Recent Advances in Computational PDEs and their Applications

Organizer: *Xinfeng Liu* (xfliu@math.sc.edu), University of South Carolina

Abstract

This minisymposium focuses on recent advances on efficient and accurate numerical methods for PDEs and their various applications in physical or biological systems. The invited researchers will discuss a wide range of computational methods ranging from efficient finite element and finite difference methods, adaptive methods, multiscale methods, to spectral methods and kinetic Monte Carlo simulations. Computational challenges will be discussed, and new computational techniques will be introduced for various applications.

<u>**Session 1:**</u>

- **Speaker:** *Hong Wang* (hwang@math.sc.edu), University of South Carolina,

  Title: A component-based Eulerian-Lagrangian formulation for multicomponent multiphase compositional flow and transport in porous media

  Abstract: We present a Eulerian-Lagrangian formulation for multicomponent multiphase compositional flow and transport in porous media, by utilizing momentum balance to define a barycentric component velocity for each component based on phase velocities and the relative presence of the component in each phase. Numerical experiments are presented to investigate the performance of the method, compared with widely used explicit and implicit upwind methods in the context of a two phase, three component compositional flow and transport process. These results demonstrate that the Eulerian-Lagrangian formulation not only represents the solutions properly, but also has obvious computational benefits.

- **Speaker:** *Lili Ju* (ju@math.sc.edu), University of South Carolina,

  Title: An Efficient and Accurate Parallel Computational Model for 3D Thermo-Mechanical Stokes Ice-Sheet Flow Simulation

  Abstract: This talk mainly focuses on the development of an efficient, three-dimensional, thermo-mechanical nonlinear-Stokes flow computational model for ice sheet simulation. The model is based on the parallel finite element model developed by Leng et. al (2012) and features high-order accurate finite element discretizations on variable resolution grids, improved iterative solution methods for treating nonlinearity of the Stokes problem, a new high-order accurate finite element solver for the temperature equation, and a new conservative finite volume solver for handling mass conservation.

- **Speaker:** *Steven Wise* (swise1@utk.edu), University of Tennessee,

  Title: A Linear Iteration Solver for a Second-Order Convex Splitting Scheme for a Thin Film Model without Slope Selection

  Abstract: I will describe a linear iteration algorithm to efficiently implement a second-order energy stable numerical scheme for a model of epitaxial thin film growth without slope selection. The PDE is a highly nonlinear, fourth-order parabolic equation that results as the L^2 gradient flow of an appropriate energy. The energy stability for the scheme is preserved by a careful choice of the second-order temporal approximation for the nonlinear term. The resulting scheme is highly nonlinear, and its implementation is non-trivial. I will describe a linear iteration algorithm to solve the resulting nonlinear system. To accomplish this we introduce an $O(s^2)$ artificial diffusion term that leads to a contraction mapping property. As a result, the highly nonlinear system can be decomposed as an iteration of purely linear solvers, which can be very efficiently implemented with the help of FFT or other fast algorithms. I will discuss the convergence analysis for the numerical scheme and show some numerical simulation results that demonstrate the efficiency of the linear iteration solver. This is joint work with Wenbin Chen, Cheng Wang, and Xiaoming Wang.

- **Speaker:** *Xinfeng Liu* (xfliu@math.sc.edu), University of South Carolina,

  Title: Operator-splitting methods for convection-reaction-diffusion equations

  Abstract: For reaction-dffusion systems with both stff reaction and diusion terms, implicit integration factor (IIF) method and its high dimensional analog compact form (cIIF) serve as an efficient class of time-stepping methods. For nonlinear hyperbolic equations, front tracking method is one of the most powerful tools to dynamically track the sharp interfaces. Meanwhile, weighted essentially non-oscillatory (WENO) methods are a class of start-of-the-art schemes with uniform high order of accuracy in smooth regions of the solution. In this talk, IIF/cIIF is coupled with front tracking or WENO by the second-order symmetric operator splitting approach to solve advection-reaction-dffusion equations. In the methods, IIF/cIIF methods treat the stff reaction-dffusion equations, and front tracking/WENO/BFECC methods handle hyperbolic equations that arise from the advection part depending on various applications.

Session 2:

- **Speaker:** *Yukun Li* (yli70@utk.edu), University of Tennessee,

  Title: Discontinuous Galerkin methods for the Allen-Cahn Equation and its sharp interface limit

  Abstract: In this presentation, we propose and analyze a fully discrete scheme for the Allen-Cahn equation arising from phase transition in material science. The Backward Euler Method in time and Discontinuous Galerkin Method in space are used. The primary goal of this presentation is to establish some useful a priori error estimates for the proposed methods by focusing on the dependence of the error bounds on ϵ, which is called interaction length in material science. Optimal order and quasi-optimal order error bounds are given under different constraints on mesh size h, time step k and different regularity assumptions on the initial function u_0, and the error bounds depend on ϵ only in some lower polynomial order for small ϵ. The key step is to establish a spectrum estimate result in broken sobolev space by using the spectrum estimate result of Feng. Finally, the error estimates are used to establish convergence and the rates of convergence of the zero level set of the fully discrete solution to the classical and generalized motions by mean curvature flow.

- **Speaker:** *Jia Zhao*, (zhao62@mailbox.sc.edu), University of South Carolina,

  Title: 3D mathematical modeling and simulation of biofilm

  Abstract: Bacteria are ubiquitous. Instead of living individually, bacteria appear to live in a society called biofilm, which is a microorganism with glue-like extra-cellular polysaccharide substance. In this talk, a 3D mathematical model by phase-field approach has been derived, together with numerical implementation. The hydrodynamic effects on biofilm will be discussed, as well as the mechanism of antibiotic persistence and quorum sensing. The biofilm spreading accounting for cell motility will be analyzed as well.

- **Speaker:** *Xiaogang Yang* (yangxiaoxiaogang@gmail.com), University of South Carolina and Nankai University (China),

  Title: Capillary instability of an active liquid crystal

  Abstract: In this talk, we study the capillary or Rayleigh instability of a cylindrical active liquid crystal jet in a passive air ambient. We adopt an active polar nematic model which is a director based active liquid crystal solution model. We first identify a set of plausible steady states for the liquid jet. Then, we conduct a linear stability analysis for the axisymmetric cylindrical free surface jet of active liquid crystals. The instability exists in a window of finite wave number. The cut-off wave number is given by the geometry of the underlining steady state while the growth rate depends on the model parameters, especially, the effective viscosity, anchoring condition at the free surface, and the activity parameter of the active material. We discuss the growth rate dependence on the model parameters in details. The role of the long range elasticity to the rheological prediction will be discussed as well.

- **Speaker:** *Che Wang* (wang324@email.sc.edu), University of South Carolina,

  Title: A fast Galerkin method with efficient matrix assembly for a nonlocal diffusion model

  Abstract: Peridynamic theory provides an appropriate description of the deformation of a continuous body involving discontinuities or other singularities. However, the models are nonlocal which require $O(N^3)$ of computational cost and $O(N^2)$ of memory where N is the number of unknowns. We develop a fast method for the model by exploiting the structure of the stiffness matrix. The method reduces the computational work from $O(N^3)$ to $O(Nlog^2N)$ and the memory requirement from $O(N^2)$ to $O(N)$ without using any lossy compression. This shows the benefit of the fast method.