# New Frontiers in Numerical Analysis and Scientific Computing

## —— A conference on the occasion of Lothar Reichel's 60th birthday and on the 20th anniversary of ETNA

April 19-20, 2013

Department of Mathematical Sciences, Kent State University

### COMPLETE LISTING OF ABSTRACTS

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**Speaker's Name:** James Baglama

**Speaker's Institution:** University of Rhode Island

**Title of Presentation:** Augmented LSQR Method

**Abstract:** The LSQR iterative method for solving least-squares problems may require many iterations to determine an approximate solution with desired accuracy. This often depends on the fact that singular vector components of the solution associated with small singular values of the matrix require many iterations to be determined. Augmentation of Krylov subspaces with harmonic Ritz vectors often makes it possible to determine the singular vectors associated with small singular values with fewer iterations than without augmentation. Computed examples illustrate the competitiveness of the augmented LSQR method proposed.

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**Speaker's Name:** Zhaojun Bai

**Speaker's Institution:** University of California, Davis

**Title of Presentation:** Minimization Principle, Interlacing Inequalities, and Computing the Smallest Positive Eigenpairs of the Linear Response Eigenvalue Problem

**Abstract:** The linear response (LR) eigenvalue problem arises from excitation state (energies) calculations in the study of collective motion of many-particle systems. There are immense interests in developing efficient simulation techniques for excitation-state calculations of molecules for materials design in energy science.

In this talk, we present theoretical results for the LR eigenvalue problem, which include a minimization principle for the sum of the smallest positive eigenvalues and interlacing inequalities associated with these eigenvalues. Although the LR eigenvalue problem is a nonsymmetric eigenvalue problem, these results mirror the well-known trace-minimization principle and Cauchy's inequalities for the symmetric eigenvalue problem. In addition, we will discuss *best* (possible) approximations of the few smallest positive eigenvalues via a structure-preserving projection, and describe conjugate gradient-like algorithms, of which the search subspace is only four in dimension, for simultaneously computing these eigenvalues and their associated eigenvectors.

This is a joint work with Ren-cang Li, Dario Rocca and Giulia Galli.

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**Speaker's Name:** Jesse Barlow

**Speaker's Institution:** The Pennsylvania State University

**Title of Presentation:** Block Gram-Schmidt Downdating

**Abstract:** The problem of deleting multiple rows from a Q-R factorization, called the block downdating problem, is considered. The problem is important in the context of solving recursive least squares problem where observations are added or deleted over time.

The problem is solved by a block classical Gram-Schmidt procedure with reorthogonalization. However, two heuristics are needed for the block downdating problem that are not needed for the cases of deleting a single row; one is a condition estimation heuristic, the other is a method for constructing a one left orthogonal matrix that is orthogonal to another. The difficulties that require these heuristic tend to occur when the block downdating operation changes the rank of the matrix.

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**Speaker's Name:** Peter Benner

**Speaker's Institution:** Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany

**Title of Presentation:** ADI for Sylvester Equations — Lothar's Contributions and New Results

**Abstract:** Large-scale Sylvester equations arise in numerous application areas like control, filtering, image processing, etc. In a series of papers in the 1990ies, Lothar Reichel has contributed to the numerical solution of Sylvester equations and its application to image restoration. Particularly, he and co-authors have devised a way to efficiently solve the special Sylvester equation arising in the restoration of noisy images via an Alternating Directions Implicit (ADI) method. These considerations have proven very useful later in solving large-scale discrete-time Lyapunov equations in the context of discrete-time control problems. We will review the earlier results of Lothar Reichel and co-workers, and will discuss some new developments in this direction obtained in the last 3 years.
This is joint work with Heike Faßbender, Patrick Kürschner, and Jens Saak.

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**Speaker's Name:** Claude Brezinski

**Speaker's Institution:** UFR of Mathematics, University of Lille I, France

**Title of Presentation:** Padé–type Rational and Barycentric Interpolation

**Abstract:** In this paper, we consider the particular case of the general rational Hermite interpolation problem where only the value of the function is interpolated at some points, and where the function and its first derivatives agree at the origin. Thus, the interpolants constructed in this way possess a Padé–type property at 0. Numerical examples show the interest of the procedure. The interpolation procedure can be easily modified to introduce a partial knowledge on the poles and the zeros of the function to approximated. A strategy for removing the spurious poles is explained. A formula for the error is proved in the real case. Applications are given. This is a joint work with Michela Redivo–Zaglia.

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**Speaker's Name:** Jie Chen

**Speaker's Institution:** Argonne National Laboratory

**Title of Presentation:** Flexible BiCGStab and Its Use in Practice

**Abstract:** BiCGStab is one of the de facto methods of choice for solving linear systems in many application domains. Motivated by recent development of flexible preconditioners in high performance computing, we study BiCGStab under flexible preconditioning. In this talk, we will present some analysis results of the convergence behavior of flexible BiCGStab, and show its successful use in practice. In an important application, PFLOTRAN, we demonstrate that the run time of flexible BiCGStab preconditioned by multigrid is significantly improved over the currently known fastest record. This is joint work with Lois Curfman McInnes and Hong Zhang from Argonne National Laboratory.

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**Speaker's Name:** Vani Cheruvu

**Speaker's Institution:** The University of Toledo

**Title of Presentation:** Nodal Discontinuous Galerkin Solutions for Shallow Water Equations on a Triangular Grid

**Abstract:** We present a triangle-based nodal discontinuous Galerkin model for the shallow-water equations in two dimensions. The model uses Lagrange polynomials on the triangle and Warburton's interpolation points. We perform a computational study of the convergence rate of the discontinuous Galerkin method in both one and two dimensions for advection and shallow-water equations. The two dimensional models are tested for problems with known analytical solution and the shallow water model is applied to the generation of Kevin and gravity waves. In this talk, I will present details involved in both the grid generation and the discretization scheme and conclude with the results. This is my postdoctoral work with Prof. Max Gunzburger at Florida State University.

