

A CPU/GPU Linear Scaling Three Dimensional Fragment Method for Large Scale Electronic Structure Calculations on Titan Supercomputer

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Abstract

In this talk, I will talk about the hybrid CPU/GPU Linear Scaling Three Dimensional Fragment (LS3DF) method implementation on Titan supercomputer. LS3DF is a Gordon Bell prize code developed by Dr. Lin-Wang Wang in 2008. it is a linear scaling total energy electronic structure calculation method based on plane wave pseudopotential density functional theory. The divide-and-conquer scheme of the LS3DF method makes it ideal to utilize the GPU computing power of a hybrid architecture supercomputer such as Titan. Our work in the hybrid implementation includes: (1) a G-parallel to band-index parallel scheme to solve the wave function FFT; (2) a new MPI communication scheme in the charge patching procedure. Our results show that we could have more than 4x speedup compared with CPU LS3DF(1500 GPU compared with 24000 CPU cores on Titan).