

# Midwest Numerical Analysis Day

May 3, 2008

Talks (other than the plenary talk) are scheduled for 25 minutes in length with a five-minute break between talks. During this time, the speaker can field a question or two, the next speaker can set up her/his presentation, and participants can move between sessions.

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## Alternating Evolution Schemes for Hyperbolic Conservation Laws

Haseena Ahmed, Iowa State University  
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A new alternating evolution (AE) system

$$\partial_t u + \partial_x f(v) = \frac{1}{\epsilon}(v - u), \quad \partial_t v + \partial_x f(u) = \frac{1}{\epsilon}(u - v),$$

is proposed which is an accurate approximation to systems of hyperbolic conservation laws

$$\partial_t \phi + \partial_x f(\phi) = 0, \quad \phi(x, 0) = \phi_0(x).$$

We develop a class of local Alternating Evolution (AE) schemes, where we take advantage of high accuracy of the proposed AE approximation. Our approach is based on a sliding average of the AE system over an interval of  $[x - \Delta x, x + \Delta x]$ . The numerical scheme is then constructed by sampling the averaged system over alternating grids. Higher order accuracy is achieved by a combination of high-order polynomial reconstruction from the obtained averages and a stable Runge-Kutta discretization in time.

The AE schemes have the advantage of easier formulation and implementation, and efficient computation of the solution. For the first and second order local AE schemes applied to scalar laws, we prove the numerical stability in the sense of satisfying the maximum principle and total variation diminishing (TVD) property. Numerical tests for both scalar conservation laws and compressible Euler equations are presented to demonstrate the high order accuracy and capacity of these AE schemes. *Session 1, 4:30 - 4:55.*

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## A Spectral Method for Elliptic Equations: The Dirichlet Problem

Kendall Atkinson, University of Iowa  
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Let  $\Omega$  be an open, simply connected, and bounded region in  $\mathbb{R}^d$ ,  $d \geq 2$ , and assume its boundary  $\partial\Omega$  is smooth. Consider solving an elliptic partial differential equation  $Lu = f$  over  $\Omega$  with zero Dirichlet boundary values. The problem is converted to an equivalent elliptic problem over the unit ball  $B$ , and then a spectral method is given that uses a special polynomial basis. With sufficiently smooth problem parameters, the method is shown to have very fast convergence. Numerical examples illustrate exponential convergence. *Session 1, 1:50 - 2:15.*

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### **Deformations of Heat-Shrinkable Thin Films**

Pavel Bělík, University of St. Thomas  
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We propose and study a model for the behavior of heat-shrinkable thin films such as PET. We compare the model to those derived rigorously through the techniques of  $\Gamma$ -convergence and give numerical results. (Joint work with M. Shvartsman (UST), C. Thomas and B. Jennings (3M).)  
*Session 2, 11:20 – 11:45.*

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### **On the Solution of Ill-Conditioned Symmetric Positive Definite Systems of Linear Equations with an Application to RBF Interpolation**

Greg Fasshauer, Illinois Institute of Technology  
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In practical computing situations one often faces the problem of having to solve an ill-conditioned system of linear algebraic equations. One of the best-known approaches to deal with such problems involves the singular value decomposition which was shown to be computationally feasible by Gene Golub, William Kahan and Christian Reinsch in the late 1960s and early 1970s. Another technique perhaps much less known is due to James Riley (*Solving Systems of Linear Equations With a Positive Definite, Symmetric, but Possibly Ill-Conditioned Matrix*, *Mathematical Tables and Other Aids to Computation* 9/51 (1955), 96–101). We will explain Rileys algorithm (which we just recently became aware of) and compare it to two SVD-implementations on a problem that arises when determining optimal shape parameters for radial basis function interpolants of scattered data. *Session 2, 2:20 – 2:45.*

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### **Eight Bit Floating Point**

James Hurt, Enventive Engineering  
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As a pedagogical tool, and to understand the impact of finite precision arithmetic on various algorithms, I have developed the concept of eight bit floating point numbers. I will outline the format of these numbers and discuss some features of floating point arithmetic, including the IEEE 64 bit system, using eight bit numbers as an illustration. *Session 2, 2:50 – 3:15.*

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### **Exponential Time Differencing for Nonlinear Reaction-Diffusion Systems-Algorithms and Implementation**

Britta Janssen, University of Wisconsin–Milwaukee  
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We discuss new versions of some exponential time differencing (ETD) schemes designed to handle various computational difficulties from nonlinear systems with irregular data. The focus of this presentation is on implementation of the ETD-Pade schemes and their performance in numerical simulation. *Session 1, 11:50 – 12:15.*

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## A New Class of Curve Search Methods in Nonlinear Optimization