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**Speaker's Name:** Sou-Cheng (Terrya) Choi

**Speaker's Institution:** University of Chicago/Argonne National Laboratory

**Title of Presentation:** Minimal Residual Methods for Singular Complex Symmetric, Skew Symmetric, and Skew Hermitian Linear Systems and Least-Squares Problems

**Abstract:** While there is no lack of efficient Krylov subspace solvers for Hermitian systems, there are few for complex symmetric systems, which are increasingly important in modern applications including quantum dynamics, electromagnetics, and power systems.

For a large consistent complex symmetric system, one may apply a non-Hermitian Krylov subspace method disregarding the symmetry of $A$, or a Hermitian Krylov solver on the equivalent normal equation or an augmented system twice the original dimension. These have the disadvantages of increasing either memory, conditioning, or computational costs. An exception is a special version of QMR by Freund (1992), but that may be affected by non-benign breakdowns unless look-ahead is implemented; furthermore, it is designed for only consistent and nonsingular problems.

We extend the symmetric and Hermitian algorithm MINRES-QLP by Choi, Paige and Saunders (2011) to complex symmetric systems. The method uses a rank-revealing QLP decomposition of the tridiagonal matrix from a three-term recurrent complex-symmetric Lanczos process. Whether the systems are real or complex, singular or invertible, compatible or inconsistent, MINRES-QLP computes the unique minimum-length, i.e., pseudoinverse, solutions. It is a significant extension of MINRES by Paige and Saunders (1975) with enhanced stability and capability.

Noting the similarities in the definitions of skew symmetric matrices and complex symmetric matrices, we further extend MINRES-QLP for skew symmetric equations. Lastly, via a simple transformation of skew Hermitian systems, we show that MINRES-QLP can readily solve this class of problems.

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**Speaker's Name:** Julianne Chung

**Speaker's Institution:** Virginia Tech

**Title of Presentation:** Windowed Regularization for Image Deblurring via Operator Approximation

**Abstract:** By windowing the components in the spectral domain of the blurring operator and employing different regularization parameters for each window, windowed regularization can be used to obtain superior image reconstructions. However, windowed regularization requires computation of the SVD of the blurring matrix. In this work, we consider suitable surrogate representations of the blurring operator, such as a Krylov subspace approximation, that allow us to make windowed regularization, as well as other SVD-based regularization methods, applicable.

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**Speaker's Name:** Antonio Cicone

**Speaker's Institution:** Georgia Institute of Technology

**Title of Presentation:** Fast computation of tight bounds for the Joint Spectral Radius

**Abstract:** Given $F$, finite set of square matrices of dimension $n$, it is possible to define the Joint Spectral Radius or simply *JSR* as a generalization of the well known spectral radius of a matrix.

The *JSR* evaluation proves to be useful for instance in the analysis of the asymptotic behavior of solutions of linear difference equations with variable coefficients, in the construction of compactly supported wavelets of and many others contexts.

This quantity proves, however, to be hard to compute in general. Gripenberg in [*Computing the joint spectral radius*, Linear Algebra Appl., 234 (1996), pp. 43–60] proposed an algorithm for the computation of lower and upper bounds to the *JSR* based on a four member inequality and a branch and bound technique.

In this talk we describe a generalization of Gripenberg's method based on ellipsoidal norms that achieve a tighter upper bound, speeding up the approximation of the *JSR*. We show the performance of this new algorithm compared with Gripenberg's one.

This talk is based on a joint work with V.Y.Protasov.

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**Speaker's Name:** Tom DeLillo

**Speaker's Institution:** Wichita State University

**Title of Presentation:** Regularization Methods Applied to an Inverse Problem in Gravimetry in Two Dimensions

**Abstract:** A numerical method is developed to locate a domain of uniform mass in two dimensions using measurements of its gravitational field. The method uses a single layer representation of the gravitational potential. The density must be found from the measurements of the field. This problem is ill-posed and requires the use of regularization techniques. Numerical examples are given comparing several methods for selecting optimal regularization parameters for the truncated SVD and conjugate gradient for the normal equations (CGNE).

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**Speaker's Name:** Eric de Sturler

**Speaker's Institution:** Virginia Tech

**Title of Presentation:** Updating Preconditioners for Parameterized Systems

**Abstract:** We will discuss our recent efforts for updating preconditioners for parameterized linear systems. Such systems arise in a range of applications such as acoustics, (parametric) model reduction, and inverse problems. We will show a very general approach to updating preconditioners for modest changes in parameters, thereby significantly reducing the cost of computing preconditioners while maintaining good convergence.

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**Speaker's Name:** Vladimir Druskin

**Speaker's Institution:** Schlumberger

**Title of Presentation:** Model Reduction of Exterior Wave Problems Using Extended Krylov Subspaces with Short Recursions

**Abstract:** Solution of wave problems in unbounded domains requires computation of the exponential of the spatial PDE operator with continuous spectrum. To avoid spurious resonances, the the reduced order model should preserve spectral continuity of the original problem. The authors earlier obtained so-called stability-corrected time-domain exponential (SCTDE) of dumped discretization matrix possessing this conservation property. However, convergence of the Krylov subspace approximation of the SCTDE

matrix function decelerated due to appearance of the square root singularity. We improve convergence by employing extended Krylov subspace algorithm with short recursion by Jagels and Reichel, LAA, 2010. This is joint work with Rob Remis and Mikhail Zaslavsky.

