

# Conference Abstracts

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### IP 1. Challenges in modern medical image reconstruction

A common problem in medical imaging is the reconstruction of one or more anomalous hot spots distinct from the background. Many such problems are severely data limited and highly noise sensitive. Thus, a voxel-based reconstruction could be both overkill and an overreach. Shape-based methods can be used as an alternative; a recent such proposal is to use a parametric level set (PaLS) approach, whereby the image is described using the level-set of a linear combination of a relatively small number of basis functions of compact support. Remaining concerns are the nonlinear least squares problem for the image model parameters and, in the case of a nonlinear forward model, the solution of the large-scale linear systems at each step of the optimization process. We report on recent advances on both fronts, notably a trust-region regularized Gauss-Newton process for the optimization, and a reduced-order modeling approach tailored to the PaLS formulation.

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### IP 2. An envelope for the spectrum of a matrix

An envelope-type region  $\mathcal{E}(A)$  in the complex plane that contains the eigenvalues of a given  $n \times n$  complex matrix  $A$  is introduced.  $\mathcal{E}(A)$  is the intersection of an infinite number of regions defined by cubic curves. The notion and method of construction of  $\mathcal{E}(A)$  extend those of the numerical range of  $A$ , which is known to be an intersection of an infinite number of half-planes; as a consequence,  $\mathcal{E}(A)$  is contained in the numerical range and represents an improvement in localizing the spectrum of  $A$ .

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### IP 3. An iterative linear algebra perspective on compressed sensing and matrix completion

Compressed sensing and matrix completion are techniques by which simplicity in data can be exploited to allow for sensing at the information rate. Compressed sensing is typically cast as seeking to measure an unknown vector that has few non-zeros, but in unknown locations, and to make the measurements through the action of a matrix. Compressed sensing establishes that when the vector to be measured is length  $n$ , but has  $k \ll n$  nonzeros, the measurement matrix need only have order  $k$

rows, which is the minimum order possible. Matrix completion is a similar question, but where the matrix measured is assumed to be of low rank, and one would like to recover the matrix from only few of its entries. Both compressed sensing and matrix completion have natural non-convex optimization formulations for the recovery of the vector and matrix respectively; typically the non-convex objections in these formulations are replaced with their convex envelope, and well studied convex optimization algorithms applied. The convex formulations are also amenable to detailed analysis, making quantitatively accurate estimates as to the number of measurements needed for the recovery using convex optimization. In this talk we consider an alternative perspective on compressed sensing and matrix completion, inspired by iterative linear algebra algorithms. We show that the average case behaviour of surprisingly simple algorithms that directly try to solve the non-convex problem can perform as well or better than can the convex approximations.

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### IP 4. Extending preconditioned GMRES to nonlinear optimization

Preconditioned GMRES is a powerful iterative method for linear systems. In this talk, I will show how the concept of preconditioned GMRES can be extended to the general class of nonlinear optimization problems. I will present a nonlinear GMRES (N-GMRES) optimization method, which combines preliminary iterates generated by a stand-alone simple optimization method (the nonlinear preconditioner) to produce accelerated iterates in a generalized Krylov space. The nonlinear acceleration process, which is closely related to existing acceleration methods for nonlinear systems, is combined with a line search in every step to obtain a general nonlinear optimization method for which global convergence can be proved when steepest-descent preconditioning is used. Numerical tests show that N-GMRES is competitive with established nonlinear optimization methods, and outperforms them for a difficult canonical tensor approximation problem when an advanced nonlinear preconditioner is used. This suggests that the real power of N-GMRES may lie in its ability to use powerful problem-dependent nonlinear preconditioners.

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### IP 5. Matrix iterations to summarize evolving networks

I will describe a new algorithm for summarizing

properties of evolving networks. This type of data, recording connections that come and go over time, is being generated in many modern applications, including telecommunications and on-line human social behavior. The algorithm computes a dynamic measure of how well pairs of nodes can communicate by taking account of routes through the network that respect the arrow of time. The conventional approach of downweighting for length (messages become corrupted as they are passed along) is combined with the novel feature of downweighting for age (messages go out of date). This allows us to generalize widely used centrality measures that have proved popular in static network science to the case of dynamic networks sampled at non-uniform points in time. In particular, indices can be computed that summarize the current ability of each node to broadcast and receive information. The computations involve basic operations in linear algebra, and the asymmetry caused by times arrow is captured naturally through the non-commutativity of matrix-matrix multiplication. I will give illustrative examples on both synthetic and real-world communication data sets. This talk covers joint work with Ernesto Estrada, Peter Grindrod and Mark Parsons.

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## IP 6. PDE-constrained optimization

The term 'PDE-constrained optimization' refers to optimization problems which involve partial differential equations as side constraints. Problems of this class arise, for instance, in parameter identification as well as optimal control. Dealing with them appropriately and efficiently touches upon a wide range of topics, such as optimization theory in function spaces, taylored discretizations, error estimation, and numerical linear algebra. In this presentation we focus on some of the properties of linear systems arising as optimality conditions for discretized optimal control problems. Particular attention will be given to problems with additional inequality constraints, which exhibit some unexpected features.

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## IP 7. Hierarchical tensor decomposition and approximation

The (numerical) linear algebra related to tensor computations plays an immensely powerful role in theoretical and applied sciences: applied mathematics, biology, chemistry, information sciences, physics and many other areas. In this talk we consider high-order or high-dimensional tensors of the form  $A \in \mathbb{R}^{n \times \dots \times n}$  as they appear in multivariate (discrete or continuous)

approximation problems. These require special techniques in order to allow a representation and approximation for high dimension  $d$  (cf. the curse of dimension). A typical example is the canonical polyadic (CP) format

$$A_{i_1, \dots, i_d} = \sum_{j=1}^r a_1^r(i_1) \cdots a_d^r(i_d)$$

that requires  $\mathcal{O}(d \cdot n \cdot r)$  degrees of freedom for the representation. However, this simple format comes along with several numerical obstructions, because it is highly non-linear.

In the last three years some new hierarchical formats (namely Tensor Train and Hierarchical Tucker) have been developed and analysed. These include as a subset all tensors of CP format (rank parameter  $r$  fixed), but in addition they allow for some nice linear algebra approaches, e.g. a hierarchical SVD in complexity  $\mathcal{O}(d \cdot n \cdot r^3)$ . The hierarchical SVD is similar to the SVD for matrices in the sense that it allows us to reliably compute a quasi-best approximation in the hierarchical format.

We will outline the basic linear algebra behind the new approaches as well as open questions and possible applications.

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## IP 8. Improving performance and robustness of incomplete factorization preconditioners

We will present methods for improving the performance and robustness of incomplete factorization preconditioners for solving both SPD and general sparse linear systems. A key technique that results in significant improvement is the use of block rows and columns, which is commonplace in direct solvers. This enables the construction of denser and more robust preconditioners without the excessive cost traditionally associated with the construction of such preconditioners. We present empirical results to show that in most cases, the preconditioner density can be increased in a memory-neutral manner for solving unsymmetric systems with restarted GMRES because the restart parameter can be reduced without compromising robustness. In addition to blocking, we will also present some relatively simple but effective adaptive heuristics for improving preconditioning based on incomplete factorization. These include robust management of breakdown of incomplete Cholesky factorization, use of a flexible fill-factor, and automatic tuning of drop tolerance and fill-factor in applications requiring solution of a sequence of linear systems.

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### IP 9. Solving nonlinear eigenvalue problems in electronic structure calculation

The Kohn-Sham density functional theory is the most widely used theory for studying electronic properties of molecules and solids. It reduces the need to solve a many-body Schrodinger's equation to the task of solving a system of single-particle equations coupled through the electron density. These equations can be viewed as a nonlinear eigenvalue problem. Although they contain far fewer degrees of freedom, these equations are more difficult in terms of their mathematical structures. In this talk, I will give an overview on efficient algorithms for solving this type of problems. A key concept that is important for understanding these algorithms is a nonlinear map known as the Kohn-Sham map. The ground state electron density is a fixed point of this map. I will describe properties of this map and its Jacobian. These properties can be used to develop effective strategies for accelerating Broyden's method for finding the optimal solution. They can also be used to reduce the computational complexity associated with the evaluation of the Kohn-Sham map, which is the most expensive step in a Broyden iteration.

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### IP 10. Randomized algorithms in linear algebra

The introduction of randomization in the design and analysis of algorithms for matrix computations (such as matrix multiplication, least-squares regression, the Singular Value Decomposition (SVD), etc.) over the last decade provided a new paradigm and a complementary perspective to traditional numerical linear algebra approaches. These novel approaches were motivated by technological developments in many areas of scientific research that permit the automatic generation of large data sets, which are often modeled as matrices.

In this talk we will outline how such approaches can be used to approximate problems ranging from matrix multiplication and the Singular Value Decomposition (SVD) of matrices to approximately solving least-squares problems and systems of linear equations. Application of the proposed algorithms to data analysis will also be discussed.

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### IP 11. Computations with some classes of matrices

### related to P-matrices

A square matrix is called a P-matrix if all its leading principal minors are positive. Sublasses of P-matrices very important in applications are the nonsingular totally nonnegative matrices and the nonsingular M-matrices. Other classes of P-matrices used for eigenvalue localization are also presented. We also present some recent results and applications of the following two classes of matrices: sign-regular matrices (which contains the class of totally nonnegative matrices) and H-matrices (which contains the class of M-matrices). Let us recall that nonsingular H-matrices are, in fact, strictly diagonally dominant matrices up to a column scaling. For diagonally dominant matrices and some subclasses of nonsingular totally nonnegative matrices, accurate methods for computing their singular values, eigenvalues or inverses have been obtained, assuming that adequate natural parameters are provided. We present some recent extensions of these methods to other related classes of matrices.

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### IP 12. Reduction of quadratic matrix polynomials to triangular form

There is no analogue of the generalized Schur decomposition for quadratic matrix polynomials in the sense that  $Q(\lambda) = \lambda^2 A_2 + \lambda A_1 + A_0 \in \mathbb{C}[\lambda]^{n \times n}$  cannot, in general, be reduced to triangular form

$T(\lambda) = \lambda^2 I + \lambda T_1 + T_0$  by equivalence transformations independent of  $\lambda$ . We show that there exist matrix polynomials  $E(\lambda), F(\lambda)$  with constant determinants such that  $E(\lambda)Q(\lambda)F(\lambda) = T(\lambda)$  is a triangular quadratic matrix polynomial having the same eigenstructure as  $Q(\lambda)$ .

For any linearization  $\lambda I_{2n} - A$  of  $Q(\lambda)$  with  $A_2$  nonsingular, we show that there is a matrix  $U \in \mathbb{C}^{2n \times n}$  with orthonormal columns such that  $S = [U \ A U]$  is nonsingular and  $S^{-1}(\lambda I_{2n} - A)S = \lambda I_{2n} - \begin{bmatrix} 0 & -T_0 \\ I & -T_1 \end{bmatrix}$  is a companion linearization of an  $n \times n$  triangular quadratic  $T(\lambda) = \lambda^2 I + \lambda T_1 + T_0$  equivalent to  $Q(\lambda)$ . Finally, we describe a numerical procedure to compute  $U$  and  $T(\lambda)$ .

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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. Gomilko, F. Greco, K. Ziętak and the paper by O. Gomilko, 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  $A^T Ax = A^T b$  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  $\mu$  as an eigenvalue of algebraic multiplicity at least  $r$  and to those that have  $\mu$  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  $\varepsilon$ -pseudospectrum of a square matrix, which is the set of eigenvalues of all real matrices that are  $\varepsilon$ -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  $\varepsilon$ -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 problems 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/Tytyshnikov (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 ( $\alpha$ SA), suffer from drawbacks, such as noisy candidate vectors (BAMG) and potentially high operator complexity, especially for scalar problems, ( $\alpha$ SA). This work is intended to address some of these drawbacks by combining elements of BAMG and  $\alpha$ 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 optimal 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. Schwartz'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 scarcely 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 talk 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  $3 \times 3$  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 devises 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  $AA^T$ ,  $A^TA$ , 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  $A^TA$ . Specifically, using techniques from combinatorial matrix theory, we characterise all pairs of (0,1) matrices  $A_1, A_2$  such that  $A_1A_1^T = A_2A_2^T$ ,  $A_1^TA_1 = A_2^TA_2$ , 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  $(\kappa, \tau)$ -regular set is a subset of the

vertices inducing a  $\kappa$ -regular subgraph such that every vertex not in the subset has  $\tau$  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  $(\kappa, \kappa)$ -regular set, then it is a core graph. By considering the walk matrix, we develop an algorithm to extract  $(\kappa, \kappa)$ -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  $\lambda_i$  and  $d_i$  are the  $i^{th}$  largest Laplacian eigenvalue and degree of  $G$ , respectively. For  $\lambda_3$  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. Proper generalized decomposition of multiscale models

In this talk the coupling of a parabolic model with a system of local kinetic equations is analyzed. A space-time separated representation is proposed for the global model (this is simply the radial approximation proposed by Pierre Ladevèze in the LATIN framework (Non-linear Computational Structural Mechanics. Springer: New York, 1999)). The originality of the present work concerns the treatment of the local problem, that is first globalized (in space and time) and then fully globalized by introducing a new coordinate related to the different species involved in the kinetic model. Thanks to the non-incremental nature of both discrete descriptions (the local and the global one) the coupling is quite simple and no special difficulties are encountered by using heterogeneous time integration

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### Talk 3. Dynamic data-driven inverse identification in dynamical systems

Dynamic Data-Driven Application Systems DDDAS appear as a new paradigm in the field of applied sciences and engineering, and in particular in simulation-based engineering sciences. By DDDAS we mean a set of techniques that allow the linkage of simulation tools with measurement devices for real-time control of systems and processes. DDDAS entails the ability to dynamically incorporate additional data into an executing application, and in reverse, the ability of an application to dynamically steer the measurement process. DDDAS needs for accurate and fast simulation tools making use if possible of off-line computations for limiting as much as possible the on-line computations. We could define efficient solvers by introducing all the sources of variability as extra-coordinates in order to solve off-line only once the model to obtain its most general solution to be then considered for on-line purposes.

However, such models result defined in highly multidimensional spaces suffering the so-called curse of dimensionality. We proposed recently a technique, the Proper Generalized Decomposition -PGD-, able to circumvent the redoubtable curse of dimensionality. The marriage of DDDAS concepts and tools and PGD “off-line” computations could open unimaginable possibilities in the field of dynamics data- driven application systems. In this work we explore some possibilities in the context of on-line inverse identification of dynamical systems that can be found in the control of industrial processes.

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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 RRGMRES 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 RRGMRES 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  $\gamma$  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. Sparse tensor approximation for uncertainty quantification

Uncertainty quantification (UQ) in complex models is typically challenged by the high-dimensionality of the input space. This is true of both forward and inverse UQ problems, and particularly so when the computational cost of a forward model evaluation is high. Despite the availability of efficient sparse-quadrature methods, it is frequently necessary to pursue sparse, low dimensional, representations of uncertain model outputs, retaining only important dependencies on the input space, in order to render the UQ problem tractable. We discuss the use of Bayesian Compressed Sensing methods for discovering sparse polynomial chaos representations in this context.

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##### Talk 2. Analysis of greedy algorithms for high-dimensional problems

We study a class of greedy algorithms for the solution of high dimensional partial differential equations. The idea is to represent the solution as a sum of tensor products and to compute iteratively the terms of this sum. Convergence results of this approach will be presented for the case of convex optimization problems. We will also analyze algorithms for the solution of nonsymmetric problems.

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##### Talk 3. Projected dynamical systems in tensor Banach spaces

Some classes of projected dynamical systems in reflexive, strictly convex and smooth Banach spaces was introduced by Guiffrè, Idone and Pia in *J. Glob. Optim.* (2008) 40:119–128. The main drawback to extend this concept in the framework of

Tensor spaces, is the use of closed convex subsets in metric projections. In this talk we discuss about the definition of a Projected Dynamical System on a Tensor Banach space using a path of idempotent operators.

