Recent Advances in Numerical Methods and Scientific Computing
Abstracts

Saturday 10:15 – 12:15
Carol Woodward, LLNL
Victoria Howle, Texas Tech
Misha Kilmer, Tufts University
Carla D. Martin, James Madison University

Saturday 3:15 – 5:15
Jingmei Qiu, Colorado School of Mines
Fengyan Li, Rensselaer Polytechnic Institute
Lorena Barba, Boston University
Sarah Olson, WPI (as of Fall 2011)

Saturday 10:15 – 12:15

Accelerated Fixed Point Methods for Subsurface Flow Problems
Carol Woodward, LLNL
Authors: P. A. Lott, H. F. Walker, C. S. Woodward, and U. M. Yang

We investigate effectiveness of an acceleration method applied to the modified Picard iteration for simulations of variably saturated flow. We solve nonlinear systems using both unaccelerated and accelerated modified Picard iteration as well as Newton's method. Since Picard iterations can be slow to converge, the advantage of acceleration is to provide faster convergence while maintaining advantages of the Picard method over the Newton method. Results indicate that the accelerated method provides a robust solver with significant potential computational advantages.

Block Preconditioners for Coupled Fluid Problems
Victoria Howle, Texas Tech

Many important engineering and scientific systems require the solution of extensions to standard incompressible flow models, whether by coupling to other processes or by incorporating additional nonlinear effects. Finite element methods and other numerical techniques provide effective discretizations of these systems, and the generation of the resulting algebraic systems may be automated by high-level software tools such those in the Sundance project, but the efficient solution of these algebraic equations remains an important challenge.

Frequently, the nonlinear equations are linearized by a fixed point or Newton technique, and then the linear systems are solved by a preconditioned Krylov method such as GMRES. In this talk, we discuss important extensions to the methodology and analysis of preconditioning such systems. In particular, we extend existing block-structured preconditioners (such as those of Elman, et al.) to address some of these coupled systems, showing how an effective preconditioner for Navier-Stokes may be combined with one for some other process such as convection-diffusion of temperature to obtain a preconditioner for the Newton linearization of a nonlinearly coupled system such as B\'enard convection.

Tensor factorizations in image processing
Misha Kilmer, Tufts University

Consider a collection of two-dimensional images. This set can be stored as a third order tensor (multi-way array). In this talk, we investigate the use of new tensor factorizations as a sum of k, product cyclic tensors, that are suitable for compression of such multiway data, and which can be tuned to preserve features such as non-negativity.

Order-p Tensors: Factoring and Applications
Carla D. Martin, James Madison University

Tensor decompositions or representations of multiway arranys have been motivated by applications. Given that data is often multidimensional, extending powerful linear algebra concepts to tensors has been crucial for interpretation of the data as well as data compression. In this talk, we describe a factorization that is SVD-like in nature, for general order-p tensors. The idea is best explained using recursive programming, but is implemented directly using the fast Fourier transform. In particular, we present an alternative representation for order-p tensors as a 'product' of tensors which is reminiscent of the matrix factorization approach. This leads to a different generalization of the matrix SVD. Furthermore, our framework allowed other matrix factorizations to be extended to tensors. We also present algorithms for computation and potential applications.

Saturday 3:15 – 5:15

Conservative high order semi-Lagrangian hybrid finite element-finite difference methods for the Vlasov equation
Jingmei Qiu, Colorado School of Mines
Authors: Jingmei Qiu and Wei Guo

We propose a novel conservative hybrid finite element-finite difference method for the Vlasov equation. The methodology uses semi-Lagrangian discontinuous Galerkin (DG) for spatial advection, and semi-Lagrangian finite difference WENO for velocity acceleration/deceleration. Such hybrid method enjoys the advantage of DG in its compactness and ability in handling complicated geometry and that of the WENO in its robustness in resolving sharp gradients. Simulation results will be demonstrated to show the performance of the proposed method.

Positive Preserving discontinuous Galerkin methods for ideal MHD equations

Fengyan Li, Rensselaer Polytechnic Institute

Ideal MHD system arises in astrophysics and energy physics, it consists of a set of nonlinear hyperbolic conservation laws. In this presentation, we report our recent progress in developing positive preserving discontinuous Galerkin (DG) and central DG methods for this system. Such methods preserve positivity of density and pressure in the simulation.

Hierarchical Algorithms in Heterogeneous Systems for the Exascale Era

Lorena Barba, Boston University

There is a potentially transformative combination in the use of fast hierarchical algorithms with heterogeneous systems. In particular, GPU-based clusters are likely to be a leading contender in the exascale era, and algorithms that adapt well to this hardware will become key players. Among these, the fast multipole method is particularly favorable for heterogeneous many-core hardware. In fact, this algorithm offers exceptional opportunities to enable exascale applications. Its exascale-suitable features include: (i) intrinsic geometric locality, and local access patterns via particle indexing techniques; (ii) temporal locality achieved via an efficient queuing of GPU tasks before execution; and (iii) global data communication and synchronization, often a significant impediment to scalability, is a soft barrier for the FMM. Recent innovations in this area indicate a potential for unprecedented performance with these algorithms

Dynamics of an elastic rod in a viscous fluid: Stokes Formulation

Sarah Olson, WPI (as of Fall 2011)

The generalized immersed boundary (IB) method simplifies the interaction of a slender, elastic rod with a surrounding fluid by representing the rod by its centerline and keeping track of an evolving orthnormal director basis. In this method, the IB applies torque and force to the surrounding fluid. Additionally, the equations of motion of the IB involve the local angular velocity and the local linear velocity of the fluid. We will present a Stokes formulation of the generalized immersed boundary method. In this formulation, the fluid velocity resulting from a distribution of regularized forces and torques is expressed in terms of regularized Stokeslets and rotlets. The dynamics of an open and closed rod with curvature and twist in a viscous fluid will be studied as a benchmark problem. This will be compared to previous generalized immersed boundary implementations that solved the full Navier-Stokes equations using finite difference methods.

This work has been in collaboration with Sookkyung Lim at University of Cincinatti, Ricardo Cortez at Tulane University, and Lisa Fauci at Tulane University.

.