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**Speaker's Name:** Michael Eiermann

**Speaker's Institution:** Technische Universität Bergakademie Freiberg, Germany

**Title of Presentation:** Parameter Identification and Matrix Functions

**Abstract:** Numerical simulation of transient electromagnetic (TEM) geophysical explorations require the computation of the time-evolution of an electrical field $\mathbf{E}(\mathbf{x}, t)$ which can be modelled via

$$\sigma \mathbf{E}_t + \nabla \times (\mu^{-1} \nabla \times \mathbf{E}) = \mathbf{0} \text{ on } \Omega \subset \mathbb{R}^3, \qquad \mathbf{E}(\mathbf{x}, 0) = \mathbf{E}_0(\mathbf{x})$$

(and boundary conditions). Discretization in space leads to a homogeneous linear initial value problem whose solution has the form $\mathbf{u}(t) = \exp(-tA(\sigma))\mathbf{u}_0$, where $A(\sigma)$ discretizes $\sigma^{-1}\nabla \times (\mu^{-1}\nabla \times \cdot)$. In addition to this forward problem, the corresponding inverse problem (parameter identification, i.e., estimating $\sigma$ from some measurements of $\mathbf{E}$) has to be solved for which the Jacobian $\partial \mathbf{u}/\partial \sigma$ or at least its action on a vector is required.

We solve these tasks using Krylov subspace methods for the evaluation of the exponential function and compare this approach to more popular techniques such as the adjoint method.

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**Speaker's Name:** Malena I. Español

**Speaker's Institution:** The University of Akron

**Title of Presentation:** Wavelet-Based Multilevel Methods for Eigenvalue Problems

**Abstract:** We investigate extensions of the wavelet-based multilevel methods introduced in [SIAM J. Sci. Comput, 32 (2010), pp. 299–319] to linear and nonlinear eigenvalue problems. We are particularly interested in eigenvalue problems arising from electronic structure computations of materials. Specifically, we study wavelet-based multilevel methods to solve the discrete time-independent linear Schrödinger equation and the nonlinear Kohn-Sham equation. In these methods, we use the discrete wavelet transform to provide restriction and prolongation operators within a multigrid-type iteration. We present practical numerical examples showing the potential of this approach.

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**Speaker's Name:** Caterina Fenu

**Speaker's Institution:** Department of Mathematics and Computer Science, University of Cagliari, Italy

**Title of Presentation:** Fast Computation of Centrality Indices in Complex Networks

**Abstract:** In complex networks theory, matrix functions are used to extract global information from an undirected unweighted graph G, when applied to its adjacency matrix. We will introduce a new computational method to rank the nodes of a network according to this kind of functions. The procedure is based on the initial approximation of the adjacency matrix, in order to obtain a list of nodes candidates to being the most important, their ranking is then refined by using an algorithm based on Gauss quadrature. The method is compared to other approaches to perform the computation, both on a set of test problems, and on real networks coming from applications, e.g. in software engineering, bibliometry and social network. This is joint work with Lothar Reichel and Giuseppe Rodriguez.

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**Speaker's Name:** Roland W. Freund

**Speaker's Institution:** University of California, Davis

**Title of Presentation:** Krylov Subspace Methods for Two Families of Structured Matrices

**Abstract:** A standard approach to model reduction of large-scale $\ell$-th-order linear dynamical systems of state-space dimension $n$ is to rewrite the system as an equivalent first-order system with state-space dimension $\ell n$ and then employ Krylov-subspace techniques for model reduction of first-order systems. In [BIT, 45 (2005), pp. 495–516], we introduced two families of matrices that exhibit the key structures of first-order formulations of $\ell$-th-order systems and proved that for both families, the Krylov subspaces (of $\ell n$-dimensional state space) can be viewed as multiple copies of certain subspaces (of $n$-dimensional state space). In particular, this result shows that significant savings in computational cost and storage are possible if one can efficiently generate basis vectors of these subspaces of $n$-dimensional state space directly, without first generating basis vectors in $\ell n$-dimensional state space. In this talk, we discuss this problem of the efficient construction of basis vectors for these subspaces. For both families of matrices, we present novel Arnoldi-type procedures for generating orthonormal basis vectors.

This is joint work with Jeffrey Anderson.

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**Speaker's Name:** Andreas Frommer

**Speaker's Institution:** Bergische Universität Wuppertal, Germany

**Title of Presentation:** Analysis of GMRES for Singular Systems

**Abstract:** It is well established that if 0 is not contained in the field of values $\mathcal{F}(\mathcal{A})$ of a square matrix $A$, one can guarantee the convergence of GMRES and restarted GMRES. Moreover, from the geometry of $\mathcal{F}(\mathcal{A})$ one can obtain estimates on the speed of convergence.

In this talk we are concerned with the case where $A$ is singular. There are several known results on the convergence of full GMRES in the singular case, but strong results on restarted GMRES and on the speed of convergence are still missing. Since $0 \in \mathcal{F}(\mathcal{A})$ if $A$ is singular, it is not possible to directly transport the known results for the non-singular case to the singular case. We show how to do so by looking at the field of values of an appropriately reduced matrix.

This work was inspired by our work on preconditioned GMRES for Markov chains where the preconditioner is obtained via an algebraic multigrid method [Bolten et al., *A bootstrap algebraic multilevel method for Markov chains*, SIAM J. Sci. Comput. 33, 3425-3446 (2011)]. It now provides an explanation of the experimentally observed excellent convergence properties.

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**Speaker's Name:** Per Christian Hansen

**Speaker's Institution:** Technical University of Denmark

**Title of Presentation:** Lothar's Sense of Krylov Subspaces

**Abstract:** Krylov subspaces are fascinating mathematical objects with many important applications in scientific computing, e.g., for solving large systems of linear equations, for computing eigenvalues, and for determining controllability in a control system. They are also important tools for regularization of large-scale discretizations of inverse problems, which is the topic of this talk.

In a number of papers, Lothar Reichel has developed theory and algorithms that utilize the efficiency of the Krylov space methods and the ability of the Krylov subspace to capture the important information in an inverse problem. Lothar's work on these algorithms, and his insight into the properties of Krylov subspace methods, has inspired a lot of work that builds on his ideas and methods.

In this talk I will survey Lothar's work on regularization via Krylov subspace methods, and I will illustrate this ideas with some simple examples.

