Matrix Computations & Scientific Computing Seminar

Organizer: James Demmel & Ming Gu

Wednesday, 12:10–1:00pm, 380 Soda

March 7 **Dr. Lin Lin**, LBNL

Adaptive local basis set for Kohn-Sham density functional theory in a discontinuous Galerkin framework

Kohn-Sham density functional theory (KSDFT) is the most widely used electronic structure theory for condensed matter systems. Uniform discretization of the Kohn-Sham Hamiltonian generally results in a large number of basis functions per atom in order to resolve the rapid oscillations of the Kohn-Sham orbitals around the nuclei even in the pseudopotential framework. Atomic orbitals and similar objects significantly reduces the number of basis functions, but these basis sets generally require fine tuning of the parameters in order to reach high accuracy. We present a novel discretization scheme that adaptively and systematically builds the rapid oscillations of the Kohn-Sham orbitals around the nuclei as well as environmental effects into the basis functions. The resulting basis functions are localized in the real space, and are discontinuous in the global domain. The continuous Kohn-Sham orbitals and the electron density are evaluated from the discontinuous basis functions using the discontinuous Galerkin (DG) framework. Our method is implemented in parallel and the current implementation is able to handle systems with at least thousands of atoms. Numerical examples indicate that our method can reach very high accuracy (less than 1meV) with a very small number ($4 \sim 40$) of basis functions per atom.