Laurent Jay, University of Iowa

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In this talk we show that the field of nonlinear optimization may benefit from techniques developed primarily for the numerical integration of ordinary differential equations (ODEs). We propose a new class of curve search methods for problems in unconstrained nonlinear optimization. A first idea is to obtain at each step the parametrization of a desired curve with better local minimization properties than a straight line obtained by line search. We show in particular that the curve corresponding to the the gradient flow is generally not the most desirable curve. A second idea is to approximate a desired curve with a curve analogous to a dense output formula of a Runge-Kutta method for ODEs. This is work in progress. *Session 1, 3:30 – 3:55.*

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## The Cell Boundary Element Method

Youngmok Jeon, Ajou University, Korea (visiting at UMN, Twin Cities)

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The Cell Boundary Element Method for elliptic PDEs is presented. The cell boundary element method can be understood as the finite element version of the finite volume method, in that it is constructed on the mesh of the FEM(no dual mesh), but it has the flux conservation property. The MsCBE, MultiScale CBEM, is also introduced. It is based on the Over Sampling technique by T. Hou. Some numerical experiments are also presented which emphasize the importance of flux conservation property for a numerical method. *Session 2, 4:30 – 4:55.*

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## Multiwavelets on a Finite Interval

Fritz Keinert, Iowa State University

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Wavelets are naturally defined on the whole real line. Using them on a finite interval requires additional endpoint functions and modifications in the decomposition and reconstruction algorithms. This talk describes one approach to constructing endpoint functions, and discuss some unexpected new features that appear in the multiwavelet case. *Session 1, 10:20 – 10:45.*

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## Inverse Scattering of Sound-Soft Obstacles in 3D

Andreas Kleefeld, University of Wisconsin–Milwaukee

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An introduction to the inverse scattering problem for sound-soft obstacles in 3D is given as well as how to solve this problem. This is achieved using integral equations over surfaces. They are solved numerically with a boundary element method (BEM). First of all, the direct scattering problem is presented. It calculates far field data for a given smooth or piecewise smooth obstacle. The far field depends on the wavenumber  $k$  and the incident wave. Afterward, the inverse scattering problem is described. It tries to find the shape of an obstacle for given far field data. Unfortunately, this problem is nonlinear and ill-posed. Therefore, we use the nonlinear Landweber method. It is an iterative regularization scheme to obtain approximations for the unknown boundary of the obstacle. 3D smooth and piecewise smooth obstacles are reconstructed with this method. The latter case is nowhere to be found in the literature. *Session 2, 1:50 – 2:15.*

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## The Direct Discontinuous Galerkin (DDG) Methods for Diffusion Problems

Hailiang Liu, Iowa State University  
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A new discontinuous Galerkin finite element method for solving diffusion problems is introduced. Unlike the traditional LDG method, the scheme, called the direct discontinuous Galerkin (DDG) method, is based on the direct weak formulation for solutions of parabolic equations in each computational cell, and let cells communicate via the numerical flux  $\widehat{u}_x$  ONLY. We propose a general numerical flux formula for the solution derivative, which is consistent, and conservative; and we then introduce a concept of admissibility to identify a class of numerical fluxes so that the nonlinear stability for both one dimensional and multi-dimensional problems are ensured. Furthermore, when applying the DDG scheme with admissible numerical flux to the one dimensional linear case,  $k$ th order of accuracy in an energy norm is proven when using  $k$ -th degree polynomials. The DDG method has the advantage of easier formulation and implementation, and efficient computation of the solution. A series of numerical examples are presented to demonstrate the high order accuracy of the method. In particular, we study the numerical performance of the scheme with different admissible numerical fluxes. *Session 1, 10:20 – 10:45.*

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## Numerical Analysis Challenges for the Quasicontinuum Method

Mitchell Luskin, University of Minnesota  
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Many challenging scientific computing problems have too many degrees of freedom and too many time scales to be accurately computed without multiscale and multiphysics computational methods. These computational methods need a solid theoretical basis to be capable of reliable scientific prediction. We need to develop numerical analysis to guide the development of algorithms to determine where to utilize more accurate, but computationally demanding, physics models.

The quasicontinuum (QC) multiscale method has been successfully used to efficiently couple atomistic and continuum models for crystalline solids. Regions with highly non-uniform deformations such as around crack tips and defects require the accuracy of atomistic models, whereas continuum models can be used in regions with nearly uniform deformations to reduce the number of degrees of freedom by piecewise linear interpolation and mesh coarsening.

It is not known how to couple the atomistic and continuum models to simultaneously satisfy conditions of accuracy, efficiency, and conservation. We will present a theoretical framework for evaluating the goal-oriented accuracy of the atomistic-continuum interface, and we will apply this theory to analyze several quasicontinuum approximations.

