Purdue University | Department of Computer Science, College of Science

Conference on Scientific Computing & Approximation in Honor of Professor Walter Gautschi

Friday, March 30

9:00-9:30 a.m., LWSN 1142
Registration and reception

9:30-10:00 a.m., LWSN 1142
Opening remarks

10:00-10:45 a.m., LWSN 1142
Keynote
Ronald DeVore, Texas A&M
Estimating a quantity of interest from data

10:45-11:10 a.m.
Break

11:10-12:00 p.m., LWSN 1142
Frank Stenger
Indefinite integration and solving ODE

Walter Gautschi, Purdue University
On a linear algebra conjecture in the theory of orthogonal polynomials

12:00-2:00 p.m., Lawson Commons
Poster session
Lunch will be provided

2:00-2:45 p.m., LWSN 1142
Keynote
Nick Higham, The University of Manchester
Matrix functions and their sensitivity

2:45-3:35 p.m., LWSN 1142
Ahmed Sameh, Purdue University (Emeritus)
A scalable parallel sparse linear system solver

Paul Fischer, University of Illinois Urbana-Champaign
Recent developments in scalable spectral element methods for turbulence

3:35-4:00 p.m.
Break

4:00 p.m.-5:40 p.m., LWSN 1142
Paul Constantine, University of Colorado, Boulder
How Stieltjes, Lanczos, and Gautschi helped me find and exploit low-dimensional structure in functions of several variables

James Lambers, University of Southern Mississippi
Rapid computation of Jacobi matrices from modification by rational weight functions

Fatih Celiker, Wayne State University
Novel nonlocal operators in arbitrary dimension enforcing local boundary conditions

Carl Jagels, Hanover College
Laurent polynomials, pentadiagonal matrices, and Radau rules

6:30 p.m.
Reception and dinner for registered participants
Lafayette Country Club
1500 S. 9th St., Lafayette, IN 47905

Saturday, March 31

8:30-9:00 a.m., LWSN 3102
Welcome reception

9:00-9:45 a.m., LWSN 3102
Keynote
Gradimir V. Milovanović, Serbian Academy of Sciences and Arts
Walter Gautschi and the constructive theory of orthogonal polynomials

9:45-10:10 a.m.
Break

10:10 a.m.-12:15 p.m., LWSN 3102
Dexuan Xie, University of Wisconsin-Milwaukee
Simple series solutions of nonlocal Poisson dielectric models in Legendre polynomials and spherical Bessel functions

Yang Qi, University of Chicago
Complex best r-term approximations almost always exist in finite dimension

Ulises Fidalgo, Case Western Reserve University
Conditions of convergence for non complete interpolatory quadrature rules

Simina Branzei, Purdue University
Universal growth in production economies

12:15 p.m.
Conference ends

Friday, March 30

9:30-10:00 a.m., LWSN 1142

Ronald DeVore
Texas A&M

Estimating a quantity of interest from data

A common scientific problem is that we are given some data about a function *f* and we wish to use this information to either (i) approximate *f* or (ii) answer some question about *f* called a quantity of interest. In approximation circles this problem is referred to as optimal recovery. Meaningful results require extra information about *f* known as model class assumptions. We discuss recent results on optimal recovery which determine optimal algorithms for the two scenarios above under the assumption that *f* is in a model class described by approximation.

11:10-12:00 p.m., LWSN 1142

Frank Stenger

Indefinite integration and solving ODE

This talk involves approximating the indefinite integrals on an interval (a, b), i.e., , $\int_0^x g(t)dt$ and $\int_x^b g(t)dt$. The method is based on n-point interpolation of g at the zeros of a polynomial $P_n(x)$, where the $\{P_n\}$ are orthogonal over (a, b) with respect to a weight function that is positive on (a, b). Demanding exactness of the indefinite integration at the zeros of P_n defines explicit $n \times n$ matrices $B^{\mp}$ with the property that if λ is any eigenvalue of $B^{\mp}$, then $\Re\lambda > 0$, at least for n sufficiently small. I offer \$300 for proof or disproof of my conjecture (to be defined more precisely during my talk), which is that this positivity property holds for all such orthogonal polynomials, and for all $n > 1$. The result yields a novel procedure for solving ODE initial value problems that has $2n - 1$ degree polynomial accuracy.

