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The Hong Kong University of Science and Technology

Department of Mathematics

Seminar on Applied Mathematics

Fast algorithms for Hartree-Fock-like equations

by

Prof. Lin LIN

University of California, Berkeley

Abstract

Hartree-Fock-like equations are very widely used in quantum chemistry and materials science, but the computational cost for solving such these equations is quite high. In a simplified mathematical setting, the solution requires the computation of low-lying eigenpairs of a large matrix in the form A+B. Here applying A to a vector is easy but A has a large spectral radius, while applying B (the Fock operator) is costly but B has a small spectral radius. It turns out that most eigensolvers are not well equipped to solve such problems efficiently. We will discuss some recently developed strategies to significantly accelerate such calculations, and to enable the solution of Hartree-Fock-like equations for more than 4000 atoms in a planewave basis set. Some of the techniques have been included in community electronic structure software packages such as Quantum ESPRESSO. We also find that the setup of the Hartree-Fock-like equations introduces interesting questions from the perspective of numerical analysis.

Date: **Wednesday, 9 May 2018**

Time: **3:30p.m. – 4:30p.m.**

Venue: **Room 2503 (Lifts 25-26), Academic Buildings, HKUST**

All are welcome!