We will also present an a posteriori goal-oriented error estimator and a corresponding adaptive atomistic-continuum modeling and mesh refinement algorithm to enable a quantity of interest to be efficiently computed to a predetermined accuracy.

Joint work with Marcel Arndt and Matthew Dobson. *Plenary Speaker, 9:00 – 9:50.*

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## On the Numerical Anisotropy of Isotropic Wave-like Partial Differential Equations

Adrian Sescu, MIME Department, University of Toledo, Ohio

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The propagation of waves in multidimensional space are mostly described by partial differential equations (PDEs) of hyperbolic type. Because of the deficiency of analytical solutions, the PDEs are most frequently solved by using numerical approximations. One such approach is the method of lines in which the spatial derivatives are discretized by using finite difference or/and volume methods, and the solution is found by an adequate time marching method. There are several errors resulting from the numerical approximation of PDEs, common to both one- and multi-dimensional problems; some examples include truncation, round-off, dispersion or dissipation errors. There is one mostly disregarded error specific to multi-dimensional problems, called numerical anisotropy or isotropy error. It is mainly related to the spatial discretization or, more specifically, to the distribution of the grid points in the spatial domain. This work tries to give an insight regarding the numerical anisotropy in two-dimensions, and finally intends to offer a way to alleviate the occurrence of this type of error. Optimized finite difference schemes are derived which are designed to have improved isotropy compared to existing schemes. The derivation is performed based on both Taylor series expansion and Fourier analysis. The isotropy corrector factor, a parameter of the schemes, can be determined by minimizing the integrated error between the phase or group velocities on different spatial directions. The schemes are restricted to equally-spaced Cartesian grids, so the generalized curvilinear transformation methods and Cartesian grid methods are good candidates. *Session 1, 2:50 – 3:15.*

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## Modeling Delay in Spiking Neurons

Mikhail Shvartsman, University of St. Thomas

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We consider the model of spiking neurons and role of the delay mechanism in neuronal signal propagation. The spatial separation of signals is taken into account and we compare the solutions generated by input in Hodgkin-Huxley and FitzHugh-Nagumo systems. *Session 1, 10:50 – 11:15.*

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## Modeling Growing Viscoelastic Tissues: Numerical Aspects

Magda Stolarska, University of St. Thomas

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Living systems are extremely complex, and to fully understand them researchers must focus on various individual areas of their internal organization. One such area that is of significant interest is cell and tissue mechanics. Single cells and tissues interact mechanically with their surroundings, yet it is often difficult to experimentally measure the nature of the forces that result from the interactions. As a result, mathematical modeling and simulation can be extremely useful. However, due to the fact that many living tissues exhibit viscoelastic response and are incompressible, simulation of their mechanical response presents significant computational difficulties. In this talk, I will present a mathematical model of the mechanics involved in a growing, viscoelastic tissue, the computational difficulties that arise in finite element simulations of such a model, and techniques that allow us to overcome some of the difficulties. *Session 2, 3:30 – 3:55.*

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## A Spectrally Accurate Boundary Integral Method for Two-Dimensional Stokes Flows

Xu Sun, Illinois Institute of Technology  
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A new numerical method is presented for interface dynamics in two-dimensional Stokes flows. It is based on the boundary integral formulation of the problem. The singular behavior of the integrands appeared in the boundary integral equations is analyzed and the equations are solved by Nystrom method. The method is spectrally accurate in space. The evolution equation is formulated in a theta-arclength coordinates and solved by Runge-Kutta method of second order. Several numerical examples are provided to verify theoretical prediction. *Session 2, 11:50 – 12:15.*

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## MIME Runge-Kutta methods for Time-Dependent PDEs

David Voss, Western Illinois University  
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Mono-Implicit-Mono-Explicit (MIME) Runge-Kutta schemes are developed for spatially discretized time-dependent partial differential equations. These implicit-explicit (IMEX) methods possess higher stage order than the typically used SDIRK methods while offering increased efficiency with the potential for parallelism. Moreover, MIME Runge-Kutta methods maintain the linear stability properties of IMEX Runge-Kutta methods based on SDIRKs. Numerical results on test problems confirm these properties. *Session 1, 4:00 – 4:25.*

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## Exponential Time Differencing for Nonlinear Reaction-Diffusion Systems- Theory and Algorithms

