Department of Mathematics
University of Texas at Arlington

Acceleration Schemes for the Nonlinear Eigenproblems in Density Functional Theory Calculations

Friday, April 24, 3:30 pm
Pickard Hall, Room 304

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Abstract:

Density functional theory (DFT) has enjoyed great success in materials science, condensed matter physics, and quantum chemistry. Central to DFT are the Kohn-Sham equations, which are nonlinear eigenvalue problems. Applying DFT to realistic materials often results in very large scale eigenproblems, solving these large scale nonlinear eigenproblems can be prohibitively expensive. We will discuss major approaches used to solve the Kohn-Sham equations. The focus will be on effective acceleration schemes for large scale nonlinear eigenproblems. One of the central themes in accelerating DFT calculations is to avoid computing explicit eigenvectors. We will present the Chebyshev polynomial filtered nonlinear subspace iteration method that is ideally suited for the acceleration. This method can routinely achieve orders of magnitude speedup over eigenvector-based methods.

The Math Department will provide refreshments 30 min. prior to the presentation.