the operator theory point of view, the perturbed Laplacians are identified with the so-called discrete Schrodinger operators of the network Γ . Our main objective is the study of positive semi-definite Schrodinger operators. In fact, many of our techniques and results appear as the discrete counterpart of the standard treatment of the resolvent of elliptic operators on Riemannian manifolds. Joint work with E. Bendito, A. Carmona and A.M. Encinas

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Talk 2. Subclasses of graphs with partial ordering with respect to the spectral radius of generalized graph Laplacians.

Brualdi and Solheid (1986) proposed the following general problem, which became a classical problem in spectral graph

theory: “Given a set G of graphs, find an upper bound for the spectral radius in this set and characterize the graphs in which the maximal spectral radius is attained.” Now there exists extensive literature that characterizes such extremal graphs for quite a couple of such sets. Moreover, the problem has been generalized to the (signless) Laplacian matrix of graphs and there even exist a few contributions that provide results for non-linear generalizations of these matrices, such as the p -Laplacian.

Many of the proofs for these results apply graph perturbations that increase or decrease the spectral radius. In graph classes, like trees, one may eventually arrive at a graph with maximum or minimum spectral radius. As a by-product we get a partial ordering of graphs in such classes. This procedure may also work for generalized graph Laplacians (symmetric matrices with non-positive off-diagonal entries) like Dirichlet matrices.

In this talk we want to find a general framework for deriving such results. We present sets of graphs and generalized Laplacians where this procedure can be applied.

This is a joint work with Türker Bıyıkoğlu.

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Talk 3. Some new results on the signless Laplacian of graphs

Since recently the signless Laplacian spectrum has attracted much attention in the literature. In this talk we will put focus on some new results about the signless Laplacian spectrum which are inspired by the results so far established for the adjacency or the Laplacian spectrum.

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Talk 4. Graph bisection from the principal normalized Laplacian eigenvector

Graph bisection is the most often encountered form of graph partitioning, which asks to divide the nodes of a network into two non-overlapping groups such that the number of links between nodes in different groups is minimized. However, graph bisection may also be understood as the search for the largest bipartite subgraph in the complement: if two groups of G should have sizes roughly equal to $n/2$, and if m_1 and m_2 are the numbers of intra-group links and inter-group links, respectively, then the numbers of intra-group and inter-group links in the complement G^C will be roughly equal to $n^2/4m_1$ and $n^2/4m_2$. Hence, the request to minimize m_2 translates into the request of maximizing $n^2/4m_2$.

Here we may relate to a well-known property of the spectrum of the normalized Laplacian matrix L^* of G , saying that G is bipartite if and only if 2 is the largest eigenvalue of L^* . If G is bipartite, then the signs of the components of the eigenvector corresponding to eigenvalue 2 of L^* , yield the bipartition of G . In the more interesting case when G is not bipartite, one may still expect that the signs of the components of the eigenvector corresponding to the largest eigenvalue of L^* will yield a large bipartite subgraph of G . For example, it yields a perfect classification of club members in the Zacharys karate club

network. More interestingly, the sizes of the bipartite subgraphs obtained in this way in instances of random networks show high similarity to those obtained by applying the old Erdős method, an iterative process which starts with a random partition in two groups and, as long as there exists a node having more than half of its neighbors in its own group, it moves such node to the other group. This similarity is explored in more detail in this talk.

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MS 72. Linear techniques for solving nonlinear equations

Talk 1. A Gauss-Seidel process in iterative methods for solving nonlinear equations

In this talk, we present a process named “Gauss-Seidelization” for solving nonlinear equations. It is an iterative process based on the well-known Gauss-Seidel method to numerically solve a system of linear equations. Together with some convergence results, we show several numerical experiments in order to emphasize how the Gauss-Seidelization process influences on the dynamical behaviour of an iterative method for solving nonlinear equations.

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Talk 2. A greedy algorithm for the convergence of a fractional blind deconvolution

In this talk we present new results on a greedy algorithm to study the convergence of the Fractional Blind Deconvolution based on fractional powers of the laplacian. Greedy algorithms perform a theoretical background to prove the convergence in a Hilbert Space. We will show the theoretical results and an application to baroque paintings.

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Talk 3. Overview of iterative methods using a variational approach

In this talk, we introduce a general framework for the approximation of nonlinear equations in Banach spaces. We adapt a variational perspective recently introduced for the analysis of differential equations. In this new approach, some classical iterative methods, including their convergence analysis, can be obtained. The method can be considered as a

generalization of the discrete least squares method, which is a standard approach to the approximate solution of many types of problems including overdetermined systems of nonlinear equations.