Walter Gautschi
Purdue University

On a linear algebra conjecture in the theory of orthogonal polynomials

The conjecture deals with the zeros x_j, $j = 1, 2, \ldots, n$, of an orthogonal polynomial of arbitrary degree $n \geq 1$ relative to any positive weight function $w(x)$ on a finite or infinite interval $[a, b]$. If $\ell_k^{(n)}$ denotes the kth elementary Lagrange interpolation polynomial of degree $n - 1$ assuming the value 1 at the zero x_k and the value 0 at all the other zeros x_j, and if $U_n = [u_{jk}^{(n)}]$ and $V_n = [v_{jk}^{(n)}]$ are the matrices of order n whose elements are, respectively, the integrals $u_{jk}^{(n)} = \int_a^{x_j} \ell_k^{(n)}(x)w(x)\mathrm{d}x$ and $v_{jk}^{(n)} = \int_{x_j}^b \ell_k^{(n)}(x)w(x)\mathrm{d}x$, then the conjecture claims that all eigenvalues of U_n and all those of V_n are located in the open right half-plane of the complex plane. The conjecture is verified computationally for a number of classical and nonclassical weight function with n as large as 75. It is also shown that for a symmetric weight function w on $[-a, a]$, $0 < a \leq \infty$, the eigenvalues of U_n and V_n are the same, and so are the matrices $U_n^{(\alpha,\beta)}$ and $V_n^{(\beta,\alpha)}$ themselves, belonging to Jacobi weight functions with parameters as indicated in the superscripts.

2:00-2:45 p.m., LWSN 1142

Nicholas J. Higham
University of Manchester
Matrix functions and their sensitivity

Functions of matrices are widely used in science, engineering and the social sciences, due to the succinct and insightful way they allow problems to be formulated and solutions to be expressed. New applications involving matrix functions are regularly being found, ranging from small but difficult problems in medicine to huge, sparse systems arising in the solution of partial differential equations. The sensitivity of a matrix function is measured by a condition number defined in terms of a Frechét derivative. I will briefly outline the history of matrix functions, summarize some applications, and describe recent developments in computation of matrix functions and estimation of their condition numbers.

2:45-3:35 p.m., LWSN 1142

Ahmed Sameh
Purdue University (Emeritus)
A scalable parallel sparse linear system solver

Numerous computational science and engineering applications give rise to large sparse linear systems for which one needs approximate solutions that yield only modest relative residuals. Further, obtaining approximate solutions for these linear systems often consumes a significant percentage of the total time required by a given simulation. Using classical Krylov subspace iterative schemes with ILU factorization or approximate sparse inverse preconditioning on parallel computing platforms, this situation is aggravated further. In this presentation, we describe a robust parallel algorithm for solving banded linear systems (SPIKE) that reduces memory references and inter-processor communications. This results in an algorithm that achieves significant speed improvement over the classical banded LU-factorization scheme used in ScaLAPACK. This banded solver is generalized to handle general sparse linear systems via the use of sparse matrix reordering schemes. The parallel scalability of our sparse linear system solver (PSPIKE) is compared with ILU- and AMG-preconditioned Krylov subspace methods.

Paul F. Fischer
University of Illinois Urbana-Champaign
Recent developments in scalable spectral element methods for turbulence

We present recent developments in application of the spectral element method (SEM) for the simulation of turbulent flows. The SEM is a high-order weighted residual technique for the solution of partial differential equations that combines local tensor-product-based element representations with globally-unstructured assembly. The local representation admits fast operator evaluations with memory counts that depend only on the total number of grid points, n, independent of the representation order, N. The work complexity is only $O(Nn)$, with very small constants. For the incompressible Navier-Stokes equations, the pressure solve presents the stiffest substep and efficient preconditioning of the associated Poisson problem is of paramount importance. We describe a hybrid Schwarz-multigrid strategy for solving this problem that has strong-scaled to over a million MPI ranks for engineering problems in complicated domains. We then explore the potential of new low- order preconditioning strategies that employ algebraic multigrid solvers. Finally, we look at Schwarz-based extensions to the overall SEM discretization of the Navier-Stokes equations.