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**Speaker's Name:** Lawrence A. Harris

**Speaker's Institution:** University of Kentucky

**Title of Presentation:** Lagrange Polynomials, Reproducing Kernels and Cubature in Two Dimensions

**Abstract:** We consider sequences of orthogonal polynomials $\{p_n(t)\}$ for weight $w(t)$ that satisfy a three-term recurrence relation with constant coefficients. For example, this includes the Geronimus class and, in particular, all four kinds of the Chebyshev polynomials. For each polynomial $p_n$, we obtain $n+1$ alternation points that are the nodes of an explicit interpolatory quadrature formula for weight $w(t)$ that is exact for all polynomials of degree $2n-1$. This is only one more point than in Gaussian quadrature.

For each $n$, we define two disjoint sets of nodes in $\mathbb{R}^2$ whose coordinates are certain pairs of the alternation points. Using the reproducing kernel, we obtain an explicit formula for Lagrange polynomials of minimal degree for each of these sets of nodes and establish a Lagrange interpolation theorem. This leads to a cubature formula for the product weight function $w(s)w(t)$ that is exact for all polynomials of degree at most $2n-1$ in two variables and has at most one more than the minimal number of nodes possible. Our work extends results of Yuan Xu and Bojanov and Petrova.

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**Speaker's Name:** Michiel Hochstenbach

**Speaker's Institution:** TU Eindhoven, Netherlands

**Title of Presentation:** Probabilistic eigenvalue bounds

**Abstract:** The Lanczos bidiagonalization method for the norm of matrix provides a lower bound for the largest singular value, but no upper bound. Bauer–Fike gives an interval in which a singular value is located, but does not insure that this is the largest one. We present a method that gives an additional probabilistic upper bound, making use of Lanczos polynomials that are implicitly generated during the process. Typical features of the method are a very short run-time and a small probabilistic interval for the largest singular value which holds with a high, user-determined probability.

Similar techniques can also be used in the Lanczos method for the largest and smallest eigenvalue of a symmetric matrix; see [SIAM J. Mat. Anal. Appl., 22 (2000), pp. 254–278].

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**Speaker's Name:** Nicholas Hurl

**Speaker's Institution:** University of Pittsburgh

**Title of Presentation:** Energy Stability of the Crank-Nicolson Leap Frog Method with Time Filters

**Abstract:** Stability is proven for the Crank-Nicolson Leap Frog (CNLF) method with the Robert-Asselin (RA) time filter for systems by energy methods. We derive an equivalent multistep method for CNLF+RA and stability regions are obtained. The time step restriction for energy stability and A-stability of CNLF+RA is smaller than CNLF. We find that RA adds numerical dissipation.

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**Speaker's Name:** Carl Jagels

**Speaker's Institution:** Hanover College

**Title of Presentation:** Krylov and Extended Krylov Subspace Methods Applied to the Approximation of Matrix Functions

**Abstract:** 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 entriesconsist of the recursion coefficients. As in the standard case, theapplication of the process to certain types of linear operators resultsin recursion formulas with few terms. One instance of this occurs whenthe operator is Hermitian. This case produces an analog of the Lanczos

process where the recursion matrix ispentadiagonal. The process applied to the approximation of matrix functions results in a rational approximation method that converges more quickly for an important class of functions than does the polynomial based Lanczos method. It also requires the availability of the inverse of the matrix. This presentation explores the viability of using a conjugate gradient scheme to compute the vectors in the extended Krylov subspace and compares the results with those obtained using the Lanczos method.

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**Speaker's Name:** Ram Jiwari

**Speaker's Institution:** Thapar University, India

**Title of Presentation:** A Differential Quadrature Algorithm for Numerical Treatment of Two-Dimensional Hyperbolic Equation

**Abstract:** The hyperbolic partial differential equations model the vibrations of structures (e.g., buildings, beams, and machines) and they are the basis for fundamental equations of atomic physics. The equations are important for modeling several relevant problems such as signal analysis [J. Appl. Phys. 85 (3) (1999), pp. 1273-1282], wave propagation [Inverse Probl. 9 (1993), pp. 789-812], random walk theory [J. Appl. Math. Stoch. Anal. 11 (1) (1998), pp. 9-28], in many branches of physics, fluid dynamics and aerodynamics, theory of elasticity, optics, electromagnetic etc. In this article, we proposed a numerical technique based on polynomial differential quadrature method (PDQM) to find the numerical solutions of two dimensional hyperbolic equations with Dirichlet and Neumann boundary conditions. The PDQM reduced the problem into a system of second order linear differential equation. Then, the obtained system is changed into a system of ordinary differential equations and lastly, RK4 method is used to solve the obtained system. Numerical results are obtained for various linear and nonlinear hyperbolic equations. The numerical results are found to be in good agreement with the exact solutions and the numerical solutions exist in literature. The technique is easy to apply for multidimensional problems.

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**Speaker's Name:** Stefan Kindermann

**Speaker's Institution:** University of Linz, Austria

**Title of Presentation:** Convergence Rates for Iterative Regularization Methods of Kaczmarz Type

**Abstract:** Kaczmarz iterations have been used for solving ill-posed problems for a long time. They are efficient and flexible methods in situation when the problem can be split into smaller subproblems. It is well-known that Kaczmarz iterations act as regularization methods in rather general situations, and convergence results are known even for nonlinear prolblems and in Banach spaces. However, there are almost no convergence rates results even in the simplest cases. We present a convergence rates analysis for linear ill-posed problems in Hilbert spaces for Landweber-Kaczmarz and iterated Tikhonov-Kaczmarz methods by viewing them as nonsymmetric preconditioned Landweber iterations. The main difficulty here is that by the lack of symmetry, classical approaches by spectral theory are of limited use.

This is joint work with Antonio Leitao, Federal University of Santa Catarina, Brazil.