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Talk 4. Iterative methods for ill-conditioned problems

In this talk we study some features related to ill-conditioned nonlinear equations. A strategy to choose iterative methods for solving these equations is developed. In particular, we analyze a variation of Newton method, the so called perturbed Newton method. Important features to achieve good performance, such as choice of pivots and parameters provide degrees of freedom that can be suited for improvement of the method. We illustrate this analysis through examples.

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MS 73. Algebraic Riccati equations associated with M-matrices: numerical solution and applications

Talk 1. Monotone convergence of Newton-like methods for M-matrix algebraic Riccati equations

The minimal nonnegative solution of an M-matrix algebraic Riccati equation can be obtained by Newton's method. Here we study Newton-like methods that have higher-order convergence and are not much more expensive each iteration, and are thus more efficient than Newton's method. For the Riccati equation, these Newton-like methods are actually special cases of the Newton–Shamanskii method. We show that, starting with zero initial guess or some other suitable initial guess, the sequence generated by the Newton–Shamanskii method converges monotonically to the minimal nonnegative solution.

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Talk 2. Accurate solution of M-matrix algebraic Riccati equation by ADDA: alternating-directional doubling algorithm

It is known that that an M-matrix Algebraic Riccati Equation (MARE) $XD\bar{X} - AX - X\bar{B} + C = 0$ has a unique minimal nonnegative solution Φ . In this talk, we will discuss two recent developments:

- a relative perturbation theory that will show that small relative perturbations to the entries of A , B , C , and D introduce small relative changes to the entries of the

nonnegative solution Φ , unlike the existing perturbation theory for (general) Algebraic Riccati Equations.

- an efficient Alternating-Directional Doubling Algorithm (ADDA) that can compute such a solution Φ as accurately as predicted by the relative perturbation theory.

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Talk 3. When fluid becomes Brownian: the morphing of Riccati into quadratic equations

Ramaswami (2011) approximates Brownian motion using a Markov-modulated linear fluid model. This is extended to approximate Markov-modulated Brownian motion (MMBM); in particular, the Laplace matrix exponent of a Markov-modulated linear fluid model converges to that of an MMBM. When the MMBM is reflected at zero, its stationary distribution is the limit of that of the fluid model also reflected at zero. Proof of convergence combines probabilistic arguments and linear algebra. Starting from the Wiener-Hopf factorization of the modulating Markov chain, expressed as an algebraic Riccati equation, key matrices in the limiting stationary distribution are shown to be solutions of a new quadratic equation.

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Talk 4. Analyzing multi-type queues with general customer impatience using Riccati equations

We consider a class of multi-type queueing systems with customer impatience, where the (phase-type) service time and (general) patience distribution is type dependent and the types of consecutive customers may be correlated.

To obtain the per-type waiting time distribution and probability of abandonment, we construct a fluid queue with r thresholds, the steady state of which can be expressed via the solution of $2r$ algebraic Riccati equations using matrix-analytic methods.

Numerical examples indicate that thousands thresholds may be required to obtain accurate results, indicating the need for fast

and numerically stable algorithms to solve large sets of Riccati equations.

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MS 74. Recent advances in the numerical solution of large scale matrix equations

Talk 1. Hierarchical and multigrid methods for matrix and tensor equations

Hierarchical and Multigrid methods are among the most efficient methods for the solution of large-scale systems that stem, e.g. from the discretization of partial differential equations (PDE). In this talk we will review the generalization of these methods to the solution of matrix equations (*L. Grasedyck, W. Hackbusch, A Multigrid Method to Solve Large Scale Sylvester Equations, SIAM J. Matrix Anal. Appl. 29, pp. 870–894, 2007; L. Grasedyck, Nonlinear multigrid for the solution of large scale Riccati equations in low-rank and H-matrix format, Num.Lin.Alg.Appl. 15, pp. 779–807, 2008*), and equations that possess a tensor structure (*L. Grasedyck, Hierarchical Singular Value Decomposition of Tensors, SIAM J. Matrix Anal. Appl. 31, pp. 2029–2054, 2010.*). The standard hierarchical and multigrid methods can perfectly be combined with low rank (matrix) and low tensor rank representations. The benefit is that the solution is computable in almost optimal complexity with respect to the amount of data needed for the representation of the solution. As an example we consider a PDE posed in a product domain $\Omega \times \Omega$, $\Omega \subset \mathbb{R}^d$ and discretized with N^d basis functions for the domain Ω . Under separability assumptions on the right-hand side the system is solved in low rank form in $\mathcal{O}(N^d)$ complexity (instead of $\mathcal{O}(N^{2d})$ required for the full solution). For a PDE on the product domain $\Omega \times \dots \times \Omega$ one can even solve the system in low tensor rank form in $\mathcal{O}(N \cdot d)$ complexity (instead of $\mathcal{O}(N^{2d})$ required for the full solution). The state of the art will be shortly summarized.

