Matrix Computations & Scientific Computing Seminar

Organizer: James Demmel & Ming Gu

Wednesday, 11:00AM–12:00Noon, 380 Soda

Nov. 27 **Zhaojun Bai**, UC Davis

Solving Algberaic Nonlinear Eigenvalue Problems via Rapid Iterative Diagonalization

The algebraic nonlinear eigenvalues problems with eigenvector nonlinearities arise from partial differential equations in modeling electronic structure and phase transition of materials to machine learning in data science. Self-Consistent Field (SCF) iteration basing on iterative diagonalization of a sequence of linear eigenvalue problems is a common technique to solve the nonlinear eigenvalue problems. The steepest descent-type algorithms with proper preconditioning are widely used as iterative diagonalizers in practice.

In this talk, we will revisit the convergence analysis of classical preconditioned steepest descent algorithms, and show the effectiveness of a locally accelerated block preconditioned steepest descent method for solving algebraic nonlinear eigenvalues problems produced by an enhanced real-space *ab initio* method for electronic structure calculations.

This is a joint work with Yunfeng Cai of Peking University, John Pask of Lawrence Livermore National Laboratory and N. Sukumar of University of California, Davis.