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#### **Talk 4. 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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#### **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  $60.000 \times 10.000$  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 adaptions 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  $A + I - AA^-$  is nonsingular, independently of the choice of  $A^-$ , where  $A^-$  denotes an inner inverse of  $A$ , i.e.  $AA^-A = A$ . Let  $B \in \mathbb{C}^{n \times r}$ ,  $C \in \mathbb{C}^{r \times n}$ , and  $r < n$ . If  $A$  and  $I - CA^{-1}B$  are nonsingular, then to adapt the inverse of the

modified matrix  $A - BC$  we can apply the Sherman-Morrison-Woodbury formula:

$(A - BC)^{-1} = A^{-1} + A^{-1}B(I - CA^{-1}B)^{-1}CA^{-1}$ ; and, hence, we need to compute the inverse of  $I - CA^{-1}B$ , which has size  $r < n$ . This talk will be focused on the group inverse of additively modified matrices,  $(A - BC)^\#$ , 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  $c_1A + c_2B$ , 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  $c_1A + c_2B$  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  $(ab)^\# = b^\#(a^\#abb^\#)^\#a^\#$  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.,

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

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 became 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:

- '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.

- 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. This paper has been partially supported by Universidad Nacional de La Pampa (Facultad de Ingeniería) of Argentina (grant Resol. N. 049/11) and by the Ministry of Education of Spain (Grant DGI MTM2010-18228).

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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  $E = \{(S_i, S_j)\} \subset V \times V$  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  $X$ ,  $A^\pi$  and  $B^\pi$  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  $2 \times 2$  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 favorable 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 unprecedent 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 l1-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 l1-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  $\epsilon$ -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  $\epsilon$ ,  $\Lambda_{\epsilon,j}(A)$ , 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: 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  $\lambda$ , 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  $(\omega, \tau, u)$  consisting of a complex eigenvector  $u \in \mathbb{C}^n$  and two *real* eigenvalues  $\omega$  and  $\tau$ .

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

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

Eigenanalysis of  $\mathcal{M}^{-1}(\omega)\mathcal{A}$  shows that the optimal  $\omega$  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  $\omega$  improves considerably the MCP performance.

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**Talk 2. Chebychev 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  $\ell^1$ -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  $4 \times 4$  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 $H_{\infty}$ norm

$H_{\infty}$  norm methods are used in control theory to design optimal controllers. The controllers are designed so as to minimize the  $H_{\infty}$  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  $H_{\infty}$  norm itself. Existing methods compute the  $H_{\infty}$  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  $H_{\infty}$  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  $\varepsilon$ -pseudospectral abscissa, i.e. the real part of a rightmost point of the  $\varepsilon$ -pseudospectrum of a certain linear operator. The fixed points of the iteration are characterized, local linear convergence of the algorithm for small enough  $\varepsilon$  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 effectiveness 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 Guglielmi 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  $\ell_1$  or  $\ell_2$  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  $\lambda_1$  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  $\epsilon$ -pseudospectral abscissa, i.e. the real part of the rightmost point in the  $\epsilon$ -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  $\epsilon$ , 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 sparses 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  $O(n^2)$  time with  $O(n)$  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  $2 \times 2$  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  $O(n)$  per iteration (and  $O(n^2)$  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-lyke 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 cancellation 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  $\Gamma$ . 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  $\Gamma$ . From the operator theory point of view, the perturbed Laplacians are identified with the so-called discrete Schrödinger operators of the network  $\Gamma$ . Our main objective is the study of positive semi-definite Schrödinger 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 Biyikoğlu.

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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)  $XDX - AX - XB + C = 0$  has a unique minimal nonnegative solution  $\Phi$ . 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  $\Phi$ , unlike the existing perturbation theory for (general) Algebraic Riccati Equations.
- an efficient Alternating-Directional Doubling Algorithm (ADDA) that can compute such a solution  $\Phi$  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  $\Omega$ . 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 Bagle” 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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**CP 1. Polynomial equations I****Talk 1. Solving multivariate vector polynomial interpolation problems**

The aim of this talk is to present an algorithm for computing a generating set for all multivariate polynomial vectors  $(g_1(\mathbf{z}), g_2(\mathbf{z}), \dots, g_m(\mathbf{z}))^T$  that satisfy the following homogeneous interpolation conditions:

$p_{k1}g_1(\omega_k) + p_{k2}g_2(\omega_k) + \dots + p_{km}g_m(\omega_k) = 0$  for all  $1 \leq k \leq l$ , where  $\omega_k$  are multivariate interpolation points with corresponding interpolation data  $p_{kj}$ . Moreover, we are interested in solutions having a specific degree structure. The algorithm will be constructed in such a way that it is easy to extract such solutions. At the same time we also look at different ways of ordering the monomials of multivariate polynomials, in order to obtain more specific information about the degree structure of our solution module. It will turn out that under certain conditions the generating set of the solution module constructed by the algorithm will form a Gröbner basis.

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**Talk 2. A general condition number for polynomial evaluation**

In this talk we present a new expression of the condition number for polynomial evaluation valid for any polynomial basis obtained from a linear recurrence. This expression extends the classical one for the power and Bernstein bases, providing a general framework for all the families of orthogonal polynomials. The use of this condition number permits to give a general theorem about the forward error in the evaluation of finite series in any of these polynomial bases by means of the extended Clenshaw algorithm. A running-error bound is also presented and all the bounds are compared in several numerical examples.

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**Talk 3. The geometry of multivariate polynomial division and elimination**

Multivariate polynomials are usually discussed in the framework of algebraic geometry. Solving problems in algebraic geometry usually involves the use of a Gröbner basis. This talk will show that linear algebra without any Gröbner basis computation suffices to solve basic problems from algebraic geometry by

describing three operations: multiplication, division and elimination. This linear algebra framework will also allow us to give a geometric interpretation. Division will involve oblique projections and a link between elimination and principal angles between subspaces (CS decomposition) will be revealed. The main computations in this framework are the QR and Singular Value Decomposition of sparse structured matrices.

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**Talk 4. Characterization and construction of classical orthogonal polynomials using a matrix approach**

We identify a polynomial sequence

$u_n(x) = a_{n,0} + a_{n,1}x + \dots + a_{n,n}x^n$  with the infinite lower triangular matrix  $[a_{n,k}]$ . Using such matrices we obtain basic properties of orthogonal sequences such as the representation as characteristic polynomials of tri-diagonal matrices and the 3-term recurrence relation  $u_{n+1}(x) = (x - \beta_n)u_n(x) - \alpha_n u_{n-1}(x)$ . Then we characterize the classical orthogonal sequences as those that satisfy the equation  $(5v + w)\alpha_2 = (v + 2w)(v^2 + \alpha_1)$ , where  $v = \beta_1 - \beta_0$ ,  $w = \beta_2 - \beta_1$ ,  $\alpha_1 > 0$ ,  $\alpha_2 > 0$ , and also give certain pair of diagonals equal to zero in a matrix constructed from  $[a_{n,k}]$ . For each choice of the parameters  $v, w, \alpha_1$ , we find explicit expressions for all the  $\alpha_k, \beta_k$ . In the case  $v = w = 0$  we obtain a one-parameter family of classical orthogonal sequences that includes the Chebyshev, Legendre, and Hermite sequences and also contains the sequence of derivatives of each of its elements. Our matrix methods can be used to study other classes of orthogonal sequences.

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**CP 2. Structured matrices I****Talk 1. Determinants and inverses of circulant matrices with Jacobsthal and Jacobsthal-Lucas numbers**

Let  $\mathbb{J}_n := \text{circ}(J_1, J_2, \dots, J_n)$  and  $\mathbb{J}_n := \text{circ}(j_0, j_1, \dots, j_{n-1})$  be the  $n \times n$  circulant matrices ( $n \geq 3$ ) whose elements are Jacobsthal and Jacobsthal-Lucas numbers, respectively. The determinants of  $\mathbb{J}_n$  and  $\mathbb{J}_n$  are obtained in terms of  $J_n$  and  $j_n$ , respectively. These imply that  $\mathbb{J}_n$  and  $\mathbb{J}_n$  are invertible. We also derive the inverses of  $\mathbb{J}_n$  and  $\mathbb{J}_n$ .

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**Talk 2. Determinants and inverses of circulant matrices with**

### Pell and Pell-Lucas numbers

In this talk, we define two  $n$ -square circulant matrices whose elements are Pell and Pell-Lucas numbers in the following form

$$\mathcal{P}_n = \begin{pmatrix} P_1 & P_2 & \cdots & P_{n-1} & P_n \\ P_n & P_1 & \cdots & P_{n-2} & P_{n-1} \\ P_{n-1} & P_n & \cdots & P_{n-3} & P_{n-2} \\ \vdots & \vdots & & \vdots & \vdots \\ P_2 & P_3 & \cdots & P_n & P_1 \end{pmatrix}$$

and

$$\mathfrak{P}_n = \begin{pmatrix} Q_1 & Q_2 & \cdots & Q_{n-1} & Q_n \\ Q_n & Q_1 & \cdots & Q_{n-2} & Q_{n-1} \\ Q_{n-1} & Q_n & \cdots & Q_{n-3} & Q_{n-2} \\ \vdots & \vdots & & \vdots & \vdots \\ Q_2 & Q_3 & \cdots & Q_n & Q_1 \end{pmatrix}$$

where  $P_n$  is the  $n$ th Pell number and  $Q_n$  is the  $n$ th Pell-Lucas number. Then we compute determinants of the matrices. We also obtain formulas which give elements of inverse of the matrices.

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### Talk 3. Eigenproblem for circulant and Hankel matrices in extremal algebra

Eigenvectors of circulant and Hankel matrices in fuzzy (max-min) algebra are studied. Both types of matrices are determined by vector of inputs in the first row. Investigation of eigenvectors in max-min algebra is important for applications connected with reliability of complex systems, with fuzzy relations and further questions. Many real systems can be represented by matrices of special form. Description of the eigenproblem for the above special types of matrices is important because for special types of matrices the computation can often be performed in a simpler way than in the general case.

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### Talk 4. Inverses of generalized Hessenberg matrices

Some constructive methods are proposed for the inversion of a generalized (upper) Hessenberg matrix (with subdiagonal rank  $\leq 1$ )  $A \in GL(n, K)$ , see e.g. L. Elsner, *Linear Algebra Appl.* 409 (2005) pp. 147-152, where a general structure theorem for such matrices was provided. They are based in its related Hessenberg-like matrix  $B = A(2:n, 1:n-1)$ . If  $B$  is also a generator representable matrix, i.e.  $a_{n,1} \neq 0$ , the form  $A^{-1} = U^{-1} + YX^T$  is easily obtained using the Sherman-Morrison-Woodbury formula. When  $B$  is strictly nonsingular, an inverse factorization  $A^{-1} = H_L H_U$ , based on Hessenberg matrices, is provided. Concerns about the remaining general situation are also outlined.

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### CP 3. Matrix factorization

#### Talk 1. Modified symplectic Gram-Schmidt process is mathematically and numerically equivalent to Householder SR algorithm

In this talk, we present two new and important results. The first is that the SR factorization of a matrix  $A$  via the modified symplectic Gram-Schmidt (MSGs) algorithm is mathematically equivalent to Householder SR algorithm applied to an embedded matrix obtained from  $A$  by adding two blocks of zeros in the top of the first half and in the top of the second half of the matrix  $A$ . The second result is that MSGs is also numerically equivalent to Householder SR algorithm applied the mentioned embedded matrix. The later algorithm is a Householder QR-like algorithm, based on some specified elementary symplectic transformations which are rank-one modification of the identity. Numerical experiments will be given.

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#### Talk 2. A multi-window approach to deflation in the QR algorithm

Aggressive Early Deflation significantly improved the performance of Francis' QR algorithm by identifying deflations in matrices 'close to' the Hessenberg iterate (see The Multishift QR Algorithm. Part II. Aggressive Early Deflation. Braman, Byers and Mathias. *SIAM J. Matrix Anal. Appl.*, 23(4):948-973, 2002). The perturbations used in AED focused on a 'deflation window' which was a trailing principal submatrix. Recently, this idea has been extended to investigate the effect of allowing simultaneous perturbations in more than one location. In this talk we present new results on this 'multi-window' approach and its effect on the performance of the QR algorithm.

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#### Talk 3. Aggregation of the compact WY representations generated by the TSQR algorithm

The TSQR (Tall-and-Skinny QR) algorithm is a parallel algorithm for the Householder QR decomposition proposed recently by Langou. Due to its large-grain parallelism, it can achieve high efficiency in both shared-memory and distributed-memory parallel environments. In this talk, we consider the situation where we first compute the QR decomposition of  $A \in \mathbf{R}^{m \times n}$  ( $m \gg n$ ) by the TSQR algorithm and then compute  $Q^T B$  for another matrix  $B \in \mathbf{R}^{m \times l}$ . We further assume that the first step is performed on a multicore processor with  $p$  cores, while the latter step is performed by an accelerator such as the GPU. In that case, the original TSQR algorithm may not be optimal, since the  $Q$  factor generated by the TSQR algorithm consists of many small Householder transformations or compact WY representations of length  $m/p$

and  $2n$ , and as a result, the vector length in the computation of  $Q^T B$  is shortened. To solve the problem, we propose a technique to aggregate the compact WY representations generated by the TSQR algorithm into one large compact-WY like representation. In this way, both the large-grain parallelism of the TSQR algorithm and the long vector length in the computation of  $Q^T B$  can be exploited. We show the effectiveness of our technique in a hybrid multicore-GPU environment.

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#### Talk 4. A generalized SVD for collections of matrices

The generalized SVD for a pair of matrices is a simultaneous diagonalization. Given matrices  $D_1$  ( $m_1 \times n$ ) and  $D_2$  ( $m_2 \times n$ ), it is possible to find orthogonal matrices  $U_1$  and  $U_2$  and a nonsingular  $X$  so that  $U_1^T D_1 X = \Sigma_1$  and  $U_2^T D_2 X = \Sigma_2$  are both diagonal. In our generalization, we are given matrices,  $D_1, \dots, D_N$  each of which has full column rank equal to  $n$ . By working implicitly (and carefully) with the eigensystem of the matrix  $\sum_{ij} (D_i^T D_i) (D_j^T D_j)^{-1}$  we are able to simultaneously “take apart” the  $D_i$  and discover common features. The new reduction reverts to the GSVD if  $N = 2$ .

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#### CP 4. Krylov methods

**Talk 1. Fixed-point Lanczos with analytical variable bounds**  
We consider the problem of establishing analytical bounds on all variables calculated during the symmetric Lanczos process with the objective of enabling fixed-point implementations with no overflow. Current techniques fail to provide practical bounds for nonlinear recursive algorithms. We employ a diagonal preconditioner to control the range of all variables, regardless of the condition number of the original matrix. Linear algebra techniques are used to prove the proposed bounds. It is shown that the resulting fixed-point implementations can lead to similar numerical behaviour as with double precision floating-point while providing very significant performance improvements in custom hardware implementations.

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#### Talk 2. An Arnoldi-based method for model order reduction of delay system

For large scale time-delay systems, Michiels, Jarlebring, and Meerbergen gave an efficient Arnoldi-based model order reduction method. To reduce the order from  $n$  to  $k$ , their method needs  $nk^2/2$  memory. In this talk, we propose a new implementation for the Arnoldi process, which is numerical stable and needs only  $nk$  memory.

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#### Talk 3. The Laurent-Arnoldi process, Laurent interpolation, and an application to the approximation of matrix functions

The Laurent-Arnoldi process is an analog of the standard Arnoldi process applied to the extended Krylov subspace. It produces an orthogonal basis for the subspace along with a generalized Hessenberg matrix whose entries consist of the recursion coefficients. As in the standard case, the application of the process to certain types of linear operators results in recursion formulas with few terms. One instance of this occurs when the operator is isometric. In this case, the recursion matrix is the pentadiagonal CMV matrix and the Laurent-Arnoldi process essentially reduces to the isometric Arnoldi process in which the underlying measures differ only by a rotation in the complex plane. The other instance occurs when the operator is Hermitian. This case produces an analog of the Lanczos process where, analogous to the CMV matrix, the recursion matrix is pentadiagonal. The Laurent polynomials generated by the recursion coefficients have properties similar to those of the Lanczos polynomials. We discuss the interpolating properties of these polynomials in order to determine remainder terms for rational Gauss and Radau rules. We then apply our results to the approximation of matrix functions and functionals.

