THE UNIVERSITY OF CHICAGO

Departments of Computer Science, Mathematics, and Statistics

SCIENTIFIC AND STATISTICAL COMPUTING SEMINAR

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Lawrence Berkeley National Laboratory

Fast Algorithms for the Electronic Structure Analysis

THURSDAY, January 17, 2013, at 4:30 PM

Eckhart 133, 5734 S. University Avenue

Joint seminar with the James Franck Institute

ABSTRACT

Kohn-Sham density functional theory (KSDFT) is the most widely used electronic structure theory for condensed matter systems. The standard method for solving KSDFT requires solving N eigenvectors for an $O(N)*O(N)$ Kohn-Sham Hamiltonian matrix, with N being the number of electrons in the system. The computational cost for such procedure is expensive and scales as $O(N^3)$. We have developed pole expansion plus selected inversion (PEXSI) method, in which KSDFT is solved by evaluating the selected elements of the inverse of a series of sparse symmetric matrices, and the overall algorithm scales at most $O(N^2)$ for all materials including metallic and insulating systems. Recently we generalize the new method to nonorthogonal basis set, with the electron density, total energy, Helmholtz free energy and atomic force calculated simultaneously and accurately. Combined with atomic orbital basis functions, the new method can be applied to study the electronic structure of boron nitride nanotube and carbon nanotube with more than 10,000 atoms on a single processor.

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