Analysis and Applied Mathematics Seminar

Efficient high-order algorithms for drift-diffusion and electromagnetic systems

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Abstract: Simulations of ion channels and metamaterial devices are of considerable technological importance and also present very interesting and challenging problems from the perspective of numerical algorithms for PDEs. Robust and rapidly convergent numerical methods are essential to solve these systems. I will discuss efficient high-order algorithms for solving drift-diffusion models that describe the transport of charge-carriers coupled with a Poisson equation for electric potential. The spatial discretization is based on a standard spectral-element formulation with body-fitted hexahedral elements. The temporal discretization is a mixed implicit-explicit method using kth-order backward-difference formulas and extralpolation as well as a pseudo-timestepping approach based on Jacobi-free Newton Krylov methods. The electric potential is governed by a Poisson equation to be solved at each timestep. This problem is solved with GMRES iteration, preconditions with spectral-element multigrid. Validation of the algorithms is demonstrated with convergence studies and computational results for potassium ion channels. A second problem of interest is the study of novel ultra-thin flat metalens and graphene-based two-dimensional materials, whose behavior is governed by the solutions to Maxwell's equations. I will discuss high-order spectral element discontinuous Galerkin schemes for solving these equations. High-order discretizations offer minimial numerical dispersion and dissipation while providing high performance to deliver fast, efficient, and accurate simulations on current and next-generation architectures. The discussion will include the aspects of high-performance algorithms and

Monday, November 20 at 4:00 PM in SEO 612 performance analysis on many-core and many-GPU cmputing platforms.

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