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#### Talk 4. On worst-case GMRES

Let a nonsingular matrix  $A$  be given. By maximizing the GMRES residual norm at step  $k$  over all right hand sides from the unit sphere we get an approximation problem called the *worst-case GMRES problem*. In this contribution we concentrate on characterization of this problem. In particular, we will show that worst-case starting vectors satisfy the so called cross-equality and that they are always right singular vectors of the matrix  $p_k(A)$  where  $p_k$  is the corresponding worst-case GMRES polynomial. While the ideal GMRES polynomial is always unique, we will show that a worst-case GMRES polynomial needs not be unique.

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### CP 5. Control systems I

#### Talk 1. Structured perturbation of a controllable pair

We study the variation of the controllability indices of a pair  $(A, B) = (A, [B_1 \ b]) \in \mathbb{C}^{n \times n} \times \mathbb{C}^{n \times (m_1+1)}$ , where  $(A, B_1)$  is controllable, when we make small additive perturbations on the last column of  $B$ . Namely, we look for necessary conditions that must be satisfied by the controllability indices of  $(A, [B_1 \ b'])$  where  $b'$  is sufficiently close to  $b$ .

On the other hand, if  $\varepsilon$  is a sufficiently small real number, we look for (necessary and sufficient) conditions that must be satisfied by a partition in order to be the partition of the controllability indices (or, equivalently, those of Brunovsky) of  $(A, [B_1 \ b'])$  for some  $b'$  such that  $\|b' - b\| < \varepsilon$ . These problems can be considered as perturbation problems as well as completion problems, since one part of the matrix remains fixed. Because of this, we talk about structured perturbation.

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#### Talk 2. Reduction to miniversal deformations of families of bilinear systems

Bilinear systems under similarity equivalence are considered. Using Arnold technique a versal deformation of a differentiable family of bilinear systems is derived from the tangent space and orthogonal bases for a normal space to the orbits of similar equivalent bilinear systems. Versal deformations provide a special parametrization of bilinear systems space, which can be applied to perturbation analysis and investigation of complicated objects like singularities and bifurcations in multi-parameter bilinear systems.

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#### Talk 3. Matrix stratifications in control applications

In this talk, we illustrate how the software tool StratiGraph can be used to compute and visualize the closure hierarchy graphs associated with different orbit and bundle stratifications. The stratification provides the user with qualitative information of a dynamical system like how the dynamics of the control problem and its system characteristics behave under perturbations. We investigate linearized models of mechanical systems which

can be represented by a linear time-invariant (LTI) system. We also analyze dynamical systems described by linear time-invariant differential-algebraic sets of equations (DAEs), which often are expressed as descriptor models.

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**Talk 4. Stratification of structured pencils and related topics**  
 In this talk we present new results on stratifications (i.e., constructing closure hierarchies) of structured pencil orbits under congruence transformations:  $O(A, B) = \{S^T(A, B)S \text{ s.t. } \det S \neq 0, \text{ and } A, B \text{ are symmetric or skew symmetric matrices}\}$ . We use the canonical forms given by Thompson [Linear Algebra Appl. 147(1991), 323–371] as the representatives of the orbits. In particular, miniversal deformations are derived and codimensions of the orbits are computed by solving associated systems of matrix equations (codimensions can also be calculated from the miniversal deformations). One goal is to reduce the stratifications of structured pencils under congruence transformations to the well studied and solved problems for stratifications of matrix pencils.

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### CP 6. Preconditioning I

**Talk 1. Memory optimization to build a Schur complement**  
 One promising algorithm for solving linear system is the hybrid method based on domain decomposition and Schur complement (used by HIPS and MAPHYS for instance).

In this method, a direct solver is used as a subroutine on each subdomain matrix; unfortunately, these calls are subject to serious memory overhead. With our improvements, the direct solver PASTIX can easily scale in terms of performances with several nodes composed of multicore chips and forthcoming GPU accelerators, and the memory peak due to Schur complement computation can be reduce by 10% to 30%.

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**Talk 2. On generalized inverses in solving two-by-two block linear systems**

The goal is to analyze a role of generalized inverses in the projected Schur complement based algorithm for solving nonsymmetric two-by-two block linear systems. The outer level of the algorithm combines the Schur complement reduction with the null-space method in order to treat the singularity of the (1,1)-block. The inner level uses a projected variant of the Krylov subspace method. We prove that the inner level is invariant to the choice of a generalized inverse to the (1,1)-block so that each generalized inverse is internally adapted to the More-Penrose one. The algorithm extends ideas used in the background of the FETI domain decomposition methods. Numerical experiments confirm the theoretical results.

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### Talk 3. Sparse direct solver on top of large-scale multicore systems with GPU accelerators

In numerical simulations, solving large sparse linear systems is a crucial and time-consuming step. Many parallel factorization techniques have been studied. In PASTIX solver, we developed a dynamic scheduling for strongly hierarchical modern architectures. Recently, we evaluated how to replace this scheduler by generic frameworks (DAGUE or STARPU) to execute the factorization tasks graph. Since sparse direct solvers are built with dense linear algebra kernels, we are implementing prototype versions of solvers on top of PLASMA and MAGMA libraries. We aim at designing algorithms and parallel programming models to implement direct methods on GPU-equipped computers.

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### Talk 4. New block distributed Schur complement preconditioners for CFD simulation on many-core architectures

At the German Aerospace Center, the parallel simulation systems TAU and TRACE have been developed for the aerodynamic design of aircrafts or turbines for jet engines. For the parallel iterative solution of large, sparse real or complex systems of linear equations, required for both CFD solvers, block-local preconditioners are compared with reformulated global block Distributed Schur Complement (DSC) preconditioning methods. Numerical, performance and scalability results of block DSC preconditioned FGMRes algorithms are presented for typical TAU and TRACE problems on many-core systems together with an analysis of the advantages of using block compressed sparse matrix data formats.

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### CP 7. Least squares

#### Talk 1. Partially linear modeling combining least squares support vector machines and sparse linear regression

In this talk we propose an algorithm to efficiently solve a partially linear optimization problem in which the linear relation will be sparse and the non-linear relation will be non-sparse. The sparsity in the linear relation will be obtained by punishing the complexity of the corresponding weight vector similarly as in LASSO or group LASSO. The non-linear relation is kernel-based and its complexity is punished similarly as in Least Squares Support Vector Machines (LS-SVM). To solve the optimization problem we eliminate the non-linear relation using a Singular Value Decomposition. The remaining optimization problem can be solved using existing solvers.

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#### Talk 2. Construction of test instances with prescribed properties for sparsity problems

For benchmarking algorithms solving

$$\min \|x\|_1 \text{ subject to } Ax = b,$$

it is desirable to create test instances containing a matrix  $A$ , a right side  $b$  and a known solution  $\tilde{x}$ . To guarantee the existence of a solution with prescribed sign pattern, the existence of a dual certificate  $w$  satisfying  $A^T w \in \partial \|\tilde{x}\|_1$  is necessary and sufficient. As used in the software package L1TestPack, alternating projections calculate a dual certificate with least squares on the complement of the support of  $\tilde{x}$ . In this talk, we present strategies to construct test instances with different additional properties such as a maximal support size or favorable dual certificate.

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#### Talk 3. Weighted total least-squares collocation with geodetic applications

The Total Least-Squares (TLS) approach to Errors-In-Variables Models is well established, even in the case of correlation among the observations, and among the elements of the coefficient matrix, as long as the two are not cross-correlated. Adding stochastic prior information transforms the fixed parameter vector into a random effects vector to be predicted rather than

estimated. Recently, Schaffrin found a TLS solution for this case, if the data were assumed iid. Here, this assumption is dropped, leading to a technique that is perhaps best called Weighted Total-Least Squares Collocation. A fairly general algorithm will be presented along with an application.

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#### Talk 4. Polynomial regression in the Bernstein basis

One important problem in statistics consists of determining the relationship between a response variable and a single predictor variable through a regression function. In this talk we consider the problem of linear regression when the regression function is an algebraic polynomial of degree less than or equal to  $n$ . The coefficient matrix  $A$  of the overdetermined linear system to be solved in the least squares sense usually is an ill-conditioned matrix, which leads to a loss of accuracy in the solution of the corresponding normal equations.

If the monomial basis is used for the space of polynomials  $A$  is a rectangular Vandermonde matrix, while if the Bernstein basis is used then  $A$  is a rectangular Bernstein-Vandermonde matrix. Under certain conditions both classes of matrices are totally positive, and this can advantageously be used in the construction of algorithms based on the  $QR$  decomposition of  $A$ .

In the talk, the advantage of using the Bernstein basis is to be shown.

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#### CP 8. Miscellaneous I

#### Talk 1. Reduced basis modeling for parametrized systems of Maxwell's equations

The Reduced Basis Method generates low-order models to parametrized PDEs to allow for efficient evaluation of parametrized models in many-query and real-time contexts. We apply the Reduced Basis Method to systems of Maxwell's equations arising from electrical circuits. Using microstrip models, the input-output behaviour of interconnect structures is approximated with low order reduced basis models for a parametrized geometry, like distance between microstrips and/or material coefficients, like permittivity and permeability of substrates.

We show the theoretical framework in which the Reduced Basis Method is applied to Maxwell's equations and present first numerical results.

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#### Talk 2. A new alternative to the tensor product in wavelet construction

Tensor product has been a predominant method in constructing multivariate biorthogonal wavelet systems. An important feature of tensor product is to transform univariate refinement filters to multivariate ones so that biorthogonality of the univariate refinement filters is preserved. In this talk, we introduce an alternative transformation, to which we refer as Coset Sum, of tensor product. In addition to preserving biorthogonality of univariate refinement filters, Coset Sum shares many other essential features of tensor product that make it attractive in practice. Furthermore, Coset Sum can even provide wavelet systems whose algorithms are faster than the ones based on tensor product.

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#### Talk 3. Purely algebraic domain decomposition methods for incompressible Navier-Stokes equation

In the context of domain decomposition methods, an algebraic approximation of the transmission condition (TC) is proposed in “F. X. Roux, F. Magoules, L. Series. Y. Boubendir, Algebraic approximations of Dirichlet-to-Neumann maps for the equations of linear elasticity, *Comput. Methods Appl. Mech. Engrg.*, 195, 3742-3759, 2006”. For the case of non overlapping domains, approximations of the TCs are analogous to the approximation of the Schur complements (SC) in the incomplete block factorization. The basic idea is to approximate the SC by a small SC approximations in patches. The computation of these local transmissions are constructed independently, thus enhancing the parallelism in the overall approximation.

In this work, a new computation of local Schur complement is proposed and the method is tested on steady state incompressible Navier-Stokes problems discretized using finite element method. The earlier attempts used in the literature approximate the TC by building small patches around each node. The method is generalized by aggregating the nodes and thus reducing the overlapping computation of local TCs. Moreover, the approach of aggregating the nodes is based on the “numbering” of the nodes rather than on the “edge connectivity” between the nodes as previously done in the reference above.

With the new aggregation scheme, the construction time is significantly less. Furthermore, the new aggregation based approximation leads to a completely parallel solve phase. The new method is tested on the difficult cavity problem with high reynolds number on uniform and stretched grid. The parallelism of the new method is also discussed.

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#### Talk 4. On specific stability bounds for linear multiresolution schemes based on biorthogonal wavelets

Some Biorthogonal bases of compactly supported wavelets can be considered as a cell-average prediction scheme within Harten's framework. In this paper we express the Biorthogonal

prediction operator as a combination of some finite differences. Through a detailed analysis of certain contractivity properties, we arrive at specific stability bounds for the multiresolution transform. A variety of tests indicate that these bounds are close to numerical estimates.

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#### CP 9. Eigenvalue problems I

##### Talk 1. Incremental methods for computing extreme singular subspaces

The oft-described family of low-rank incremental SVD methods approximate the truncated singular value decomposition of a matrix  $A$  via a single, efficient pass through the matrix. These methods can be adapted to compute the singular triplets associated with either the largest or smallest singular values. Recent work identifies a relationship with an optimizing eigensolver over  $A^T A$  and presents multi-pass iterations which are provably convergent to the targeted singular triplets. We will discuss these results, and provide additional analysis, including circumstances under which the singular triplets are exactly computed via a single pass through the matrix.

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##### Talk 2. An efficient implementation of the shifted subspace iteration method for sparse generalized eigenproblems

We revisit the subspace iteration (SI) method for symmetric generalized eigenvalue problems in the context of improving an existing solver in a commercial structural analysis package. A new subspace algorithm is developed that increases the efficiency of the naïve SI by means of novel shifting techniques and locking. Reliability of results is ensured using stronger convergence criterion and various control parameters are exposed to the end user. The algorithm is implemented in software using the C++ library ‘Eigen’. Results are presented and we end with an introduction to a new, communication reducing method for sparse matrix-vector multiplication that we envisage will increase efficiency further.

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#### Talk 3. Recursive approximation of the dominant eigenspace of an indefinite matrix

We consider here the problem of tracking the dominant eigenspace of an indefinite matrix by updating and downsizing recursively a low rank approximation of the given matrix. The tracking uses a window of the given matrix, which is adapted at every step of the algorithm. This increases the rank of the approximation, and hence requires a rank reduction of the approximation. In order to perform the window adaptation and the rank reduction in an efficient manner, we make use of a new anti-triangular decomposition for indefinite matrices. All steps of the algorithm only make use of orthogonal transformations, which guarantees the stability of the intermediate steps.

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#### Talk 4. Jacobi-Davidson type methods using a shift invariance property of Krylov subspaces for eigenvalue problems

The Jacobi-Davidson method is a subspace method for a few eigenpairs of a large sparse matrix. In the method, one has to solve a nonlinear equation, the so-called correction equation, to generate subspaces. The correction equation is approximately solved after a linearization that corresponds to replacing a desired eigenvalue with its approximation. In this talk, we focus on the nonlinear correction equation. Here, a Krylov subspace is generated, not only to compute approximate eigenvalues which lead to a class of linearized correction equations, but also to solve the linearized correction equations. Our approach reproduces the Jacobi-Davidson method and the Riccati method, and derives new efficient variants.

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#### CP 10. Miscellaneous II

##### Talk 1. Phylogenetic trees via latent semantic indexing

In this talk we discuss a technique for constructing phylogenetic trees from a set of whole genome sequences. The method does not use local sequence alignments but is instead based on latent semantic indexing, which involves a reduction of dimension via the singular value decomposition of a very large polypeptide-by-genome frequency matrix. Distance measures between species are then obtained. These are used to generate a phylogenetic tree relating the species under consideration.

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### Talk 2. Synchronization of rotations via Riemannian trust-regions

We estimate unknown rotation matrices  $R_i \in \text{SO}(n = 2, 3)$  from a set of measurements of relative rotations  $R_i R_j^T$ . Each measurement is either slightly noisy, or an outlier bearing no information. We study the case where most measurements are outliers. In (A. Singer, *Angular Synchronization by Eigenvectors and Semidefinite Programming*, ACHA 30(1), pp. 20–36, 2011), an estimator is computed from a dominant subspace of a matrix. We observe this essentially results in least-squares estimation, and propose instead a Maximum Likelihood Estimator, explicitly acknowledging outliers. We compute the MLE via trust-region optimization on a matrix manifold. Comparison of our estimator with Riemannian Cramér-Rao bounds suggests efficiency.

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### CP 11. Miscellaneous III

#### Talk 1. A new multi-way array decomposition

This talk draws a new perspective on multilinear algebra and the multi-way array decomposition. A novel decomposition technique based on Enhanced Multivariate Product Representation (EMPR) is introduced. EMPR is a derivative of High Dimensional Model Representation (HDMR), which is a divide-and-conquer algorithm. The proposed technique provides a decomposition by rewriting multi-way arrays in a form that consists of outer products of certain support vectors. Each support vector corresponds to a different subspace of the original multi-way array. Such an approach can improve the semantic meaning of the decomposition by eliminating rank considerations. Compression of animations is performed as an initial experimental evaluation.

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#### Talk 2. Towards more reliable performances of accurate floating-point summation algorithms

Several accurate algorithms to sum IEEE-754 floating point numbers have been recently published, *e.g.* Rump-Ogita-Oishi (2008, 2009), Zhu-Hayes (2009, 2010). Since some of these actually compute the correct rounding of the exact sum, run-time and memory performances become the discriminant property to decide which one to choose. In this talk we focus the difficult problem of presenting reliable measures of the run-time performances of such core algorithms. We present an almost machine independent analysis based on the instruction-level

parallelism of the algorithm. Our PerPI software tool automatizes this analysis and provides a more reliable performance analysis.