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**Speaker's Name:** Michaela Kubacki

**Speaker's Institution:** University of Pittsburgh

**Title of Presentation:** Uncoupling Groundwater-Surface Water Flow Using Partitioned Methods

**Abstract:** Partitioned methods for the fully evolutionary Stokes-Darcy equations uncouple the system so that at each time step we solve one groundwater and one surface water problem using codes highly optimized for the physics in each sub-domain. Challenges include maintaining stability and accuracy along the interface and maintaining stability given small parameters. The Crank-Nicolson

Leapfrog method uncouples the system and is second order convergent, however, it is only conditionally stable and the resulting time-step condition is restrictive in regards to certain problem parameters. In addition, even when the stability condition is met the method may become unstable because of spurious oscillations in the unstable mode due to Leapfrog. Time filtering provides added stability, but decreases the order of convergence. By adding stabilization terms to CNLF we create a new method, CNLF-stab, and gain unconditional stability while maintaining second order convergence. Analysis of CNLF-stab is joint work with Marina Moraiti (University of Pittsburgh).

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**Speaker's Name:** Scott Ladenheim

**Speaker's Institution:** Temple University

**Title of Presentation:** A Locally Optimal Combination Preconditioner for GMRES

**Abstract:** A new method for preconditioning GMRES involving two preconditioners is presented. The method applies a linear combination of two preconditioners, called a combined preconditioner. The coefficients for this linear combination are determined at each iteration so as to minimize the residual over an augmented space of search directions. We present how this search space is constructed and how the coefficients for the linear combination are determined. Numerical experiments are provided to demonstrate the potential of this method. This is joint work with Daniel B. Szyld.

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**Speaker's Name:** William Layton

**Speaker's Institution:** University of Pittsburgh

**Title of Presentation:** Nonlinear Filter Algorithms for Modeling and Approximation of High Reynolds Number Flows

**Abstract:** This talk will present a recent approach to modeling turbulence that is modular, allows model accuracy to evolve as understanding of turbulence improves, possesses a strong mathematical foundation characterizing stability, model and numerical energy dissipation, convergence and error estimates. The approach is joint work with Catalin Trenchea (Pitt) and Leo Rebholz (Clemson) and an outgrowth of previous work with Monika Neda (UNLV) and Vince Ervin (Clemson).

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**Speaker's Name:** Xiezhang Li

**Speaker's Institution:** Georgia Southern University

**Title of Presentation:** An Iterative Algorithm for Solving Underdetermined Linear Systems in Computed Tomography

**Abstract:** The sparse solutions of an underdetermined linear system $Ax = b$ under certain condition can be obtained by solving a constrained $l_1$-minimization problem: $\min ||x||_1$ subject to $Ax = b$. An generalized $l_1$ greedy algorithm is proposed. It is implemented as a generalized total variation minimization for reconstruction of medical images with sparse gradients in computed tomography. Numerical experiments are also given to illustrate the advantage of the new iterative algorithm.

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**Speaker's Name:** Nathaniel Mays

**Speaker's Institution:** Wheeling Jesuit University

**Title of Presentation:** Iterated Deconvolution Methods for Turbulence Modeling with Time-Relaxation

**Abstract:** The Navier-Stokes equations (NSE) constitute a well-accepted continuum model for incompressible, viscous, Newtonian fluids with a wide range of applications in climate modeling, energy

sciences, and bio-engineering. Regularization methods are an enticing approach of approximating the NSE solutions due to their simple and efficient implementation. In this talk, we will look at a particular method, the Iterated-Tikhonov deconvolution model to the Leray approximation model of the NSE. We will show convergence of the method, and a numerical experiment supporting the theoretical results.

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**Speaker's Name:** Marina Moraiti

**Speaker's Institution:** University of Pittsburgh

**Title of Presentation:** Effect of Small Parameters and Numerical Methods for the Evolutionary Stokes-Darcy Problem

**Abstract:** In the fully evolutionary Stokes-Darcy problem that models the coupling between groundwater and surface-water flows, certain physical parameters can take very small values. This talk will present the effect of small parameters on the solution as well as a numerical scheme that is unconditionally stable and second order convergent.

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**Speaker's Name:** James Nagy

**Speaker's Institution:** Emory University

**Title of Presentation:** Hybrid Krylov Subspace Methods for Inverse Problems

**Abstract:** Hybrid Krylov subspace methods for inverse problems apply a standard regularization method, such as Tikhonov, to projected least squares problems at each iteration. In this talk we review some previous work on hybrid methods, and describe some new preconditioning approaches. This is joint work with Silvia Gazzola, University of Podova.

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**Speaker's Name:** Akil Narayan

**Speaker's Institution:** University of Massachusetts Dartmouth

**Title of Presentation:** Polynomial Approximation on Nested Unstructured Meshes

**Abstract:** We present a novel method for construction of polynomial interpolation grids on arbitrary Euclidean geometries on which there is a probability density. These grids are very suitable for approximation in high dimensions, constructed using orthogonal polynomial basis sets, and are nested so that refinement strategies can be employed. The construction of these grids is accomplished by combining the Least Orthogonal Interpolant formulation, allowing interpolation on an arbitrary distribution of nodes, and weighted Leja Sequence methods, allowing the well-behaved construction of nested approximation sequences.

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**Speaker's Name:** Silvia Noschese

**Speaker's Institution:** SAPIENZA Università di Roma, Italy

**Title of Presentation:** Some Applications of Inverse Invariant Subspace Problems

**Abstract:** We investigate properties of Krylov subspace methods for large-scale linear systems of equations and eigenvalue problems, by considering how they relate to inverse invariant subspace problems. Given a square matrix $A$, the inverse invariant subspace problem is concerned with determining a closest matrix to $A$ with a prescribed invariant subspace. When $A$ is Hermitian, the closest matrix may be required to be Hermitian. We measure distance in the Frobenius norm. Both the Arnoldi and Lanczos methods determine low-rank approximations of $A$. These low-rank matrices have a Krylov subspace as an invariant subspace. We are interested in whether there are matrices much closer to $A$

with the same invariant subspace. We also are concerned with extensions that allow the matrix $A$ to be rectangular and with applications to Lanczos bidiagonalization, as well as to the recently proposed subspace-restricted SVD method for the solution of linear discrete ill-posed problems. Joint work with Lothar Reichel.

