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Accelerating Orbital-Free DFT Calculation with a heterogeneous multi-core system MASARU AOKI, Shizuoka Sangyo Univ., Japan, HIDEKAZU TOMONO, KAZUO TSUMURAYA, Meiji Univ., Japan — Computational material design requires efficient algorithms and high-speed computers to calculate and to predict material properties. The orbital-free first principles calculation (OF-FPC) method, which is a tool for calculating and designing the properties, is an $O(N)$ method and is a powerful tool to study large-scaled systems. We implement a CUFFT routine, which is an FFT library of CUDA (Compute Unified Device Architecture) for GPGPU (General-Purpose Graphics Processing Unit), into our in-house OF-FPC code. We evaluate the computation time to optimize the electron charge density of the sodium crystal systems containing 2, 16, 128, 1024, and 6750 atoms. The GPU-CPU system reduces the time to half of that of the CPU system for the system with 6750 atoms. The GPGPU is effective in accelerating the OF-FPC code.

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