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### CP 12. Matrix norms

#### Talk 1. Numerical solutions of singular linear matrix differential equations

The main objective of this talk is to provide a procedure for discretizing an initial value problem of a class of linear matrix differential equations whose coefficients are square constant matrices and the matrix coefficient of the highest-order derivative is degenerate. By using matrix pencil theory, first we give necessary and sufficient conditions to obtain a unique solution for the continuous time model. After by assuming that the input vector changes only at equally space sampling instants we shall derive the corresponding discrete time state equation which yield the values of the solutions of the continuous time model.

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#### Talk 2. Matrix version of Bohr's inequality

The classical Bohr's inequality states that for any  $z, w \in \mathbb{C}$  and for  $p, q > 1$  with  $\frac{1}{p} + \frac{1}{q} = 1$ ,

$$|z + w|^2 \leq p|z|^2 + q|w|^2$$

with equality if and only if  $w = (p - 1)z$ . Several operator generalizations of the Bohr inequality have been obtained by some authors. Vasić and Kečkić, (Math. Balkanica, 1(1971) 282–286), gave an interesting generalization of the inequality of the following form

$$\left| \sum_{j=1}^m z_j \right|^r \leq \left( \sum_{j=1}^m p_j^{\frac{1}{1-r}} \right)^{r-1} \sum_{j=1}^m p_j |z_j|^r,$$

where  $z_j \in \mathbb{C}$ ,  $p_j > 0$ ,  $r > 1$ .

In this talk we aim to give weak majorization inequalities for matrices and apply it to prove eigenvalue extension of the result by Vasić and Kečkić and unitarily norm extensions.

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### CP 13. Code theory

#### Talk 1. Linear codes in LRTJ spaces

In [S. Jain, *Array Codes in the Generalized-Lee-RT-Pseudo-Metric (the GLRTP-Metric)*, to appear in Algebra Colloquium.], Jain introduced a new metric viz. LRTJ-metric on the space  $\text{Mat}_{m \times s}(\mathbf{Z}_q)$ , the module space of all  $m \times s$  matrices with entries from the finite ring  $\mathbf{Z}_q$  ( $q \geq 2$ ) generalizing the classical one dimensional Lee metric [C. Y. Lee, *Some properties of non-binary error correcting codes*, IEEE Trans. Information Theory, IT-4 (1958), 77–82] and the two-dimensional RT-metric [M.Yu. Rosenbloom and M.A.

Tsfasman, *Codes for m-metric*, Problems of Information Transmission, 33 (1997), 45-52] which further appeared in [E. Deza and M.M. Deza, Encyclopedia of Distances, Elsevier, 2008, p.270]. In this talk, we discuss error control techniques viz. error detection and error correction in linear codes equipped with LRTJ-metric in communication channels[S. Jain, *Array Codes in the Generalized-Lee-RT-Pseudo-Metric (the GLRTP-Metric)*, to appear in Algebra Colloquium]. We further discuss various properties of the dual code of an LRTJ code and obtain the relation for the complete weight enumerator of the dual code of an array code in LRTJ spaces in the form of MacWilliams duality relations[S. Jain, *MacWilliams Duality in LRTJ-Spaces*, to appear in Ars Combinatoria].

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#### **Talk 2. On turbo codes of rate $1/n$ from linear systems point of view**

Turbo codes were introduced by Berrou, Glavieux and Thitimajshima in 1993. Their idea of using parallel concatenation of recursive systematic convolutional codes with an interleaver was a major step in terms of achieving low bit error rates at signal to noise ratios near the Shannon limit. One of the most important parameter of turbo codes is the effective free distance, introduced by Berrou and Montorsi. It plays a role similar to that of the free distance for convolutional codes. Campillo, Devesa, Herranz and Perea developed turbo codes in the framework of the input-state-output representation for convolutional codes. In this talk, using this representation, we present conditions for a turbo code with rate  $1/n$  in order to achieve maximum effective free distance.

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#### **CP 14. Iterative methods II**

##### **Talk 1. Meshless method for steady Burgers' equation: a matrix equation approach**

In this talk we present some numerical linear algebra methods to solve a Burgers equations. A meshless method based on thin plate splines is applied to a non homogeneous steady Burgers' equation with Dirichlet boundary condition. The numerical approximation of the solution leads to a large-scale nonlinear matrix equation. In order to implement the inexact Newton algorithm to solve this equation, we focus ourselves on the jacobian matrix related to this method and establish some interesting matrix relations. The obtained linear matrix equation

will be solved using a global GMRES method. Numerical examples will be given to illustrate our method.

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#### **Talk 2. Tuned preconditioners for inexact two-sided inverse and Rayleigh quotient iteration**

We consider two-sided inner-outer iterative methods based on inverse and Rayleigh quotient iteration for the numerical solution of non-normal eigenvalue problems. There, in each outer iterations two adjoint linear systems have to be solved, but it is often sufficient to solve these systems inexactly and still preserve the fast convergence of the original exact algorithm. This can, e.g., be accomplished by applying a limited number of steps of a Krylov subspace method for linear systems. To reduce the number of these inner iterations, preconditioners are usually applied. In the one-sided case it is even possible to keep the number of inner iterations almost constant during the course of the inner-outer method by applying so called tuned preconditioners. We investigate how these ideas can be carried over to the two-sided case. A special interest there is the simultaneous solution of the occurring adjoint linear systems using methods based on the two-sided Lanczos process, e.g., BiCG and QMR.

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#### **CP 15. Polynomial equations II**

##### **Talk 1. Standard triples of structured matrix polynomials**

The notion of standard triples plays a central role in the theory of matrix polynomials. We study such triples for matrix polynomials  $P(\lambda)$  with structure  $\mathcal{S}$ , where  $\mathcal{S}$  is the Hermitian, symmetric, adj-even, adj-odd, adj-palindromic or adj-antipalindromic structure (with  $\text{adj} = *, T$ ). We introduce the notion of  $\mathcal{S}$ -structured standard triple. With the exception of  $T$ -(anti)palindromic matrix polynomials of even degree with both  $-1$  and  $1$  as eigenvalues, we show that  $P(\lambda)$  has structure  $\mathcal{S}$  if and only if  $P(\lambda)$  admits an  $\mathcal{S}$ -structured standard triple, and moreover that every standard triple of a matrix polynomial with structure  $\mathcal{S}$  is  $\mathcal{S}$ -structured. We investigate the important special case of  $\mathcal{S}$ -structured Jordan triples.

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### Talk 2. Solving systems of polynomial equations using (numerical) linear algebra

Solving multivariate polynomial equations is central in optimization theory, systems and control theory, statistics, and several other sciences. The task is phrased as a (numerical) linear algebra problem involving a large sparse matrix containing the coefficients of the polynomials. Two approaches to retrieve all solutions are discussed: In the nullspace-based algorithm an eigenvalue problem is obtained by applying realization theory to the nullspace of the coefficient matrix. Secondly in the data-driven approach one operates directly on the coefficient matrix and solves linear equations using the QR-decomposition yielding an eigenvalue problem in the triangular factor R. Ideas are developed on the levels of geometry (e.g., column/row spaces, orthogonality), numerical linear algebra (e.g., Gram-Schmidt orthogonalization, ranks) and algorithms (e.g., sparse nullspace computations, power method).

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### CP 16. Matrices and algebraic structures

#### Talk 1. Determinantal range and Frobenius endomorphisms

For  $A, C \in M_n$  the set

$W_C(A) = \{Tr(AUCU^*) : UU^* = I_n\}$  is the  $C$ -numerical range of  $A$  and it reduces to the classical numerical range, when  $C$  is a rank one Hermitian orthogonal projection. A variation of  $W_C(A)$  is the  $C$ -determinantal range of  $A$ , that is,  $\Delta_C(A) = \{\det(A - UCU^*) : UU^* = I_n\}$ . We present some properties of this set and characterize the additive Frobenius endomorphisms for the determinantal range on the whole matrix algebra  $M_n$  and on the set of Hermitian matrices  $H_n$ .

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#### Talk 2. On algorithms for constructing $(0, 1)$ -matrices with prescribed row and column sum vectors

Given partitions  $R$  and  $S$  with the same weight and  $S \preceq R^*$  let  $\mathcal{A}(R, S)$  be the class of the  $(0, 1)$ -matrices with row sum  $R$  and column sum  $S$ . These matrices play an active role in modern mathematics and the applications extend from their natural context (Matrix Theory, Combinatorics or Graph Theory) to many other areas of knowledge as Biology or Chemistry. The

Robinson-Schensted-Knuth correspondence establishes a bijection between the class  $\mathcal{A}(R, S)$  and pairs of Young tableaux with conjugate shape  $\lambda$  and  $\lambda^*$  with  $S \preceq \lambda \preceq R^*$ . We give a canonical construction for matrices in  $\mathcal{A}(R, S)$  whose insertion tableau has a prescribed shape  $\lambda$ , with  $S \preceq \lambda \preceq R^*$ . This algorithm generalizes some recent constructions due to R. Brualdi for the extremal cases  $\lambda = S$  and  $\lambda = R^*$ .

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#### Talk 3. Elementary matrices arising from unimodular rows

Let  $(R, \mathfrak{m})$  be a commutative local ring with maximal ideal  $\mathfrak{m}$ . Let  $A = R[X]$  be a  $R$ -algebra and  $f$  be a monic polynomial of  $R[X]$ . Assume that

1.  $A/fA$  is finitely generated  $R$ -module.
2.  $R(X)$  contains a subalgebra  $B$  such that  $R(X) = R[X] + B$  and  $\mathfrak{m}B \subset J(B)$  (the Jacobson radical of  $B$ ).
3.  $SL_r(K(X)) = E_r(K(X))$  for every  $r \geq 1$ , where  $K = R/m$ .
4.  $SL_n(R[X]) \cap E_n(R(X)) = E_n(R[X])$ .

Let  $F = (f_1, f_2, \dots, f_n)$  be a unimodular row in  $R[X]$  which can be completed to a matrix  $C_1$  belonging to  $E_n(R(X))$  and a matrix  $C_2$  belonging to  $E_n(K[X])$ . Then  $F$  can also be completed to a matrix belonging to  $E_n(R[X])$ .

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#### Talk 4. Nonsingular ACI-matrices over integral domains

An ACI-matrix is a matrix whose entries are polynomials of degree at most one in a number of indeterminates where no indeterminate appears in two different columns. Consider the next two problems: (a) characterize the ACI-matrices of order  $n$  all of whose completions have the same nonzero constant determinant; (b) characterize the ACI-matrices of order  $n$  all of whose completions are nonsingular. In 2010 Brualdi, Huang and Zhan solved both problems for fields of at least  $n + 1$  elements. We extend their result on problem (a) to integral domains, and extend their result on problem (b) to arbitrary fields.

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### CP 17. Lyapunov equations

#### Talk 1. Lyapunov matrix inequalities with solutions sharing a common Schur complement

The square matrices  $A_1, A_2, \dots, A_N$  are said to be stable with respect of the positive definite matrices  $P_1, \dots, P_N$  if the Lyapunov inequalities  $A_i^T P_i + P_i A_i < 0$ , with  $i = 1, \dots, N$ , are satisfied. In this case, the matrices  $P_i$  are called Lyapunov solutions for the matrices  $A_i$ , with  $i = 1, \dots, N$ , respectively. In this work, we investigate when the Lyapunov solutions  $P_i$  share the same Schur complement of certain order. The existence problem of a set of Lyapunov solutions sharing a common Schur complement arises, for instance, in the stabilization of a switched system, under arbitrary switching signal for which discontinuous jumps on some of the state components are allowed, during the switching instants.

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#### Talk 2. Solving large scale projected periodic Lyapunov equations using structure-exploiting methods

Simulation and analysis of periodic systems can demand to solve the projected periodic Lyapunov equations associated with those periodic systems, if the periodic systems are in descriptor forms. In this talk, we discuss the iterative solution of large scale sparse projected periodic discrete-time algebraic Lyapunov equations which arise in periodic state feedback problems and in model reduction of periodic descriptor systems. We extend the Smith method to solve the large scale projected periodic discrete-time algebraic Lyapunov equations in lifted form. The block diagonal structure of the periodic solution is preserved in every iteration steps. A low-rank version of this method is also presented, which can be used to compute low-rank approximations to the solutions of projected periodic discrete-time algebraic Lyapunov equations. Numerical results are given to illustrate the efficiency and accuracy of the proposed method.

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#### Talk 3. A new minimal residual method for large scale Lyapunov equations

The solution of large scale algebraic Lyapunov equations is important in the stability analysis of linear dynamical systems. We present a projection-based residual minimizing procedure for solving the Lyapunov equation. As opposed to earlier methods

(e.g., [I.M. Jiamouka and E.M. Kasenally, SIAM J. Numer. Anal., 1994]), our algorithm relies on an inner iterative solver, accompanied with a selection of preconditioning techniques that effectively exploit the structure of the problem. The residual minimization allows us to relax the coefficient matrix passivity constraint, which is sometimes hard to meet in real application problems. Numerical experiments with standard benchmark problems will be reported.

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#### Talk 4. Contributions to the analysis of the extended Krylov subspace method (EKSM) for Lyapunov matrix equations

The EKSM is an iterative method which can be used to approximate the solution of Lyapunov matrix equations and extract reduced order models of linear time invariant systems (LTIs). We explain why any positive residual curve is possible and we show how to construct LTIs for which the approximations of the Gramians returned by the EKSM are orthogonal in exact arithmetic. Finally, we build an electrical circuit for which the Gramians  $P$  and  $Q$  satisfy  $\text{fl}(P \text{ fl}(Qx)) = 0$ , where  $\text{fl}(x)$  denotes the floating point representation of  $x$ .

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### CP 18. Eigenvalue problems II

#### Talk 1. Differentials of eigenvalues and eigenvectors under nonstandard normalizations with applications

We propose a new approach to the identification of the change in eigenvalues and eigenvectors as a consequence of a perturbation applied to the eigenproblem. The approach has three differences with respect to most previous literature that allow for covering several intricate normalizations previously adopted and simplify the proofs. First, we start from the differentials, and not from the derivatives. Second, in our more general result, we explicitly consider two normalization functions, one for the right and one for the left eigenvector. Third, using complex differentials, we explicitly allow for nonanalytic normalization functions. Several applications are discussed in detail.

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#### Talk 2. A solution to the inverse eigenvalue problem for certain singular Hermitian matrices

We present the solution to Inverse Eigenvalue problem of certain singular Hermitian matrices by developing a method in the context of consistency conditions, for solving the direct

Eigenvalue problem for singular matrices. Based on this method, we propose an algorithm to reconstruct such matrices from their eigenvalues. That is, we develop algorithms and prove that they solve special  $2 \times 2$ ,  $3 \times 3$  and  $4 \times 4$  singular symmetric matrices. In each case, the number of independent matrix elements would reduce to the extent that there would be an isomorphism between the seed elements and the eigenvalues. We also initiate a differential geometry and, a numerical analytic interpretation of the Inverse Eigenvalue problem using fiber bundle with structure group  $O(n)$ . A simple and more practicable algorithm based on the Newtons iterative method would be developed to construct symmetric matrices using singular symmetric matrices as the initial matrices.

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### Talk 3. Divide and conquer the CS decomposition

The CS decomposition factors a unitary matrix into simpler components, revealing the principal angles between certain linear subspaces. We present a divide-and-conquer algorithm for the CS decomposition and the closely related generalized singular value decomposition. The method is inspired by the work of Gu and Eisenstat and others. Novel representations enforce orthogonality.

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### Talk 4. The optimal perturbation bounds of the Moore-Penrose inverse under the Frobenius norm

We obtain the optimal perturbation bounds of the Moore-Penrose inverse under the Frobenius norm by using Singular Value Decomposition, which improved the results in the earlier paper [P.-Å. Wedin, Perturbation theory for pseudo-inverses, BIT 13 (1973) 217-232]. In addition, a perturbation bound of the Moore-Penrose inverse under the Frobenius norm in the case of the multiplicative perturbation model is also given.