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**Speaker's Name:** Duk-Soon Oh

**Speaker's Institution:** Louisiana State University

**Title of Presentation:** A Balancing Domain Decomposition Method by Constraints for Raviart-Thomas Vector Fields

**Abstract:** A balancing domain decomposition by constraints (BDDC) preconditioner is defined by a coarse component, expressed in terms of primal constraints across the interface between the subdomains, and local components given in terms of Schur complements of local subdomain problems. A BDDC method for vector field problems discretized with Raviart-Thomas finite elements is introduced. Our method is based on a new type of weighted average developed to deal with more than one variable coefficient. A bound on the condition number of the preconditioned linear system is also provided which is independent of the values and jumps of the coefficients across the interface and has a polylogarithmic condition number bound in terms of the number of degrees of freedom of the individual subdomains. Numerical experiments are also presented, which support the theory and show the effectiveness of our algorithm. This is joint work with Olof Widlund and Clark Dohrmann.

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**Speaker's Name:** Gerhard Opfer

**Speaker's Institution:** University of Hamburg, Germany

**Title of Presentation:** Linear Systems in Coquaternions

**Abstract:** Coquaternions, invented 1849 by Sir James Cockle (1819–1895), six years after Hamilton's famous work on quaternions, were mentioned in a recent article related to physics: Dorje C Brody and Eva-Maria Graefe [*On complexified mechanics and coquaternions*, J. Phys. A: Math. Theory, 44 (2011), 072001 (9pp)]. In the abstract the authors write: "In particular, quantum theories characterized by complex Hamiltonians invariant under spacetime reflection are shown to be equivalent to certain coquaternionic extensions of Hermitian quantum theories."

The algebraic structure of coquaternions is similar to that of quaternions, it is an algebra in $\mathbb{R}^4$ but it is not a field. The main algebraic rules are

$$\mathbf{i}^2 = -1,\ \mathbf{j}^2 = 1,\ \mathbf{k}^2 = 1,\ \mathbf{ijk} = 1.$$

We denote the space of coquaternions by $\mathbb{H}_{\text{coq}}$. Linear coquaternionic equations in one variable have the form $l(x) := \sum_{j=1}^{\nu} a_j x b_j$, where $a_j, b_j, x \in \mathbb{H}_{\text{coq}}$ and $\nu \in \mathbb{N}$ is a variable, positive integer. A system in $n$ variables and $m$ equations will be described in the lecture. The matrix case $\mathbf{Ax} = \mathbf{b}$ is only a special case. We will show how to solve all these equations including the Kronecker case $\mathbf{AXB} = \mathbf{C}$, where the main tool is the transition of the coquaternionic system to a real matrix problem.

The paper is jointly written by D. Janovská, Prague. The research was supported by the German Science Foundation, DFG, GZ: OP 33/19-1.

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**Speaker's Name:** Surya Prasath

**Speaker's Institution:** University of Missouri-Columbia

**Title of Presentation:** Multiresolution Regularization Methods for Image Deblurring

**Abstract:** We study the image deblurring problem using multiresolution regularization techniques. To avoid the ringing artifacts associated with the traditional regularization techniques, we introduce gradient fitting regularizer term with a multiresolution strategy. Assuming a convolution based blur kernel $h$, the forward imaging equation reads $f = h \star u + n$ with random noise $n$. We consider an energy minimization scheme based on the total variation to obtain an estimate for the latent image $u$ as well as the kernel $h$:

$$\min_{u,h \in BV(\Omega)} \left\{ \int_\Omega |h \star u - f|^2 + \alpha \int_\Omega |\nabla u| + \beta \int_\Omega |\nabla h| + \gamma \int_\Omega \psi(|\nabla u \downarrow - \nabla f|) \right\}$$

where $\psi$ a convex function, $\nabla u \downarrow$ represents a down-sampled gradient and $\alpha$, $\beta$, $\gamma \geq 0$ are regularization parameters. The minimization is carried out by alternating for the image $u$ and the blur kernel $h$ and we utilize an operator splitting scheme for solving it. In this talk I will provide the convergence result of the iterative scheme along with some latest advances made in regularization based image deblurring techniques. This is a joint work with K. Palaniappan, University of Missouri-Columbia.

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**Speaker's Name:** Ronny Ramlau

**Speaker's Institution:** Johannes Kepler University Linz, Austria

**Title of Presentation:** Inverse Problems in Adaptive Optics

**Abstract:** Large earthbound astronomical telescopes rely on adaptive optics systems in order to achieve a good image quality. The resolution of telescopes depends mainly on its diameter but it is further degraded by atmospheric turbulences. Adaptive optics systems correct for the influence of the atmosphere by measuring the incoming wavefront from bright guide stars. Based on the measurements, an optimal shape of deformable mirrors is computed such that the influence of the atmosphere is corrected after reflection on the deformable mirrors. Several inverse problems are associated to adaptive optics, e.g., wavefront reconstruction from different types of wavefront sensors, atmospheric tomography or optimal mirror fitting. In the talk, we will present new reconstruction methods for these inverse problems. The focus will be on methods that are able to perform the reconstruction in real time, which is a requirement for telescopes as the atmosphere changes rapidly.

