Matrix Computations & Scientific Computing Seminar

Organizer: James Demmel & Ming Gu

Wednesday, 12:00–1:00PM, 380 Soda

Sept. 21 **Lin Lin**, LBNL

Numerical algorithms for the electronic structure analysis

Kohn-Sham density functional theory (KSDFT) is by far the most widely used electronic structure theory for condensed matter systems. The computational time of KSDFT increases as $O(N^3)$ with respect to the number of electrons (N), which hinders its practical application to systems of large size. We have developed an accurate and efficient algorithm to solve KSDFT which is uniformly applicable to insulating and metallic systems. Our method directly uses the property that the electron density and the electron energy are fully characterized by the diagonal elements and the nearest off diagonal elements of the single particle density matrix. This property is not reflected in the current $O(N^3)$ scaling methods. Our new method achieves $O(N)$ scaling for quasi 1D systems, $O(N^1.5)$ scaling for quasi 2D systems and $O(N^2)$ scaling for 3D bulk systems.