4:00-5:40 p.m., LWSN 1142

Paul Constantine
University of Colorado, Boulder
How Stieltjes, Lanczos, and Gautschi helped me find and exploit low-dimensional structure in functions of several variables

In computational science applications, we often represent the map from a model's input parameters to its output predictions as a function of several variables. This representation facilitates methods for uncertainty quantification, design optimization, and sensitivity analysis. However, tools for such studies become prohibitively expensive when the number of inputs is more than a handful. One way to deal with this issue is to identify low-dimensional structure in map from inputs to output that the tools can exploit to enable otherwise infeasible computations. For example, a function's active subspace is the span of important directions in the input space. To exploit such structure when present, the practitioner must know how to transform the model's input space to the reduced input space with a change of measure. Gautschi helped show that Lanczos' method can be interpreted as a discretization of Stieltjes' procedure for computing polynomials that are orthogonal to a given measure. I will show how this work can be applied to help solve high-dimensional problems that arise in uncertainty quantification.

James Lambers
University of Southern Mississippi
Rapid computation of Jacobi matrices from modification by rational weight functions

Given a Jacobi matrix for some measure, the modified Jacobi matrix corresponding to the measure obtained through multiplication by a polynomial weight function can be obtained in linear time. The case of a rational weight function, however, is considerably more difficult. The Minimal Solution method of Gautschi, and the Inverse Cholesky method due to Elhay and Kautsky, require substantially more computational effort, and also perform best in complementary scenarios. In this talk, we explore an alternative approach based on the attempted reversal of the procedure for polynomial modification. This reversal introduces unknown parameters, which are obtained through a rapidly convergent iteration. The resulting procedure completes in linear time. The cases of division by linear and irreducible quadratic factors will be considered.

Joint work with Amber Sumner

Fatih Celiker
Wayne State University
Novel nonlocal operators in arbitrary dimension enforcing local boundary conditions

We present novel nonlocal governing operators in 2D/3D for wave propagation and diffusion that enforce local boundary conditions (BC). The main ingredients are periodic, antiperiodic, and mixed extensions of kernel functions together with even and odd parts of bivariate functions. We present all possible 36 different types of BC in 2D which include pure and mixed combinations of Neumann, Dirichlet, periodic, and antiperiodic BC. Our construction is systematic and easy to follow. We provide numerical experiments that validate our theoretical findings. We also compare the solutions of the classical wave and heat equations to their nonlocal counterparts.

Carl Jagels
Hanover College
Laurent polynomials, pentadiagonal matrices, and Radau rules

Professor Gautschi has investigated extensively modifications of Gaussian quadrature rules. These modifications generally involve an augmentation of the tridiagonal recursion matrix whose spectral decomposition yields the nodes and weights of the Gaussian rule. Analogous rules exist for Laurent polynomials, polynomials that contain reciprocal powers. The analog of the tridiagonal recursion matrix is a pentadiagonal matrix. This talk discusses augmentations of the pentadiagonal matrix that yields a Radau rule that integrates exactly one more positive power and a similar rule for a negative power.

Saturday, March 31

9:00-9:45 a.m., LWSN 3102

Gradimir V. Milovanović
Serbian Academy of Sciences and Arts
Walter Gautschi and the constructive theory of orthogonal polynomials

The central part of this lecture is devoted to Gautschi's constructive theory of orthogonal polynomials on the real line. Beside the basic facts on the coefficients in the three-term recurrence relation for such polynomials, we present the basic procedures for their numerical generation for arbitrary measures, some details on the stability analysis of such algorithms, Christoffel modifications of the measure and corresponding algorithms, as well as available software. Gautschi's theory enables the construction of many interesting classes of non-classical orthogonal polynomials and the corresponding quadratures of Gaussian type, as well as a number of new nonstandard applications of orthogonal polynomials. Some typical examples, further extensions, and applications are also given.

10:10 a.m.-12:15 p.m., LWSN 3102

Dexuan Xie
University of Wisconsin-Milwaukee
Simple series solutions of nonlocal Poisson dielectric models in Legendre polynomials and spherical Bessel functions

The nonlocal dielectric approach has led to new models and solvers for predicting electrostatics of proteins (or other biomolecules), but how to validate and compare them remains a challenge. In this talk, two typical nonlocal dielectric models with multiple point charges inside a dielectric sphere are first introduced. Their analytical solutions are then presented in the expressions of simple series in terms of Legendre polynomials and modified spherical Bessel functions. As a special case, the analytical solution of the classic Poisson dielectric model is also reported in simple series, which significantly improves the well-known Kirkwood's double series expansion. These new series solutions have been programed as a FORTRAN software package, which can input point charge data directly from a protein data bank file. Thus, they can be easily applied to the study of electrostatic continuum models.