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**Speaker's Name:** Michela Redivo-Zaglia

**Speaker's Institution:** Department of Mathematics, University of Padova, Italy

**Title of Presentation:** Vector Generalizations of Shanks' Transformation Applied to Kaczmarz' Method

**Abstract:** The method of alternation projections (MAP) [R. Escalante, M. Raydan, *Alternating Projection Methods*, SIAM, Philadelphia, 2011] is an iterative procedure for finding the projection of a point on the intersection of closed subspaces of an Hilbert space. The convergence of this method is usually slow, and several methods for its acceleration have already been proposed. In this work, we consider a special MAP, namely Kaczmarz' method for solving systems of linear equations [S. Kaczmarz, Angenäherte Auflösung von Systemen linearer Gleichungen, Bull. Acad. Polon. Sci., A35 (1937), pp. 355–357. English translation: Approximate solution of systems of linear equations, Int. J. Control, 57 (1993), pp. 1269–1271]. The convergence of this method is discussed. After giving its matrix formulation and its projection properties, we consider several procedures for accelerating its convergence. They are based on sequence transformations whose kernels contain sequences of the same form as the sequence of vectors generated by Kaczmarz' method. Acceleration can be achieved either directly, that is without modifying the sequence obtained by the method (AK algorithm), or by restarting it from the vector obtained by acceleration (RK algorithm). Numerical examples show the effectiveness of both procedures. This is a joint work with Claude Brezinski.

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**Speaker's Name:** Yousef Saad

**Speaker's Institution:** University of Minnesota, Twin Cities

**Title of Presentation:** Multilevel Low-Rank Approximation Preconditioners

**Abstract:** A new class of preconditioning methods for solving linear systems of equations will be introduced. These methods, which are based on exploiting low-rank approximations to certain matrices, have a number of appealing features. They handle indefiniteness quite well and they are amenable to SIMD computations such as those inherent to GPUs. We will first describe the methods for symmetric positive definite model problems arising from finite difference discretizations of PDEs. We will then show how to extend them to general situations, by exploiting the domain decomposition framework.

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**Speaker's Name:** Hassane Sadok

**Speaker's Institution:** LMPA, Université du Littoral, France

**Title of Presentation:** Review of the Convergence of the Conjugate Gradient Method

**Abstract:** Krylov subspace methods are widely used for the iterative solution of a large variety of linear systems of equations with one or several right hand sides or for solving nonsymmetric eigenvalue problems.

Known as one of the best iterative methods for solving symmetric positive definite linear systems, CG generates as FOM an Hessenberg matrix which is symmetric then triangular. This specific structure may be really helpful to understand how does behave the convergence of the conjugate gradient method and its study gives an interesting alternative to Chebyshev polynomials. The talk deals about some new bounds on residual norms and error $A$-norms using essentially the condition number. We will show how to derive a bound of the $A$- norm of the error by solving a constrained optimization problem using Lagrange multipliers.

This is joint work with Mohammed Bellalij from University of Valenciennes, France.

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**Speaker's Name:** Michael Saunders

**Speaker's Institution:** Stanford University

**Title of Presentation:** Generalized MINRES or Generalized LSQR?

**Abstract:** Given a general matrix $A$, we can construct orthogonal matrices $U$, $V$ that reduce $A$ to tridiagonal form: $U^TAV = T$. We can also arrange that the first columns of $U$ and $V$ are proportional to given vectors $b$ and $c$. For square $A$, an iterative form of this orthogonal tridiagonalization was given by Saunders, Simon, and Yip (SINUM 1988) and used to solve square systems $Ax = b$ and $A^Ty = c$ simultaneously. (One of the resulting solvers becomes MINRES when $A$ is symmetric and $b = c$.)

The approach was rediscovered by Reichel and Ye (NLAA 2008) with emphasis on rectangular $A$ and least-squares problems $Ax \approx b$. The resulting solver was regarded as a generalization of LSQR (although it doesn't become LSQR in any special case). Careful choice of $c$ was shown to improve convergence.

In his last year of life, Gene Golub became interested in "GLSQR" for estimating $c^Tx$ and $b^Ty$ without computing $x$ or $y$ (Golub, Stoll, and Wathen (ETNA 2008)). We review the tridiagonalization process and Gene et al.'s insight into its true identity.

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**Speaker's Name:** Fiorella Sgallari

**Speaker's Institution:** University of Bologna, Italy

**Title of Presentation:** Cascadic Alternating Krylov Subspace Image Restoration Methods

**Abstract:** In this talk we present a cascadic image restoration method which at each level applies a two-way alternating denoising and deblurring procedure. The denoising step is based on wavelet

transforms that allows us also to determine a suitable estimated noise level value which will be used in the Krylov-subspace iterative method for the deblurring step. The cascadic multilevel methods proceed from coarse to fine image resolution levels, with suitable restriction and prolongation operators. The choice of the latter is critical and in this work we introduce a special deblurring procedure based on TV regularization. Computed examples demonstrate the effectiveness of the method proposed for determining high-quality restorations.

Joint work with Serena Morigi and Lothar Reichel.

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**Speaker's Name:** Stephen Shank

**Speaker's Institution:** Temple University

**Title of Presentation:** Krylov Subspace Methods for Large-Scale Constrained Sylvester Equations

**Abstract:** We consider the numerical approximation to the solution of the following system of matrix equations

$$\begin{aligned} A_1X + XA_2 - YC &= 0 \\ XB &= 0 \end{aligned}$$

given $A_1 \in \mathbb{R}^{n\times n}, A_2 \in \mathbb{R}^{m\times m}$ large and sparse and $B, C$ of full rank but having few columns and rows, respectively, for the unknown matrices $X$ and $Y$. We propose a new formulation of the problem that entails the numerical solution of an unconstrained Sylvester equation. The structure of the resulting coefficient matrices call for appropriately designed variants of projection methods. To this end, we propose new enriched approximation spaces, and provide experimental evidence of their effectiveness on benchmark problems. Joint work with Valeria Simoncini.