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Talk 2. A survey on Newton-ADI based solvers for large scale AREs

Newton based solvers for the algebraic Riccati equation (ARE) have been around for several decades. Only roughly one decade ago these have become applicable to large and sparse AREs when combined with the low rank Cholesky factor alternating directions implicit (LRCF-ADI) iteration for solving the Lyapunov equations arising in every Newton step. In this contribution we give a survey on accelerated variants of the low rank Cholesky factor Newton method (LRCF-NM) developed over the recent years. These include projection based methods and inexact Newton-like approaches.

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Talk 3. An invariant subspace method for large-scale algebraic Riccati and Bernoulli equations

We present a new family of low-rank approximations of the solution of the algebraic Riccati equation based on stable invariant subspaces of the Hamiltonian matrix (*L. Amodei and J.-M. Buchot, An invariant subspace method for large-scale algebraic Riccati equations, Appl. Numer. Math., 60 (11), 1067–1082, 2010.*). The approximations are given by a factorized form which preserves the positive semi-definiteness of the exact solution. By using the same general factorization, we deduce a reduced rank expression of the exact solution of the Bernoulli equation. We illustrate the effectiveness of this formulation by considering the stabilization of the nonstationary incompressible Navier-Stokes equations by a boundary feedback control obtained from the solution of the Bernoulli equation (*L. Amodei and J.-M. Buchot, A stabilization algorithm of the Navier-Stokes equations based on algebraic Bernoulli equation, Numer. Linear Algebra Appl., DOI: 10.1002/nla.799, 2011.*).

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Talk 4. Delay Lyapunov equations and model order reduction of time delay systems

We present a version of balanced truncation for model order reduction of linear time-delay systems. The procedure is based on a coordinate transformation of the position and preserves the delay structure of the system. To every position we associate quantities representing energies for the *controllability* and *observability* of the position. We show that these energies can be expressed explicitly in terms of Gramians which are given as solutions to corresponding *delay Lyapunov equations*. Balanced truncation can be based on these Gramians in the usual way.

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MS 75. Points that minimize potential functions

Talk 1. Discretizing compact manifolds with minimal energy

One approach to generate “good” point configurations is inspired by physics: points emulate repelling unit point charges interacting through a Coulomb potential $1/r$, where r measures the Euclidean distance between points in the ambient space. Points on the sphere that minimize the corresponding energy (potential energy) are uniformly distributed even if a Riesz s -potential $1/r^s$ governs the point interaction. On other compact manifolds minimal energy systems are uniformly distributed if s is greater than the dimension d of the manifold (“Poppy Seed Bagel” theorem).

This talk gives an introduction into the discrete minimal Riesz s -energy problem on compact manifolds.

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Talk 2. Well conditioned spherical designs and potential functions

A spherical t -design is a set of N points on the unit sphere such that equal weighted numerical integration at these points is exact for all spherical polynomials of degree at most t . This talk will look at the calculation and properties of spherical designs with N between $t^2/2$ and $(t+1)^2$, their characterization by different potential functions, and using any degrees of freedom to also minimize the condition number of the basis matrix or maximize the determinant of the associated Gram matrix.

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Talk 3. Probabilistic frames in the 2-Wasserstein metric

In this talk I will review the notion of probabilistic frames and indicate how it is a natural generalization of frames. In addition, I will show how within the framework of the 2-Wasserstein metric, probabilistic frames can be constructed and analyzed. This is based on joint work with M. Ehler.

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Talk 4. Numerical minimization of potential energies on specific manifolds

In this talk we consider the problem of computing local minimizers of potential energies of the form

$$E(\mathbf{x}_1, \dots, \mathbf{x}_M) := \sum_{i,j=1; i \neq j}^M K(\mathbf{x}_i, \mathbf{x}_j),$$

with $\mathbf{x}_i \in \mathcal{M}$, $i = 1, \dots, M$, where $\mathcal{M} \subset \mathbb{R}^n$ is a d -dimensional compact manifold and $K : \mathcal{M} \times \mathcal{M} \rightarrow \mathbb{R}$ is a given function. The optimization approach is based on a nonlinear conjugate gradient method on Riemannian manifolds, which is a generalization of the CG-method in Euclidean space. This method was already successfully applied to the computation of spherical t -designs in [Numer. Math., 119:699 – 724, 2011] and low discrepancy points for polynomial kernels K , cf. [TU Chemnitz, Preprint 5, 2011]. Now, we present interesting numerical results for localized non-polynomial discrepancy kernels K .

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