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### CP 19. Positivity I

#### Talk 1. Positivity preserving simulation of differential-algebraic equations

We discuss the discretization of differential-algebraic equations with the property of positivity, as they arise e.g. in chemical reaction kinetics or process engineering. For index-1 problems, in which the differential and algebraic equations are explicitly given, we present conditions for a positive numerical approximation that also meets the algebraic constraints. These results are extended to higher index problems, i.e., problems in which some algebraic equations are hidden in the system, by a

positivity preserving index reduction. This remodeling procedure filters out the hidden constraints without destroying the positivity property and admits to trace back these systems to the index-1 case.

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### Talk 2. Computing the exponentials of essentially nonnegative matrices with high relative accuracy

In this talk we present an entry-wise forward stable algorithm for computing the exponentials of essentially nonnegative matrices (Metzler matrices). The algorithm is a scaling-and-squaring approach built on Taylor expansion and non-diagonal Padé approximation. As an important feature, we also provide an entry-wise error estimate to the user. Both rounding error analysis and numerical experiments demonstrate the stability of the new algorithm.

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### Talk 3. Sparse and unique nonnegative matrix factorization through data preprocessing

Nonnegative matrix factorization (NMF) has become a very popular technique in data mining because it is able to extract meaningful features through a sparse and part-based representation. However, NMF has the drawback of being highly ill-posed and there typically exist many different but equivalent factorizations. In this talk, we introduce a preprocessing technique leading to more well-posed NMF problems whose solutions are sparser. It is based on the theory of M-matrices and the geometric interpretation of NMF, and requires to solving constrained linear least squares problems. We theoretically and experimentally demonstrate the effectiveness of our approach.

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### Talk 4. Iterative regularized solution of linear complementarity problems

For Linear Complementarity Problems (LCP) with a positive semidefinite matrix  $M$ , iterative solvers can be derived by a process of regularization. In [R. W. Cottle et al., The LCP, Academic Press, 1992] the initial LCP is replaced by a sequence of positive definite ones, with the matrices  $M + \alpha I$ . Here we analyse a generalization of this method where the identity  $I$  is replaced by a positive definite diagonal matrix  $D$ . We prove that the sequence of approximations so defined converges to the minimal  $D$ -norm solution of the initial LCP. This extension opens the possibility for interesting applications in the field of rigid multibody dynamics.

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## CP 20. Control systems II

### Talk 1. Disturbance decoupling problem for singular switched linear systems

In this paper, a geometric approach to disturbance decoupling problem for switched singular linear systems is made. A *switched singular linear system with disturbance* is a system which consists of several linear subsystems with disturbance and a piecewise constant map  $\sigma$  taking values into the index set  $M = \{1, \dots, \ell\}$  which indexes the different subsystems. In the continuous case, such a system can be mathematically described by  $E_\sigma \dot{x}(t) = A_\sigma x(t) + B_\sigma u(t) + G_\sigma g(t)$  where  $E_\sigma, A_\sigma \in M_n(\mathbb{R})$ ,  $B_\sigma \in M_{n \times m}(\mathbb{R})$ ,  $G_\sigma \in M_{n \times p}(C)$  and  $\dot{x} = dx/dt$ . The term  $g(t)$ ,  $t \geq 0$ , may represent modeling or measuring errors, noise, or higher order terms in linearization. In the case of standard state space systems the disturbance decoupling problem has been largely studied. The problem of constructing feedbacks that suppress this disturbance in the sense that  $g(t)$  does not affect the input-output behaviour of the switched singular linear system with disturbance is analyzed and a solvability condition for the problem is obtained using invariant subspaces for singular switched linear systems.

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### Talk 2. Invariant subspaces of switched linear systems

Invariant subspaces under a linear transformation were defined by von Neumann (1935) and generalized to linear dynamical systems: G. Basile and G. Marro (1969) defined the concept of controlled and conditioned invariant subspaces for control linear systems, I.M. Buzurovic (2000) studied (controlled and conditioned) invariant subspaces for singular linear systems. They are connected to a great number of disciplines, for example in the geometric study of control theory of linear time-invariant dynamical systems (in particular, controllability and observability). This notion was extended also to linear parameter-varying systems by introducing the concept of parameter-varying invariant subspaces. Recently, several authors such as A.A. Julius, A.J. van der Schaft, E. Yurtseven, W.P.M.H. Heemels, M.K. Çamlibel, among others, introduced invariant subspaces for switched linear systems (those containing any trajectory which originates on it) and applied them to different topics! , disturbance decoupling and observer design problems, for example. In this work we study properties and algorithms to determine the set of all invariant subspaces for a given switched linear system using linear algebra tools, providing a computational alternative to theoretical results.

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### Talk 3. On the pole placement problem for singular systems

Let us consider a singular system with outputs

$E\dot{x} = Ax + Bu$ ,  $y = Cx$ , with  $E, A \in F^{h \times n}$ ,  $B \in F^{h \times m}$ ,  $C \in F^{p \times n}$ . For  $r$  regular systems ( $E$  non singular), the pole assignment problem by state feedback, and by state feedback and output injection was solved a few decades ago. Recently, the pole assignment problem by state feedback has been solved for singular systems ( $E$  singular). We try to extend the solution to the pole assignment problem to singular systems by state feedback and output injection: Given a monic homogeneous polynomial  $f \in F[x, y]$ , we study the existence of a state feedback matrix  $F$  and an output injection  $K$  such that the state matrix  $sE - (A + BF + KC)$  has  $f$  as characteristic polynomial, under a regularizability condition on the system.

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### Talk 4. Coordination control of linear systems

Coordinated linear systems are particular hierarchical systems, characterized by conditional independence and invariance properties of the underlying linear spaces. Any distributed linear system can be transformed into a coordinated linear system, using observability decompositions. The motivation behind studying these systems is that some global control objectives can be achieved via local controllers: E.g., global stabilizability reduces to local stabilizability of all subsystems. The corresponding LQ problem separates into independent LQ problems on the lower level, and a more involved control problem on the higher level. For the latter problem, possible approaches include using subsystem observers, numerical optimization, and event-based feedback.

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## CP 21. Matrix pencils

### Talk 1. Looking at the complexity index as a matrix measure

In this paper we discuss a matrix measure based on a matrix norm. This measure, named complexity index, has been presented by Amaral et al., in 2007. In their study the authors consider that an economic system is represented by a square nonnegative matrix and their aim is to quantify complexity as

interdependence in an IO system. However for large dimension matrices the computation of this complexity index is almost impossible. In order to contribute to a better perception of this measure in an economic context and to overcome this difficulty we present some properties and bounds for this index.

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### Talk 2. A matrix pencil tool to solve a sampling problem

In sampling theory, the available data are often samples of some convolution operator acting on the function itself. In this talk we use the oversampling technique for obtaining sampling formulas involving these samples and having compactly supported reconstruction functions. The original problem reduces to finding a polynomial left inverse of a matrix pencil intimately related to the sampling problem. We obtain conditions for computing such reconstruction functions to be possible in a practical way when the oversampling rate is minimum. This solution is not unique, but there is no solution with fewer non-zero consecutive terms than the one obtained.

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### Talk 3. A duality relation for matrix pencils with applications to linearizations

Let  $A(x) = \sum_{i=0}^d A_i x^i$  be a  $n \times n$  regular matrix polynomial,  $Q \in \mathbb{C}^{(n+1)d, (n+1)d}$  the QR factor of

$$\begin{bmatrix} A_0 \\ A_1 \\ \vdots \\ A_d \end{bmatrix},$$

and  $Q_{SE}$  (resp.  $Q_{NE}$ ) the  $nd \times nd$  matrix obtained by removing the first  $n$  columns and the first (resp. last)  $n$  rows from  $Q$ .

Then,  $Q_{SE} - xQ_{NE}$  is a linearization of  $A(x)$ . This interesting result is a consequence of a new method for generating equivalent pencils, which is related to the so-called ‘‘pencil arithmetic’’ [Benner, Byers, ’06]. This provides a new interesting framework for studying many known families of linearizations (Fiedler pencils,  $M^4$  vector spaces). In the talk we present this technique and study the numerical stability of the QR-based linearization above.

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### Talk 4. Stability of reducing subspaces of a pencil

Let  $\lambda B - A$  be a pencil of  $m \times n$  complex matrices. We call *reducing subspace* of the pencil  $\lambda B - A$  to any subspace  $\mathcal{N}$  of  $\mathbb{C}^n$  such that

$$\dim(A\mathcal{N} + B\mathcal{N}) = \dim\mathcal{N} - \dim_{\mathbb{C}(\lambda)} \text{Ker}(\lambda B - A)$$

where  $\mathbb{C}(\lambda)$  is the field of rational fractions in  $\lambda$  (P. Van Dooren, 1983).

In this talk we analyze the existence of stable reducing subspaces of the pencil  $\lambda B - A$ , except for the case in which  $\lambda B - A$  has only one column minimal index and only one row minimal index, and this last index is nonzero, as a complete system of invariants for the strict equivalence.

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### CP 22. Matrix functions

#### Talk 1. Improved Schur-Padé algorithm for fractional powers of a matrix

We present several improvements to the Schur-Padé algorithm for computing arbitrary real powers  $A^s$  of a matrix  $A \in \mathbb{C}^{n \times n}$  developed by the first two authors in [SIAM J. Matrix Anal. Appl., 32 (2011), pp. 1056-1078]. We utilize an error bound in terms of the quantities  $\|A^p\|^{1/p}$ , for several small integers  $p$ , instead of  $\|A\|$ , extend the algorithm to allow real arithmetic to be used throughout when the matrix is real, and provide an algorithm that computes both  $A^s$  and the Fréchet derivative at  $A$  in the direction  $E$  at a cost no more than three times that for computing  $A^s$  alone. These improvements put the algorithm’s development on a par with the latest (inverse) scaling and squaring algorithms for the matrix exponential and logarithm.

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#### Talk 2. An automated version of rational Arnoldi for Markov matrix functions

The Rational Arnoldi method is powerful one for approximating functions of large sparse matrices times a vector  $f(A)v$  by means of Galerkin projection onto a subspace  $\text{span}\{(A + s_1 I)^{-1}v, \dots, (A + s_m I)^{-1}v\}$ . The selection of asymptotically optimal shifts  $s_j$  for this method is crucial for its convergence rate. We present and investigate a heuristic for the

automated shift selection when the function to be approximated is of Markov type,  $f(z) = \int_{-\infty}^0 \frac{d\gamma(x)}{z-x}$ , such as the matrix square root or other impedance functions. The performance of this approach is demonstrated at several numerical examples involving symmetric and nonsymmetric matrices.

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**Talk 3. Ranking hubs and authorities using matrix functions**

The notions of subgraph centrality and communicability, based on the exponential of the adjacency matrix of the underlying graph, have been effectively used in the analysis of undirected networks. In this talk we propose an extension of these measures to directed networks, and we apply them to the problem of ranking hubs and authorities. The extension is achieved by bipartition, i.e., the directed network is mapped onto a bipartite undirected network with twice as many nodes in order to obtain a network with a symmetric adjacency matrix. We explicitly determine the exponential of this adjacency matrix in terms of the adjacency matrix of the original, directed network, and we give an interpretation of centrality and communicability in this new context, leading to a technique for ranking hubs and authorities. The matrix exponential method for computing hubs and authorities is compared to the well known HITS algorithm, both on small artificial examples and on more realistic real-world networks. This is joint work with Michele Benzi (Emory University) and Ernesto Estrada (University of Strathclyde).

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**Talk 4. The geometric mean of two matrices from a computational viewpoint**

We consider the geometric mean of two matrices with an eye on computation. We discuss and analyze several numerical algorithms based on different properties and representations of the geometric mean and we show that most of them can be classified in terms of the rational approximations of the inverse square root function. Finally, a review of relevant applications is given.

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**CP 23. Applications**

**Talk 1. Study on efficient numerical simulation methods of dynamic interaction system excited via moving contact points**

When a railway train is travelling on the track, vehicles and the track are excited via moving contact points between wheels and a rail. A numerical simulation of this dynamic interaction is formulated to the problem of solving a large-scale, time-dependent linear or nonlinear system of equations. For the linear case, two methods of a direct method using the Sherman-Morrison-Woodbury formula and a PCG (Preconditioned Conjugate Gradient) method have been

comparatively investigated. In the PCG method, by carrying out the Cholesky decomposition of the time-independent part of the coefficient matrix and constructing the preconditioner from it, a very efficient numerical simulation has been attained. In this talk, numerical simulation methods for nonlinear case will be also described.

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**Talk 2. A matrix version of a digital signature scheme based on pell equation**

Cryptography had been evolved by using different types of special matrices at Vandermonde matrix, febonacci Q-matrix, latin square etc. and based on these, various types of cryptosystems and digital signature scheme have been proposed. We apply the idea of Elliptic Curve Digital Signature Algorithm (ECDSA) on the solution space of Pell equation to designed digital signature scheme and then produce a matrix version of it. Also we compare the security of our signature and its matrix version to DSA and ECDSA. We show that the signature scheme based on Pell equation is more efficient than its analogue to elliptic curve i.e. ECDSA.

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**Talk 3. Accelerating electronic structure calculation with pole expansion plus selected inversion method**

Kohn-Sham density functional theory (KSDFT) is the most widely used electronic structure theory. However, the standard method for solving KSDFT scales cubically with respect to system size. In the recently developed pole expansion plus selected inversion (PEpSI) method, KSDFT is solved by evaluating the diagonal elements of the inverse of a series of sparse symmetric matrices, and the overall algorithm scales at most quadratically with respect to system size for all materials. In this talk I will introduce the PEpSI method, and present the parallel performance of the new method with applications to real materials.

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**Talk 4. Evaluating computer vision systems**

As computer vision systems advance technologically and become more pervasive, the need for more sophisticated and

effective methods to evaluate their accuracy grows. One method to evaluate the accuracy of a given computer vision system is to solve the “robot-world/hand-eye calibration problem” which has the form  $\mathbf{AX} = \mathbf{YB}$  for unknown homogeneous matrices  $\mathbf{X}$  and  $\mathbf{Y}$ . In this talk, I will present a closed-form solution to this problem using the Kronecker Product.

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#### CP 24. Preconditioning II

##### Talk 1. Overlapping blocks by growing a partition with applications to preconditioning

Starting from a partitioning of an edge-weighted graph into subgraphs, we develop a method which enlarges the respective sets of vertices to produce a decomposition with overlapping subgraphs. In contrast to existing methods, we propose that the vertices to be added when growing a subset are chosen according to a criterion which measures the strength of connectivity with this subset. We obtain an overlapping decomposition of the set of variables which can be used for algebraic Schwarz preconditioners. Numerical results show that with these overlapping Schwarz preconditioners we usually substantially improve GMRES convergence when compared with preconditioners based on a non-overlapping decomposition, an overlapping decomposition based in adjacency sets without other criteria, or incomplete LU.

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##### Talk 2. Communication avoiding ILU(0) preconditioner

In this talk we present a general communication-avoiding Incomplete LU preconditioner for the system  $\mathbf{Ax} = \mathbf{b}$ , where communication-avoiding means reducing data movement between different levels of memory, in serial or parallel computation. We implement our method for ILU(0) preconditioners on matrices  $\mathbf{A}$  that have a regular grid (2D 5-point stencil,...). The matrix  $\mathbf{A}$  is reordered using nested dissection, then a special block and separator reordering is applied that allows to avoid communication. Finally, we show that our reordering of  $\mathbf{A}$  does not affect the convergence rate of the ILU preconditioned systems as compared to the natural ordering of  $\mathbf{A}$ , while it reduces data movement and improves the time needed for convergence.

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#### Talk 3. Preconditioning for large scale $\mu$ FE analysis of bone poroelasticity

The mixed finite element discretization of Biot's model of poroelasticity in the displacement-flow-pressure ( $\mathbf{u}$ - $\mathbf{f}$ - $\mathbf{p}$ ) formulation leads to linear systems of the form

$$\begin{bmatrix} \mathbf{A}_{uu} & \mathbf{O} & \mathbf{A}_{pu}^T \\ \mathbf{O} & \mathbf{A}_{ff} & \mathbf{A}_{pf}^T \\ \mathbf{A}_{pu} & \mathbf{A}_{pf} & -\mathbf{A}_{pp} \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{f} \\ \mathbf{p} \end{bmatrix} = \begin{bmatrix} \mathbf{g} \\ \mathbf{0} \\ \mathbf{b} \end{bmatrix}, \quad (1)$$

where all diagonal blocks are positive definite. We solve (1) with MINRES and GMRES and preconditioners composed of AMG preconditioners for the individual diagonal blocks. We show optimality of the preconditioners and scalability of the parallel solvers. We also discuss more general inner-outer iterations.

