



復旦大學
FUDAN UNIVERSITY

Applied Math Ph.D. Seminar

Parallel Multi-Coordinate Descent Methods for Full Configuration Interaction

Speaker: Yuejia Zhang (Fudan University)

Time: 2025-02-27, 16:10 to 17:00

Location: Rm 1801, Guanghua East Tower

Advisor:

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Abstract: Solving the time-independent Schrödinger equation gives us full access to the chemical properties of molecules. Among all the ab-initio methods, full configuration interaction (FCI) provides the numerically exact solution under a predefined basis set. However, the FCI problem scales exponentially with respect to the number of bases and electrons and suffers from the curse of dimensionality. We develop a multi-threaded parallel coordinate descent full configuration interaction algorithm, for the electronic structure ground-state calculation in the configuration interaction framework. The algorithm solves an unconstrained nonconvex optimization problem, via a modified block coordinate descent method with a deterministic compression strategy. CDFCI captures and updates appreciative determinants with different frequencies proportional to their importance. We demonstrate the efficiency of the algorithm on practical systems.