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**Speaker's Name:** Daniel B. Szyld

**Speaker's Institution:** Temple University

**Title of Presentation:** On Two Practical Methods for the Numerical Solution of Riccati Equations

**Abstract:** The inexact Newton-Kleinman method is an iterative scheme for numerically solving large scale algebraic Riccati equations. At each iteration, the approximate solution of a Lyapunov linear equation is required. Specifically designed projection of the Riccati equation onto an iteratively generated approximation space provides a possible alternative. Our numerical experiments with enriched approximation spaces seem to indicate that this latter approach is superior to Newton-type strategies on realistic problems, thus giving experimental ground for recent developments in this direction. As part of an explanation of why this is so, we derive several matrix relations between the iterates produced by the same projection approach applied to both the (quadratic) Riccati equation and its linear counterpart, the Lyapunov equation.
Joint work with Valeria Simoncini (Bologna) and Marlliny Monsalve (Caracas).

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**Speaker's Name:** Gerd Teschke

**Speaker's Institution:** Institute for Computational Mathematics in Science and Technology, University of Applied Sciences Neubrandenburg, Germany

**Title of Presentation:** Generalized Sampling: Extension to Frames and Inverse Problems

**Abstract:** Generalized sampling is new framework for sampling and reconstruction in infinite-dimensional Hilbert spaces. Given measurements (inner products) of an element with respect to one basis, it allows one to reconstruct in another, arbitrary basis, in a way that is both convergent and numerically stable. However, generalized sampling is thus far only valid for sampling and reconstruction in systems that comprise bases. We extend this framework from bases to frames, and provide fundamental sampling theorems for this more general case. Moreover, we are concerned with extending the idea of generalized sampling to the solution of inverse and ill-posed problems. We furnish evidence of the usefulness of the proposed theories by providing a number of numerical experiments.

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**Speaker's Name:** Yuanzhe Xi

**Speaker's Institution:** Purdue University

**Title of Presentation:** Superfast Randomized Algorithms for Toeplitz Matrices

**Abstract:** We present some superfast and stable algorithms for Toeplitz linear systems, least squares and eigenvalue problems. Based on the displacement equation, a Toeplitz matrix $T$ is first transformed into a Cauchy-like matrix $\mathcal{C}$, which has the properties of fast matrix-vector multiplication and small off-diagonal numerical ranks. By exploring these two properties, the hierarchically semiseparable (HSS) matrix approximation to $\mathcal{C}$ can be constructed in nearly linear complexity. Then one linear complexity linear system solver, three linear complexity least squares solvers and one linear complexity (for each eigenvalue) eigensolver are proposed. The efficiency and stability of our algorithms are studied through various classical numerical tests on matrices varying from well-conditioned to very ill-conditioned ones. In these tests, our new methods are generally much faster and more accurate than some recent solvers.

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**Speaker's Name:** Jianlin Xia

**Speaker's Institution:** Purdue University

**Title of Presentation:** Superfast Selected Sparse Inversion

**Abstract:** We show some ideas of reduced structures for efficiently simplifying or sparsifying the dense matrices (e.g., fill-in) arising in large matrix computations such as sparse solution or inversion. Structured matrix techniques are used to derive and prove the concepts, which result in nearly linear time and storage in the computations. Selected applications include preconditioning, density functional theory, uncertainty quantification, etc. Part of the work is joint with Yuanzhe Xi.

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**Speaker's Name:** Hongguo Xu

**Speaker's Institution:** University of Kansas

**Title of Presentation:** A Factorization Method for Eigenvalues of An Orthogonal Matrix

**Abstract:** The eigenvalue problem of a unitary matrix is a topic that Lothar and his colleagues have been studied for decades. Here we consider the real orthogonal case. We show that a real $2n \times 2n$ orthogonal matrix $Q$ (without $\pm 1$ as eigenvalues) is orthogonally similar to an orthogonal matrix in the product form $\Sigma Z \Sigma Z^T$, where

$$\Sigma = \begin{bmatrix} I_n & 0 \\ 0 & -I_n \end{bmatrix}, \quad Z = \begin{bmatrix} C_1 & S_2^T \\ S_1 & C_2^T \end{bmatrix},$$

where $C_1, C_2, S_1, S_2$ are all upper bidiagonal and $n \times n$, and $Z$ is real orthogonal. Then, the eigenvalues of $Q$ can be obtained by computing a CS decomposition of $Z$.

We borrow the idea from Demmel-Kahan SVD algorithm, and construct a CS decomposition method so that the small singular values of the blocks in $Z$ can be computed accurately. In this way the accuracy of both the real and imaginary parts of eigenvalues are improved.

This is a joint work with Daniela Calvetti and Lothar Reichel.

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**Speaker's Name:** Qiang Ye

**Speaker's Institution:** University of Kentucky

**Title of Presentation:** Accurate Computations of Matrix Eigenvalues with Applications to Differential Operators

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

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**Speaker's Name:** Wenjun Ying

**Speaker's Institution:** Shanghai Jiao Tong University, China

**Title of Presentation:** A Kernel-free Boundary Integral Method for Variable Coefficient Elliptic PDE

**Abstract:** In this talk, I will present a kernel-free boundary integral (KFBI) method for the variable coefficient elliptic partial differential equation on complex domains. The KFBI method is a generalization of the standard boundary integral method. But, unlike the standard boundary integral method, the method does not need to know an analytical expression for the kernel of the boundary integral operator or the Green's function associated with the elliptic PDE. It is not limited to the constant coefficient PDEs. The KFBI method solves the discrete integral equations by an iterative method, in which only the part of the matrix vector multiplication involves the discretization of the boundary integral. With the KFBI method, the evaluation of the boundary integral is replaced by interpolation from a structured grid based solution to an equivalent interface problem, which is solved with a Fourier transform or geometric multigrid based fast elliptic solver. The computational work involved with the KFBI method is essentially linearly proportional to the node number of the structured grid. Even for the PDE with a non-trivial source, the KFBI method also solves the problem efficiently. At the end of the talk, the accuracy and efficiency of the algorithm will be demonstrated with numerical examples for both boundary value problems and (homogeneous and heterogeneous) interface problems.