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#### Talk 4. Block-triangular preconditioners for systems arising from edge-preserving image restoration

Signal and image restoration problems are often solved by minimizing a cost function consisting of an  $\ell_2$  data-fidelity term and a regularization term. We consider a class of convex and edge-preserving regularization functions. In specific, half-quadratic regularization as a fixed point iteration method is usually employed to solve this problem. We solve the above-described signal and image restoration problems with the half-quadratic regularization technique by making use of the Newton method. At each iteration of the Newton method, the Newton equation is a structured system of linear equations of a symmetric positive definite coefficient matrix, and may be efficiently solved by the preconditioned conjugate gradient method accelerated with the modified block SSOR preconditioner. The experimental results show that this approach is more feasible and effective than the half-quadratic regularization approach.

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#### CP 25. Tensors and multilinear algebra

##### Talk 1. Decomposition of semi-nonnegative semi-symmetric three-way tensors based on LU matrix factorization

CANDECOMP/PARAFAC (CP) decomposition of semi-symmetric three-way tensors is an essential tool in signal processing particularly in blind source separation. However, in many applications, such as magnetic resonance spectroscopy, both symmetric modes of the three-way array are inherently nonnegative. Existing CP algorithms, such as gradient-like approaches, handle symmetry and nonnegativity but none of them uses a Jacobi-like procedure in spite of its good convergence properties. First we rewrite the considered optimization problem as an unconstrained one. In fact, the nonnegativity constraint is ensured by means of a square change of variable. Second we propose a Jacobi-like approach using LU matrix factorization, which consists in formulating a high-dimensional optimization problem into several sequential rational subproblems. Numerical experiments emphasize the advantages of the proposed method, especially in the case of degeneracies such as bottlenecks.

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#### Talk 2. Random matrices and tensor rank probabilities

By combining methods for tensors (multiway arrays) developed by ten Berge and recent results by Forrester and Mays on the number of real generalised eigenvalues of real random matrices, we show that the probability for a real random Gaussian  $n \times n \times 2$  tensor to be of real rank  $n$  is  $P_n = (\Gamma((n+1)/2))^n / ((n-1)!(n-2)!\dots1!)$ , where  $\Gamma$  is the gamma function, i.e.,  $P_2 = \pi/4$ ,  $P_3 = 1/2$ ,  $P_4 = 3^3\pi^2/2^{10}$ ,  $P_5 = 1/3^2$ , etc. [ref: G. Bergqvist, Lin. Alg. Appl. to appear, 2012 (doi:10.1016/j.laa.2011.02.041); G. Bergqvist and P. J. Forrester, Elect. Comm. in Probab. 16, 630-637, 2011]. Previously such probabilities were only studied using numerical simulations. We also show that for large  $n$ ,  $P_n = (e/4)^{n^2/4} n^{1/12} e^{-1/12 - \zeta'(-1)} (1 + O(1/n))$ , where  $\zeta$  is the Riemann zeta function.

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#### Talk 3. A new truncation strategy for the higher-order singular value decomposition of tensors

We present an alternative strategy to truncate the higher-order singular value decomposition (T-HOSVD) [De Lathauwer *et al.*, SIMAX, 2000]. Our strategy is called the sequentially truncated HOSVD (ST-HOSVD). It requires less operations to compute

and often improves the approximation error w.r.t. T-HOSVD. In one experiment we performed, the results of a numerical simulation of a partial differential equation were compressed by T-HOSVD and ST-HOSVD yielding similar approximation errors. The execution time, on the other hand, was reduced from 2 hours 45 minutes for T-HOSVD to one minute for ST-HOSVD, representing a speedup of 133.

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#### Talk 4. Probabilistic matrix approximation

This talk will present new results from the computer vision domain. We define a probabilistic framework in which the full range of an incomplete matrix is approximated by incorporating a prior knowledge from similar matrices. Considering the low-rank matrix approximation inequality  $\|\mathbf{A} - \mathbf{Q}\mathbf{Q}^T\mathbf{A}\| < \epsilon$ , where the projection of  $\mathbf{A}$  into the subspace spanned by  $\mathbf{Q}$  is used as an approximation, the proposed framework derives  $\mathbf{Q}$  having only a submatrix  $\mathbf{A}(:, J)$  (*i.e.* given only a few columns) by utilizing a prior distribution  $p(\mathbf{Q})$ . Such an approach provides useful results in face recognition tasks when we deal with variations like illumination and facial expression.

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#### CP 26. Eigenvalue problems III

##### Talk 1. Eigenvalues of matrices with prescribed entries

An important motivation for our work is the description of the possible eigenvalues or the characteristic polynomial of a partitioned matrix of the form  $A = [A_{i,j}]$ , over a field, where the blocks  $A_{i,j}$  are of type  $p_i \times p_j$  ( $i, j \in \{1, 2\}$ ), when some of the blocks  $A_{i,j}$  are prescribed and the others are unknown. Our aim is to describe the possible list of eigenvalues of a partitioned matrix of the form  $C = [C_{i,j}] \in F^{n \times n}$ , where  $F$  is an arbitrary field,  $n = p_1 + \dots + p_k$ , the blocks  $C_{i,j}$  are of type  $p_i \times p_j$  ( $i, j \in \{1, \dots, k\}$ ), and some of its blocks are prescribed and the others vary. In this talk we provide some solutions for the following situations:

- (i)  $p_1 = \dots = p_k$ ;
- (ii) A diagonal of blocks is prescribed;
- (iii)  $k = 3$ .

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##### Talk 2. Characterizing and bounding eigenvalues of interval

**matrices**

In this talk we give a characterization of the eigenvalue set of an interval matrix and present some outer approximations on the eigenvalue set. Intervals represent measurement errors, estimation of unknown values or other kind of uncertainty. Taking into account all possible realizations of interval values is necessary to obtain reliable bounds on eigenvalues. This approach helps in robust stability checking of dynamical systems, and in many other areas, where eigenvalues of matrices with inexact entries are used.

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**Talk 3. Lifted polytopes methods for the computation of joint spectral characteristics of matrices**

We describe new methods for computing the joint spectral radius and the joint spectral subradius of arbitrary sets of matrices. The methods build on two ideas previously appeared in the literature: the polytope norm iterative construction, and the lifting procedure. Moreover, the combination of these two ideas allows us to introduce a pruning algorithm which can importantly reduce the computational burden. We prove several appealing theoretical properties of our methods, and provide numerical examples of their good behaviour.

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**Talk 4. An improved dqds algorithm**

In this talk we present a new deflation strategy and some modified shift strategies for dqds algorithm. We call our implementation DLASQ2, which is faster and more accurate than current routines DLASQ of LAPACK. For some tough matrices for which DLASQ shows very slow convergence, DLASQ2 can be 2-6 times faster. For the matrices collected for testing DLASQ and random matrices, DLASQ2 can also achieve more than 15% speed up on average. More importantly, we prove that DLASQ2 has linear complexity.

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**CP 27. Multigrid I****Talk 1. Algebraic multigrid for solution of discrete adjoint****Reynolds-averaged Navier-Stokes (RANS) equations in compressible aerodynamics**

In this work, solution to the adjoint equations for second-order accurate unstructured finite volume discretizations of RANS equations is investigated. For target applications, the corresponding linear systems are very large and bad-conditioned, and finding an efficient solver for them is a challenging task. Here, we suggest a solution approach, based on algebraic multigrid (AMG), because AMG has potential for dealing with problems on unstructured grids. Combining AMG with defect correction helps to handle second-order accurate discretizations. The approach can be used in parallel, allowing solution of problems involving several million grid points, which we demonstrate on a number of test cases.

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**Talk 2. Symmetric multigrid theory for deflation methods**

In this talk we present a new estimate for the speed of convergence of deflation methods, based on the idea of Nicolaides, for the iterative solution of linear systems of equations. This is done by using results from classical algebraic multigrid theory. As a further result we obtain that many prolongation operators from multigrid methods can be used to span the deflation subspace, which is needed for deflation methods.

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**Talk 3. Aggregation-based multilevel methods for lattice QCD**

In this talk, we present a multigrid solver for application in Quantum Chromodynamics (QCD), a theory that describes the strong interaction between subatomic particles. In QCD simulations a substantial amount of work is spent in solving Dirac equations on regular grids. These large sparse linear systems are often ill conditioned and typical Krylov subspace methods (e.g. CGN, GCR, BiCGStab) tend to be slow. As a solution to their bad scaling behavior we present an aggregation based multigrid method with a domain decomposition smoother and show numerical results for systems up to the size of 450 million of unknowns.

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**Talk 4. Adaptive algebraic multigrid methods for Markov chains**

We present an algebraic multigrid approach for computing the stationary distribution of an irreducible Markov chain. This method can be divided into two main parts, namely a multiplicative bootstrap algebraic multigrid (BAMG) setup

phase and a Krylov subspace iteration, preconditioned by the previously developed multigrid hierarchy. In our approach, we propose some modifications to the basic BAMG framework, e.g., using approximations to singular vectors as test vectors for the adaptive computation of the restriction and interpolation operators. Furthermore, new results concerning the convergence of the preconditioned Krylov subspace iteration for the resulting singular linear system will be shown.

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#### CP 28. Structured matrices II

##### Talk 1. Structured matrices and inverse problems for discrete Dirac systems with rectangular matrix potentials

Inverse problems for various classical and non-classical systems are closely related to structured operators and matrices. See, e.g., the treatment of such problems for discrete systems (where structured matrices appear) and additional references in A. Sakhnovich, *Inverse Problems* 22 (2006), 2083-2101 and a joint work of authors: *Operators and Matrices* 2 (2008), 201-231.

In this talk we consider an important case of discrete Dirac systems with rectangular matrix potentials and essentially develop in this way the results from the author's recent paper (see *Inverse Problems* 28 (2012), 015010) on continuous systems. The research was supported by the Austrian Science Fund (FWF) under Grant no. Y330, and German Research Foundation (DFG) under grant no. KI 760/3-1.

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#### Talk 2. Applications of companion matrices

Companion matrices are commonly used to estimate or compute polynomial zeros. We obtain new polynomial zero inclusion regions by considering appropriate polynomials of companion matrices, combined with similarity transformations. Our main tools are Gershgorin's theorem and Rouché's theorem: the former to show the way and the latter to prove the results. In addition, our techniques uncover geometric aspects of Pellet's and related theorems about the separation of zeros that were apparently not noticed before. Along the way, we encounter nontrivial root-finding problems that are currently solved with heuristic methods. We briefly show how they can be solved without heuristics.

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#### Talk 3. On factorization of structured matrices and GCD evaluation

The paper gives a self-contained survey of fast algorithms for factorization of structured matrices. Algorithms of Sylvester- and Hankel-type are discussed. Sylvester-based algorithms reduce the required complexity of classical methods per one order and the Hankel-based algorithm keeps the same complexity with respect to the classical one, triangularizing the initial matrices in  $O(n^2)$  flops. Their connections with the evaluation of GCD (Greatest common divisor) of two polynomials are demonstrated. The presented procedures are studied and compared in respect of their error analysis and complexity. Numerical experiments performed with a wide variety of examples show the effectiveness of these algorithms in terms of speed, stability and robustness.

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#### Talk 4. An anti-triangular factorization of symmetric matrices

Indefinite symmetric matrices occur in many applications, such as optimization, least squares problems, partial differential equations and variational problems. In these applications one is often interested in computing a factorization that puts into evidence the inertia of the matrix or possibly provides an estimate of its eigenvalues. In this talk we present an algorithm that provides this information for any symmetric indefinite matrix by transforming it to a block anti-triangular form using orthogonal similarity transformations. We show that the algorithm is backward stable and that it has a complexity that is comparable to existing matrix decompositions for dense indefinite matrices.

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#### CP 29. Miscellaneous IV

##### Talk 1. Structure exploited algorithm for solving palindromic quadratic eigenvalue problems

We study a palindromic quadratic eigenvalue problem (QEP) occurring in the vibration analysis of rail tracks under excitation arising from high speed train

$$(\lambda^2 A^T + \lambda Q + A)z = 0,$$

where  $A, Q \in C^{m \times n}$  and  $Q^T = Q$ . The coefficient matrices  $Q$  and  $A$  have special structure: the matrix  $Q$  is block tridiagonal and block Toeplitz, and the matrix  $A$  has only one nonzero  $q \times q$  block in the upper-right corner, where  $n = mq$ . In using the solvent approach to solve the QEP, we fully exploit the special

structures of the coefficient matrices to reduce the  $n \times n$  matrix equation  $X + A^T X^{-1} A = Q$  into a  $q \times q$  matrix equation of the same form. The numerical experiment is given to show that our method is more efficient and has better accuracy in computed results than existing methods.

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**Talk 2. A spectral multi-level approach for eigenvalue problems in first-principles materials science calculations**

We present a multi-level approach in Fourier space to solve the Kohn-Sham equations from Density Functional Theory (DFT) using a plane wave basis and replacing the ionic cores by pseudopotentials. By increasing the cutoff energy and associated other parameters in subsequent level, we demonstrate that this approach efficiently speeds up solving the Kohn-Sham equations. The method was implemented using the PARATEC first principles plane wave code. Examples of multi-level calculations for bulk silicon, quantum dots and an aluminum surface are presented. In some case using the multilevel approach the total computation time is reduced by over 50%. The connection to multigrid approaches in real space is also discussed.

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**Talk 3. Spectrum of Sylvester operators on triangular spaces of matrices**

We present recent results on the spectrum of the operator  $T$  given by  $T(X) = AX + XB$  defined on spaces of matrices with triangular shape, e.g., block upper triangular matrices and other related spaces. We also discuss the spectrum of the multiplication operator  $X \mapsto AXB$  on the same spaces.

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**Talk 4. Modulus-based successive overrelaxation method for pricing american options**

Since the Chicago Board Options Exchange started to operate in 1848, the trading of options has grown to tremendous scale and plays an important role in global economics. Various type of mathematical models for the prices of different kinds of options are proposed during the last decades, and the valuation of options has been topic of active research.

Consider the Black-Scholes model for American option, a high order compact scheme with local mesh refinement is proposed and analyzed. Then, Modulus-based successive overrelaxation method is taken for the solution of linear complementarity problems from discrete Black-Scholes American options model. The sufficient condition for the convergence of proposed methods is given. Numerical experiment further show that the

high order compact scheme is efficient, and modulus-based successive overrelaxation method is superior to the classical projected successive overrelaxation method.

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**CP 30. Iterative methods II**

**Talk 1. On convergence of MSOR-Newton method for nonsmooth equations**

Motivated by [X.Chen, On the convergence of SOR methods for nonsmooth equations. Numer. Linear Algebra Appl. 9 (2002) 81-92], we further investigate a Modified SOR-Newton (MSOR-Newton) method for solving a system of nonlinear equations  $F(x) = 0$ , where  $F$  is strongly monotone, locally Lipschitz continuous but not necessarily differentiable. The convergence interval of the parameter in the MSOR-Newton method is given. Compared with SOR-Newton method, this interval can be larger and the algorithm can be more stable because of large denominator. Furthermore, numerical examples show that this MSOR-Newton method can converge faster than the corresponding SOR-Newton method by choosing a suitable parameter.

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**Talk 2. A framework for deflated BiCG and related solvers**

For solving ill-conditioned nonsymmetric linear algebraic systems, we introduce a general framework for applying augmentation and deflation to Krylov subspace methods based on a Petrov-Galerkin condition. In particular, the framework can be applied to the biconjugate gradient method (BiCG) and some of its generalizations, including BiCGStab and IDR( $s$ ). Our abstract approach does not depend on particular recurrences and thus simplifies the derivation of theoretical results. It easily leads to a variety of realizations by specific algorithms. We avoid algorithmic details, but we show that for every method there are two approaches for extending it by augmentation and deflation.

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**Talk 3. Prescribing the behavior of the GMRES method and the Arnoldi method simultaneously**

In this talk we first show that the Ritz values generated in the subsequent iterations of the Arnoldi method can be fully independent from the eigenvalues of the input matrix. We will give a parametrization of the class of matrices and starting vectors generating prescribed Ritz values in all iterations. This result can be seen as an analogue of the parametrization that closed a series of papers by Arioli, Greenbaum, Pták and Strakoš (published in 1994, 1996 and 1998) on prescribing GMRES residual norm curves and spectra. In the second part of the talk we show, using the first part, that any GMRES convergence history is possible with any Ritz values in all iterations, provided we treat the GMRES stagnation case properly. We also present a parametrization of the class of matrices and right hand sides generating prescribed Ritz values and GMRES residual norms in all iterations.