Yang Qi
University of Chicago
Complex best r-term approximations almost always exist in finite dimension

In this talk, we show that in finite-dimensional nonlinear approximations, the best r-term approximation of a function f almost always exists over complex numbers but that the same is not true over the reals, i.e., the infimum $\inf_{f_1,\ldots,f_r \in Y} \|f - f_1 - \cdots - f_r\|$ is almost always attainable by complex-valued functions $f_1, \ldots, f_r$ in Y, a set of functions that have some desired structures. Our result extends to functions that possess special properties like symmetry or skew-symmetry under permutations of arguments. For the case where Y is the set of separable functions, the problem becomes that of best rank-r tensor approximations. We show that over the complex numbers, any tensor almost always has a unique best rank-r approximation. This extends to other notions of tensor ranks such as symmetric rank and alternating rank, and to best r-block-terms approximations. When applied to sparse-plus-low-rank approximations, we obtain that for any given r and k, a general matrix has a unique best approximation by a sum of a rank-r matrix and a k-sparse matrix with a fixed sparsity pattern; this arises in, for example, estimation of covariance matrices of a Gaussian hidden variable model with k observed variables conditionally independent of given r hidden variables.

Ulises Fidalgo
Case Western Reserve University
Conditions of convergence for non-complete interpolatory quadrature rules

Non-complete interpolatory quadrature rules were introduced in the 90's by Bloom, Lubinsky, and Stahl. With this type of rules we can compute approximation of integrals with Riemann integrable functions, where the evaluation nodes distribution has an appreciable flexibility. In this context we find a wide family of convergent schemes of nodes. To this end we use some results on the orthogonal polynomial theory, such as: strong asymptotic behavior of orthogonal polynomial with respect to varying measures, and the Wendroff theorem.

Simina Branzei
Purdue University
Universal growth in production economies

We study a basic model of an economy that develops over time, in which players invest their money in different goods and use the bundles obtained for production. We show that a simple decentralized dynamic, where players update their bids proportionally to how useful the investments were, leads to growth of the economy in the long term (whenever growth is possible) but also creates unbounded inequality, i.e., very rich and very poor players emerge. We analyze several other phenomena, such as how the relation of a player with others influences its development and the Gini index of the system.

Joint work with Ruta Mehta and Noam Nisan

Poster Session

1. Ahmed Al-Herz, Purdue University
2/3-Approximation for vertex weighted matching

2. Yu-Hong Yeung, Purdue University
Updating linear systems of equations with augmented matrices

3. S M Ferdous, Purdue University
New approximation algorithms for minimum weighted b-Edge Cover problem

4. Xin Cheng, Purdue University
Graphs for testing parallel coloring algorithms

5. Hessah Alqahtani, Kent State University
Simplified anti-Gauss quadrature rules with applications in linear algebra

6. Mykhailo Kuian, Kent State University
Fast factorization of rectangular Vandermonde matrices with Chebyshev nodes
(joint work with Lothar Reichel and Sergij V. Shiyanovskii)

7. Zhen Chao, University of Wisconsin-Milwaukee
On the semi-convergence of regularized HSS iteration methods for singular saddle point problems

8. Aritra Bose, Purdue University
TeraPCA: A fast and scalable method to study genetic variation in Tera-scale genotypes

9. Agniva Chowdhury, Purdue University
An iterative, sketching-based framework for ridge regression

10. Evgenia-Maria Kontopoulou, Purdue University
Randomized algorithms to approximate logarithm-based matrix functions

11. Duo Cao, Purdue University
Efficient numerical methods for computing structures of quasicrystals

12. Yiqi Gu, Purdue University
An accurate spectral solver for elliptic PDEs in irregular domains

13. Nicole Eikmeier, Purdue University
The cost of a least-squares solution

14. Huda Nassar, Purdue University
Multimodal network alignment