Bruce Wade, University of Wisconsin-Milwaukee  
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We introduce a new version of some exponential time differencing (ETD) schemes designed to handle various computational difficulties from nonlinear systems with irregular data. The ETD scheme uses a Pade approximation of matrix exponential functions with operator splitting, and to deal with the problem of nonsmooth data it employs several steps of an ETD scheme using a sub-diagonal Pade formula for damping. In this first part of the presentation, theory and algorithm development will be discussed. *Session 1, 11:20 – 11:45.*

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## A Field Space-Based Level Set Method for Computing Multi-Valued Solutions to 1D Euler-Poisson Equations

Zhongming Wang, Iowa State University  
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We present a field space based level set method for computing multi-valued solutions to one-dimensional Euler-Poisson equations. The system of these equations has many applications, and in particular arises in semiclassical approximations of the Schrödinger-Poisson equation. The proposed approach involves an implicit Eulerian formulation in an augmented space — called field space, which incorporates both velocity and electric fields into the configuration. Both velocity and electric fields are captured through common zeros of two level set functions, which are governed by a field transport equation. Simultaneously we obtain a weighted density  $f$  by solving again the field transport equation but with initial density as starting data. The averaged density is then resolved by the integration of the obtained  $f$  against the Dirac delta-function of two level set functions in the field space. Moreover, we prove that such obtained averaged density is simply a linear superposition of all multi-valued densities; and the averaged field quantities are weighted superposition of corresponding multi-valued ones. Computational results are presented and compared with some exact solutions which demonstrate the effectiveness of the proposed method. *Session 2, 10:50 – 11:15.*

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## An Efficient Parallel Algorithm for a General Blood-Tissue Transport and Metabolism Model Governed by a System of Nonlinear Hyperbolic Equations

Dexuan Xie, University of Wisconsin–Milwaukee  
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Fast algorithms for simulating mathematical models of coupled blood-tissue transport and metabolism are critical for the analysis of data on transport and reaction in tissues. This talk will present a novel parallel algorithm for solving a general blood-tissue transport and metabolism model, governed by a large system of one-dimensional hyperbolic partial differential equations. The key part of the algorithm is to approximate the model as a group of independent ordinary differential equation (ODE) systems such that each ODE system has the same size as the model and can be integrated independently. Thus the method is easily implemented on a parallel machine by using domain decomposition techniques. The accuracy of the algorithm is demonstrated for solving a simple blood-tissue transport model introduced by Sangren and Sheppard (Bull. Math. Biophys. 15:387-394, 1953), which has an analytical solution. A parallel Fortran-MPI program package was also developed and applied to solving a large-scale coupled blood-tissue transport and metabolism model (Beard, PLoS Comp Biol 2(9):e107, 1093-1106, 2006), which simulates advective oxygen transport and oxidative energy metabolism by a system of 30 nonlinear hyperbolic equations. Numerical experiments made on a distributed-memory parallel computer (an HP Linux cluster) and a shared-memory parallel computer (a SGI Origin 2000) demonstrate the computational efficiency of the algorithm. *Session 2, 4:00 – 4:25.*

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## Convergence Analysis of Truncated Incomplete Hessian Newton Minimization

Mazen Zarrouk, University of Wisconsin–Milwaukee

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In a recent paper, we proposed and analyzed a new type of a modified Newton line-search method for minimizing a twice continuously differentiable real-valued function  $f$  defined on a bounded domain  $\mathcal{D}$  of  $R^n$  which contains a minimum point  $x^*$  of  $f$ , where the Hessian matrix  $H(x)$  in  $\mathcal{D}$  (i.e., the second derivative of  $f$  at  $x \in \mathcal{D}$ ) is dense but can be well approximated by a sparse incomplete Hessian matrix,  $M(x)$ . This method is called the truncated incomplete Hessian Newton method (T-IHN). We proved that T-IHN is globally convergent even with an indefinite incomplete Hessian matrix or an indefinite preconditioner, which may happen in practice. We also proved that when the T-IHN iterates are close enough to a minimum point then T-IHN admits a steplength of one that satisfies the Wolfe's conditions and that T-IHN has a Q-linear rate of convergence. As an application and to demonstrate the efficiency of T-IHN, we constructed a particular T-IHN algorithm for minimizing a biomolecular potential energy function, and numerically tested it for a protein model problem based on a widely used molecular simulation package, CHARMM. Numerical results confirm the theoretical results, and demonstrate that T-IHN can have a better performance (in terms of computer CPU time) than most CHARMM minimizers. In this talk, we will describe the T-IHN method, show its major analytical convergence results, briefly describe the construction of the incomplete Hessian matrix for the energy problem using a simple cutoff strategy as well as the implementation of the particular T-IHN algorithm based on CHARMM, and present some of promising numerical results of T-IHN in comparison with the other CHARMM minimizers. *Session 1, 2:20 – 2:45.*