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**Talk 4. Efficient error bounds for linear systems and rational matrix functions**

Does it make sense to run Lanczos on a (hermitian) tridiagonal matrix? This talk will give the answer 'yes'. If  $T$  is the tridiagonal matrix arising from the standard Lanczos process for the matrix  $A$  and a starting vector  $v$ , running Lanczos on the trailing  $(2m+1) \times (2m+1)$  submatrix of  $T$  and with its start vector the  $m+1$ st unit vector, we obtain information that allows to devise lower and upper bounds on the error of the Lanczos approximations to solutions of linear systems  $A^{-1}$  and, more generally, rational function evaluations  $r(A)b$ . The approach proceeds in a manner related to work of Golub and Meurant on the theory of moments and quadrature and allows in particular to obtain upper error bounds, provided a lower bound on the spectrum is known. The computational work is very low and independent of the dimension of the matrix  $A$ . We will present several numerical results, including linear systems and rational approximations to the exponential and the sign function.

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**CP 31. Direct methods**

**Talk 1. On sparse threaded deterministic lock-free Cholesky and  $LDL^T$  factorizations**

We consider the design and implementation of sparse threaded deterministic Cholesky and  $LDL^T$  factorizations using lock-free algorithms. The approach is based on DAG representation of the factorization process and uses static scheduling mechanisms. Results show that the new solvers are comparable in quality to the existing nondeterministic ones with mean scalability degradation of about 15% over 150 instances from the University of Florida collection.

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**Talk 2. A fast algorithm for constructing the solution operator for homogeneous elliptic boundary value problems**

The large sparse linear system arising from the finite element or finite difference discretization of an elliptic PDE is typically solved with iterative methods such as GMRES or multigrid (often with the aid of a problem specific preconditioner). An alternative is solve the linear system directly via so-called nested dissection or multifrontal methods. Such techniques reorder the discretization nodes to reduce the asymptotic complexity of Gaussian elimination from  $O(N^3)$  to  $O(N^{1.5})$  for two dimensional problems, where  $N$  is the number of discretization points. By exploiting the structure in the dense matrices that arise in the computations (using, e.g.,  $\mathcal{H}$ -matrix arithmetic) the complexity can be further reduced to  $O(N)$ . In this talk, we will demonstrate that such accelerated nested dissection techniques become particularly effective for homogeneous boundary value problems when the solution is sought on the boundary for several different sets of boundary data. In this case, a modified version of the accelerated nested dissection scheme can execute any solve beyond the first in  $O(N_{\text{boundary}})$  operations, where  $N_{\text{boundary}}$  denotes the number of points on the boundary. Typically,  $N_{\text{boundary}} \sim N^{0.5}$ . Numerical examples demonstrate the effectiveness of the procedure for a broad range of elliptic PDEs that includes both the Laplace and Helmholtz equations.

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**Talk 3. Eliminate last variable first!**

When solving linear equations, textbooks typically start the elimination of variables from the top. We suggest, however, to start from the bottom, that is, we suggest to solve for the last variable from the last equation, and eliminate it from all other equations, then do the same for the second last equation, and so on. In particular, when solving the equilibrium equations arising from ergodic queueing systems, starting from the top can be proven to be unstable for large systems, whereas starting from the bottom is stable. Heuristic arguments show that starting from the bottom is also preferable in other cases.

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#### Talk 4. Sharp estimates for the convergence rate of Orthomin( $k$ ) for a class of linear systems

In this work we show that the convergence rate of Orthomin( $k$ ) applied to systems of the form  $(I + \rho U)x = b$ , where  $U$  is a unitary operator and  $0 < \rho < 1$ , is less than or equal to  $\rho$ . Moreover, we give examples of operators  $U$  and  $\rho > 0$  for which the asymptotic convergence rate of Orthomin( $k$ ) is exactly  $\rho$ , thus showing that the estimate is sharp. While the systems under scrutiny may not be of great interest in themselves, their existence shows that, in general, Orthomin( $k$ ) does not converge faster than Orthomin(1). Furthermore, we give examples of systems for which Orthomin( $k$ ) has the same asymptotic convergence rate as Orthomin(2) for  $k \geq 2$ , but smaller than that of Orthomin(1). The latter systems are related to the numerical solution of certain partial differential equations.

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#### CP 32. Nonlinear methods

##### Talk 1. On the performance of the algebraic optimized Schwarz methods with applications

In this paper we investigate the performance of the algebraic optimized Schwarz methods. These methods are based on the modification of the transmission blocks. The transmission blocks are replaced by new blocks to improve the convergence of the corresponding algorithms. In the optimal case, convergence in two iterations can be achieved. We are interested in analyzing how the algebraic optimized Schwarz methods perform as preconditioners solving differential equations. We are also interested in their asymptotic behavior with respect to change in the problems parameters. We present different numerical simulations corresponding to different type of problems in two- and three-dimensions.

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##### Talk 2. Optimizing additive Runge-Kutta smoothers for unsteady flow problems

We consider the solution of unsteady flow problems using implicit time integration schemes. Typically the appearing nonlinear systems are solved using the FAS variant of multigrid, where the steady state algorithm is reused without changes. Significant speedup can be obtained by redesigning the multigrid method for unsteady problems. In this talk, we discuss possibilities of finding optimal smoothers from the class of additive Runge-Kutta schemes, using the linear advection

diffusion equation as model problem. In particular, options for the target function are discussed, as the spectral radius of the smoother or the spectral radius of the multigrid iteration matrix.

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##### Talk 3. On convergence conditions of waveform relaxation methods for linear differential-algebraic equations

Waveform relaxation methods are successful numerical methods originated from the basic fixed-point idea in numerical linear algebra for solving time-dependent differential equations, which was first introduced for simulating the behavior of very large electrical networks. For linear constant-coefficient differential-algebraic equations, we study the waveform relaxation methods without demanding the boundedness of the solutions based on infinite time interval. In particular, we derive explicit expressions and obtain asymptotic convergence rates of this class of iteration schemes under weaker assumptions, which may have wider and more useful application extent. Numerical simulations demonstrate the validity of the theory.

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##### Talk 4. On sinc discretization and banded preconditioning for linear third-order ordinary differential equations

Some draining or coating fluid-flow problems and problems concerning the flow of thin films of viscous fluid with a free surface can be described by third-order ordinary differential equations. In this talk, we solve the boundary value problems of such equations by sinc discretization and prove that the discrete solutions converge to the true solutions of the ordinary differential equations exponentially. The discrete solution is determined by a linear system with the coefficient matrix being a combination of Toeplitz and diagonal matrices. The system can be effectively solved by Krylov subspace iteration methods such as GMRES preconditioned by banded matrices. We demonstrate that the eigenvalues of the preconditioned matrix are uniformly bounded within a rectangle on the complex plane independent of the size of the linear system. Numerical examples are given to illustrate the effective performance of our method.

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### CP 33. Matrices and graphs

#### Talk 1. Complex networks metrics for software systems

The study of large software systems has recently benefited from the application of complex graph theory. In fact, it is possible to describe a software system by a complex network, where nodes and edges represent software modules and the relationships between them, respectively. In our case, the goal is to study the occurrence of bugs in the software development and to relate them to some metrics, either old or recently introduced, used to characterize the nodes of a graph. This will be done through the application of numerical linear algebra techniques to the adjacency matrix associated to the graph.

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#### Talk 2. On Euclidean distance matrices of graphs

A matrix  $D \in \mathbb{R}^{n \times n}$  is *Euclidean distance matrix (EDM)*, if there exist points  $\mathbf{x}_i \in \mathbb{R}^r$ ,  $i = 1, 2, \dots, n$ , such that  $d_{ij} = \|\mathbf{x}_i - \mathbf{x}_j\|^2$ . Euclidean distance matrices have many interesting properties, and are used in various applications in linear algebra, graph theory, bioinformatics, e.g., where frequently a question arises, what can be said about a configuration of points  $\mathbf{x}_i$ , if only distances between them are known.

In this talk some results on Euclidean distance matrices, arising from the distances in graphs, will be presented. In particular, the distance spectrum of the matrices will be analysed for some families of graphs and it will be proven, that their distance matrices are EDM. A generalization to distance matrices of weighted graphs will be tackled.

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#### Talk 3. Evaluating matrix functions by resummations on graphs: the method of path-sums

We introduce the method of path-sums which is a tool for analytically evaluating a function of a square matrix, based on the closed-form resummation of infinite families of terms in the corresponding Taylor series. For finite matrices, our approach yields the exact result in a finite number of steps. We achieve this by combining a mapping between matrix powers and walks on a weighted graph with a universal result on the structure of such walks. This result reduces a sum over weighted walks to a sum over weighted paths, a path being forbidden to visit any vertex more than once.

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#### Talk 4. An estimation of general interdependence in an open linear structure

The open linear structures have many applications in sciences. Especially, the social sciences - including economics - have made extensive use of them.

Starting from the biunivocal correspondence between a square matrix and a graph, this paper aims to establish several theorems linking components, sub-structures, loops and circuits of the graph with certain characteristics of the exchange matrix. That correspondence focuses particularly on the determinant of the matrix and its sub-matrices. Hence, the determinant is a specific function of the possible arrangements in the graph (open, closed, linear, triangular, circular, autarkic, etc.).

A matrix appears as an orderly and intelligible articulation of sub-structures, themselves divisible until elementary coefficients. Hence it comes a possible measure of general interdependence between the elements of a structure. Multiple uses can be deduced (inter-industry trade, international trade, strategic positioning, pure economic theory, etc.).

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### CP 34. PageRank

#### Talk 1. On the complexity of optimizing PageRank

We consider the PageRank Optimization problem in which one seeks to maximize (or minimize) the PageRank of a node in a graph through adding or deleting links from a given subset. The problem is essentially an eigenvalue maximization problem and has recently received much attention. It can be modeled as a Markov Decision Process. We provide provably efficient methods to solve the problem on large graphs for a number of cases of practical importance and we show using perturbation analysis that for a close variation of the problem, the same

techniques have exponential worst case complexity.

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### Talk 2. Optimization of the HOTS score of a website's pages

Tomlin's HOTS algorithm is one of the methods allowing search engines to rank web pages, taking into account the web graph structure. It relies on a scalable iterative scheme computing the dual solution (the HOTS score) of a nonlinear network flow problem. We study here the convergence properties of Tomlin's algorithm as well as of some of its variants. Then, we address the problem of optimizing the HOTS score of a web page (or site), given a set of controlled hyperlinks. We give a scalable algorithm based on a low rank property of the matrix of partial derivatives of the objective function and report numerical results on a fragment of the web graph.

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### Talk 3. An inclusion set for the personalized PageRank

The Personalized Page Rank (PPR) was one of the first modifications introduced to the original formulation of the PageRank algorithm. PPR is based on a probability distribution vector that bias the PR to some nodes. PPR can be used as a centrality measure in complex networks. In this talk, we give some theoretical results for the PPR considering a directed graph with dangling nodes (nodes with zero out-degree). Our results, derived by using matrix analysis, lead to an inclusion set for the entries of the PPR. These bounds for the PPR, for a given distribution for the dangling nodes, are independent of the personalization vector. We use these results to give a theoretical justification of a recent model that uses the PPR to classify users of Social Network Sites. We give examples of how to use these results in some networks.

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### CP 35. Matrix equations

### Talk 1. Upper bounds on the solution of the continuous algebraic Riccati matrix equation

In this paper, by considering the equivalent form of the continuous algebraic Riccati matrix equation and using matrix properties and inequalities, we propose new upper matrix bounds for the solution of the continuous algebraic Riccati matrix equation. Then, we give numerical examples to show the effectiveness of our results.

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### Talk 2. A large-scale nonsymmetric algebraic Riccati equation from transport theory

We consider the solution of the large-scale nonsymmetric algebraic Riccati equation  $XCX - XD - AX + B = 0$  from transport theory (Juang 1995), with

$M \equiv [D, -C; -B, A] \in \mathbb{R}^{2n \times 2n}$  being a nonsingular M-matrix. In addition,  $A, D$  are rank-1 corrections of diagonal matrices, with the products  $A^{-1}u, A^{-\top}u, D^{-1}v$  and  $D^{-\top}v$  computable in  $O(n)$  complexity, for some vectors  $u$  and  $v$ , and  $B, C$  are rank 1. The structure-preserving doubling algorithm by Guo, Lin and Xu (2006) is adapted, with the appropriate applications of the Sherman-Morrison-Woodbury formula and the sparse-plus-low-rank representations of various iterates. The resulting large-scale doubling algorithm has an  $O(n)$  computational complexity and memory requirement per iteration and converges essentially quadratically, as illustrated by the numerical examples.

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### Talk 3. A stable variant of the biconjugate A-orthogonal residual method for non-Hermitian linear systems

We describe two novel iterative Krylov methods, the biconjugate A-orthogonal residual (BiCOR) and the conjugate A-orthogonal residual squared (CORS) methods, developed from variants of the nonsymmetric Lanczos algorithm. We discuss both theoretical and computational aspects of the two methods. Finally, we present an algorithmic variant of the BiCOR method which exploits the composite step strategy employed in the development of the composite step BCG method, to cure one of the breakdowns called as pivot breakdown. The resulting interesting variant computes the BiCOR iterates stably on the assumption that the underlying Biconjugate A-orthonormalization procedure does not break down.

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**Talk 4. On Hermitian and skew-Hermitian splitting iteration methods for the equation  $AXB = C$**

In this talk we present new results on iteration method for solving the linear matrix equation  $AXB = C$ . This method is formed by extending the corresponding HSS iterative methods for solving  $Ax = b$ . The analysis shows that the HSS iteration method will converge under certain assumptions. Moreover, the optimal parameter of this iteration method is presented in the latter part of this paper. Numerical results for the new method show that this new method is more efficient and robust compared with the existing methods.

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**CP 36. Positivity II**

**Talk 1. A note on  $B$ -matrices and doubly  $B$ -matrices**

A matrix with positive row sums and all its off-diagonal elements bounded above by their corresponding row means was called in Peña, J.M., *A class of  $P$ -matrices with applications to the localization of the eigenvalues of a real matrix*, SIAM J. Matrix Anal. Appl. 22, 1027-1037 (2001) a  $B$ -matrix. In Peña, J.M., *On an alternative to Gershgorin circles and ovals of Cassini*, Numer. Math. 95, 337-345 (2003), the class of doubly  $B$ -matrices was introduced as a generalization of the previous. In this talk we present several characterizations and properties of these matrices and for each of these classes we consider corresponding questions for subdirect sums of two matrices (a general ‘sum’ of matrices introduced by S.M. Fallat and C.R. Johnson, of which the direct sum and ordinary sums are special cases).

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**Talk 2. Accurate computations for rational Bernstein-Vandermonde and Said-Ball-Vandermonde matrices**

Gasca and Peña showed that nonsingular totally nonnegative (TNN) matrices and its inverses admit a bidiagonal decomposition. Koev, in a recent work, assuming that the

bidiagonal decompositions of a TNN matrix and its inverse are known with high relative accuracy (HRA), presented algorithms for performing some algebraic computations with high relative accuracy: computing the eigenvalues and the singular values of the TNN matrix, computing the inverse of the TNN matrix and obtaining the solution of some linear systems whose coefficient matrix is the TNN matrix.

Rational Bernstein and Said-Ball bases are usual representations in Computer Aided Geometric Design (CAGD). Solving some of the algebraic problems mentioned above for the collocations matrices of those bases (RBV and RSBV matrices, respectively) is important for some problems arising in CAGD. In our talk we will show how to compute the bidiagonal decomposition of the RBV and RSBV matrices with HRA. Then we will apply Koev’s algorithms showing the accuracy of the obtained results for the considered algebraic problems.

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**Talk 3. On properties of combined matrices**

The combined matrix of a nonsingular matrix  $A$  is the Hadamard (entry wise) product  $A \circ (A^{-1})^T$ . It’s well known that all row (column) sums of combined matrices are constant and equal to one. Recently, some results on combined matrices of various classes of matrices has been done in LAA-430 (2009) and LAA-435 (2011). In this work, we analyze similar properties (characterizations, positiveness, spectrum) when the matrix  $A$  belongs to some kind of matrices.

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**Talk 4. Computing the Jordan blocks of irreducible totally nonnegative matrices**

In 2005 Fallat and Gekhtman fully characterized the Jordan Canonical Form of the irreducible totally nonnegative matrices. In particular, all nonzero eigenvalues are simple and the possible Jordan structures of the zero eigenvalues are well understood and described. Starting with the bidiagonal decomposition of these matrices, we present an algorithm for computing all the eigenvalues, including the Jordan blocks, to high relative accuracy in what we believe is the first example of Jordan structure being computed accurately in the presence of roundoff errors.

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**CP 37. Matrix computations**

**Talk 1. Computation of the matrix  $p$ th root and its Fréchet derivative by integrals**

We present new integral representations for the matrix  $p$ th root

and its Fréchet derivative and then investigate the computation of these functions by numerical quadrature. Three different quadrature rules are considered: composite trapezoidal, Gauss-Legendre and adaptive Simpson. The problem of computing the matrix  $p$ th root times a vector without the explicit evaluation of the  $p$ th root is also analyzed and bounds for the norm of the matrix  $p$ th root and its Fréchet derivative are derived.

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**Talk 2. An algorithm for the exact Fisher information matrix of vector ARMAX time series processes**

In this paper an algorithm is developed for the exact Fisher information matrix of a vector ARMAX Gaussian process, VARMAX. The algorithm is composed by recursion equations at a vector-matrix level and some of these recursions consist of derivatives. For that purpose appropriate differential rules are applied. The derivatives are derived from a state space model for a vector process. The chosen representation is such that the recursions are given in terms of expectations of derivatives of innovations and not the process and observation disturbances. This enables us to produce an implementable algorithm for the VARMAX process. The algorithm will be illustrated by an example.

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**Talk 3. An algorithm to compute the matrix logarithm and its Fréchet derivative for use in condition number estimation**

Recently there has been a surge of interest in the logarithm from within the finance, control and machine learning sectors. We build on work by Al-Mohy and Higham to give an algorithm for computing the matrix logarithm and its Fréchet derivative simultaneously. We will show that the new algorithm is significantly more efficient than existing alternatives and explain how it can be used to estimate the condition number of the logarithm. We also derive a version of the algorithm that works entirely in real arithmetic where appropriate.

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**Talk 4. High-order iterative methods for the matrix  $p$ th root**

The main goal of this paper is to approximate the principal  $p$ -th root of a matrix by high-order iterative methods. We analyse the semilocal convergence and the speed of convergence of these methods. Concerning stability, it is well known that even the simplified Newton iteration is unstable. Despite it, we are able to

present stable versions of our algorithms. Finally, we test numerically the methods. We check the numerical robustness and stability of the methods by considering matrices that are close to be singular and are badly conditioned. We find algorithms in the family with better numerical behavior than both Newton and Halley methods. These two last algorithms are basically the iterative methods proposed in the literature to solve this problem.

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**CP 38. Eigenvalue problems IV**

**Talk 1. An efficient way to compute the eigenvalues in a specific region of complex plane**

Spectral projectors are efficient tools for extracting spectral information of a given matrix or a matrix pair. On the other hand, these types of projectors have huge computational costs due to the matrix inversions needed by the most computation methods. The Gaussian quadratures can be combined with the sparse approximate inversion techniques to produce accurate and sparsity preserved spectral projectors for the computation of the needed spectral information. In this talk we will show how one can compute spectral projectors efficiently to find the eigenvalues in a specific region of the complex plane by using the proposed computational approach.

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**Talk 2. A divide, reduce and conquer algorithm for matrix diagonalization in computer simulators**

We present a new parallel algorithm for an efficient way to find a subset of eigenpairs for large hermitian matrices, such as Hamiltonians used in the field of electron transport calculations. The proposed algorithm uses a Divide, Reduce and Conquer (DRC) method to decrease computational time by keeping only the important degrees of freedom without loss of accuracy for the desired spectrum, using a black-box diagonalization subroutine (LAPACK, ScaLAPACK). Benchmarking results against diagonalization algorithms of LAPACK/ScaLAPACK will be presented.

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**Talk 3. A rational Krylov method based on Newton and/or Hermite interpolation for the nonlinear eigenvalue problem**  
 In this talk we present a new rational Krylov method for solving the nonlinear eigenvalue problem (NLEP):

$$A(\lambda)x = 0.$$

The method approximates  $A(\lambda)$  by polynomial Newton and/or Hermite interpolation. It uses a companion-type reformulation to obtain a linear generalized eigenvalue problem (GEP). This GEP is solved by a rational Krylov method, where the number of iteration points is not fixed in advance. As a result, the companion form grows in each iteration. The number of interpolation points is dynamically chosen. Each iteration requires a linear system solve with  $A(\sigma)$  where  $\sigma$  is the last interpolation point. We illustrate the method by numerical examples and compare with residual inverse iteration. We also give a number of scenarios where the method performs very well.

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**Talk 4. The rotation of eigenspaces of perturbed matrix pairs**  
 We present new  $\sin \Theta$  theorems for relative perturbations of Hermitian definite generalized eigenvalue problem  $A - \lambda B$ , where both  $A$  and  $B$  are Hermitian and  $B$  is positive definite. The rotation of eigenspaces is measured in the matrix dependent scalar product. We assess the sharpness of the new estimates in terms of the effectivity quotients (the quotient of the measure of the perturbation with the estimator). The known  $\sin \Theta$  theorems for relative perturbations of the single matrix Hermitian eigenspace problem are included as special cases in our approach. We also present the upper bound for the norm of  $J$ -unitary matrix  $F$  ( $F^* J F = J$ ), which plays important role in the relative perturbation theory for *quasi-definite* Hermitian matrices  $H$ , where  $H_{qd} \equiv P^T H P = [H_{11}, H_{12}; H_{12}^*, -H_{22}]$  and  $J = \text{diag}(I_k, -I_{n-k})$ , for some permutation matrix  $P$  and  $H_{11} \in \mathbb{C}^{k \times k}$  and  $H_{22} + H_{12}^* H_{11}^{-1} H_{12} \in \mathbb{C}^{n-k \times n-k}$  positive definite.

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### CP 39. Probabilistic equations

#### Talk 1. Banded structures in probabilistic evolution equations for ODEs

Quite recently a novel approach to solve ODEs with initial conditions, using Probabilistic Evolution Equations which can be considered as the ultimate linearisation has been proposed and investigated in many details. One of the most important agents is the evolution matrix in this approach. The solution of the initial value problem of the infinite set of ODEs is basically determined by this matrix. The influence of the initial conditions is just specification of the initial point in infinite dimensional space. If the evolution matrix has a banded structure then the solution can be constructed recursively and the convergence analysis becomes quite simplified.

In this presentation we focus on the triangular evolution matrices which have just two diagonals. The construction of the truncation approximants over finite submatrices and the convergence of their sequences will be focused on.

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#### Talk 2. Space extensions in the probabilistic evolution equations of ODEs

The evolution matrix appearing in the method, which has been recently developed and based on probabilistic evolution equations for the initial value problems of ODEs, can be controlled in structure at the expense of the dimension increase in the space. Certain function(s) of the unknown functions are deliberately added to the unknowns. This results in the simplification of the right hand side functions of the ODE(s). The basic features desired to be created in the evolution are triangularity and conicality to facilitate the construction of the solutions.

In this presentation we exemplify the utilization of the space extension to get the features mentioned above by focusing on the singularity and uniqueness issues.

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#### Talk 3. Triangularity and conicality in probabilistic evolution equations for ODEs

We have recently shown that all the explicit ordinary differential equations can be investigated through infinite linear ODE systems with a constant matrix coefficient (evolution matrix) under appropriately defined infinitely many initial conditions. The evolution matrix is the basic determinating agent for the characteristics of the solution. For a Taylor basis set it is in upper Hessenberg form which turns out to be triangular if the right hand side functions of the considered ODE(s) vanish at the expansion point. Even though the triangularity facilitates the analysis very much, the conicality, that is, the second degree multinomial right hand side structure is the best nontrivial case (linear case can be considered trivial in this perspective) to get simple truncation approximants. Talk will try to focus on these types of issues.

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#### CP 40. Control systems III

##### Talk 1. $\mathcal{H}_2$ approximation of linear time-varying systems

We consider the problem of approximating a linear time-varying  $p \times m$  discrete-time state space model  $\mathcal{S}$  of high dimension by another linear time-varying  $p \times m$  discrete-time state space model  $\hat{\mathcal{S}}$  of much smaller dimension, using an error criterion defined over a finite time interval. We derive the gradients of the norm of the approximation error for the case with nonzero initial state. The optimal reduced order model is computed using a fixed point iteration. We compare this to the classical  $\mathcal{H}_2$  norm approximation problem for the infinite horizon time-invariant case and show that our solution extends this to the time-varying and finite horizon case.

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##### Talk 2. Analysis of behavior of the eigenvalues and eigenvectors of singular linear systems

Let  $E(p)\dot{x} = A(p)x + B(p)u$  be a family of singular linear systems smoothly dependent on a vector of real parameters  $p = (p_1, \dots, p_n)$ . In this work we construct versal deformations of the given differentiable family under an equivalence relation, providing a special parametrization of space of systems, which can be effectively applied to perturbation analysis. Furthermore in particular, we study of behavior of a simple eigenvalue of a singular linear system family  $E(p)\dot{x} = A(p)x + B(p)u$ .

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##### Talk 3. Stabilization of controllable planar bimodal linear systems

We consider planar bimodal linear systems consisting of two linear dynamics acting on each side of a given hyperplane,

assuming continuity along the separating hyperplane.

We obtain an explicit characterization of their controllability, which can be reformulated simply as  $\det \mathcal{C}_1 \cdot \det \mathcal{C}_2 > 0$ , where  $\mathcal{C}_1, \mathcal{C}_2$  mean the controllability matrices of the subsystems. In particular, it is obvious from this condition that both subsystems must be controllable.

Moreover, this condition allows us to prove that both subsystems can be stabilized by means of the same feedback. In contrast to linear systems, the pole assignment is not achieved for bimodal linear systems and we can only assure the stabilization of these kind of systems.

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#### Talk 4. A combinatorial approach to feedback equivalence of linear systems

The feedback class of a reachable linear control system over a vector space is given by its Kronecker Invariants or equivalently by its Ferrers Diagram. We generalize the notion to a linear control system over a vector bundle (over a compact space) and obtain also a combinatorial invariant in a semigroup. Moreover we point out that this new invariant may be simplified by using algebraic  $K$ -theory.

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#### CP 41. Miscellaneous V

##### Talk 1. Randomized distributed matrix computations based on gossiping

We discuss new randomized algorithms for distributed matrix computations which are built on gossip-based data aggregation. In contrast to approaches where randomization in linear algebra algorithms is primarily utilized for approximation purposes, we investigate the *flexibility* and *fault tolerance* of distributed algorithms with randomized communication schedules. In our algorithms, each node communicates only with its neighborhood. Thus, they are attractive for decentralized and dynamic computing networks and they can heal from hardware failures occurring at runtime.

As case studies, we discuss distributed QR decomposition and distributed orthogonal iteration, their performance, their resilience to hardware failures, and the influence of asynchrony.

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### Talk 2. A tabular methodology for matrix Padé approximants with minimal row degrees

In this paper we propose a tabular procedure to make easier the interpretation and application of a type of Matrix Padé Approximants associated to Scalar Component Models. The originality of these approximants lies in the concept of minimality defined and in the normalization associated. Considering matrix functions with  $k$  rows, to know the sets of minimal row degrees associated with an approximant, we study algebraic properties: it is relevant the number and the position of the linear depending rows that are in the block of the last  $k$  rows, in certain Hankel matrices. We illustrate this procedure with several examples.

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### Talk 3. Sublinear randomized algorithms for skeleton decompositions

A skeleton decomposition is any factorization of the form  $A = CUR$  where  $C$  comprises columns, and  $R$  comprises rows of  $A$ . Much is known on how to choose  $C$ ,  $U$ , and  $R$  in complexity superlinear in the number of elements of  $A$ . In this paper we investigate the sublinear regime where much fewer elements of  $A$  are used to find the skeleton. Under an assumption of incoherence of the generating vectors of  $A$  (e.g., singular vectors), we show that it is possible to choose rows and columns, and find the middle matrix  $U$  in a well-posed manner, in complexity proportional to the cube of the rank of  $A$  up to log factors. Algorithmic variants involving rank-revealing QR decompositions are also discussed and shown to work in the sublinear regime.

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### Talk 4. Preconditioners for strongly non-symmetric linear systems

Consider the system  $Au = f$ , where  $A$  is non-symmetric positive real matrix. The matrix  $A$  is decomposed in a sum of the symmetric matrix  $A_0$  and the skew-symmetric  $A_1$  matrix. When solving such linear systems, difficulties grow up because the coefficient matrices can lose the diagonal dominance property. Consider the preconditioner (TPT)

$P = (B_C + \omega K_U)B_C^{-1}(B_C + \omega K_L)$ , where  $K_L + K_U = A_1$ ,  $K_L = -K_U^*$ ,  $B_C = B_C^*$ . We use TPT as preconditioner for GMRES (m) and BiCG methods and compare it with conventional SSOR preconditioner.

The standard 5-point central difference scheme on the regular mesh has been used for approximation of the convection-diffusion equation with Dirichlet boundary conditions. Numerical experiments of strongly nonsymmetric systems are presented.

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### CP 42. Multigrid II

#### Talk 1. Adaptive smoothed aggregation multigrid for nonsymmetric matrices

We investigate algebraic multigrid (AMG) methods, in particular those based on the smoothed aggregation approach, for solving linear systems  $Ax = b$  with a general, nonsymmetric matrix  $A$ . Recent results show that in this case it is reasonable to demand that the interpolation and restriction operators are able to accurately approximate singular vectors corresponding to the smallest singular values of  $A$ . Therefore, we present an extension of the *bootstrap AMG* setup, which is geared towards the singular vectors of  $A$  instead of the eigenvectors as in the original approach. We illustrate the performance of our method by considering highly nonsymmetric linear systems originating in the discretization of convection diffusion equations, which show that our algorithm performs very well when compared with established methods. In another series of numerical experiments, we present results which indicate that our method can also be used as a very efficient preconditioner for the *generalized minimal residual* (GMRES) method.

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#### Talk 2. Local Fourier analysis for multigrid methods on semi-structured triangular grids

Since the good performance of geometric multigrid methods depends on the particular choice of the components of the algorithm, the local Fourier analysis (LFA) is often used to predict the multigrid convergence rates, and thus to design suitable components. In the framework of semi-structured grids, LFA is applied to each triangular block of the initial unstructured grid to choose suitable local components giving rise to a block-wise multigrid algorithm which becomes a very efficient solver. The efficiency of this strategy is demonstrated for a wide range of applications. Different model problems and discretizations are considered.

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**Talk 3. Approach for accelerating the convergence of multigrid methods using extrapolation methods**

In this talk we present an approach for accelerating the convergence of multigrid methods. Multigrid methods are efficient methods for solving large problems arising in the discretization of partial differential equations, both linear and nonlinear. In some cases the convergence may be slow (with some smoothers). Extrapolation methods are of interest whenever an iteration process converges slowly. We propose to formulate the problem as a fixed point problem and to accelerate the convergence of fixed-point iteration by vector extrapolation. We revisit the polynomial-type vector extrapolation methods and apply them in the MGLab software.

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**Talk 4. Algebraic multigrid (AMG) for saddle point systems**

We present a self-stabilizing approach to the construction of AMG for Stokes-type saddle point systems of the form

$$\mathcal{K} = \begin{pmatrix} A & B \\ B^T & -C \end{pmatrix}$$

where  $A > 0$  and  $C \geq 0$ . Our method is purely algebraic and does not rely on geometric information.

We will show how to construct the interpolation and restriction operators  $\mathcal{P}$  and  $\mathcal{R}$  such that an inf-sup condition for  $\mathcal{K}$  automatically implies an inf-sup condition for the coarse grid operator  $\mathcal{K}^C = \mathcal{R}\mathcal{K}\mathcal{P}$ . In addition, we give a two-grid convergence proof.

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