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GPU Based Acceleration of First Principles Calculations
HIDEKAZU TOMONO, Meiji University, JAPAN, TOSHIAKI IITAKA, RIKEN, JAPAN, KAZUO TSUMURAYA, Meiji University, JAPAN — The saturation of the acceleration using the silicon devices has required the parallel computing using multiple CPU's (central processing units). The parallel computing has been widely used in the field of the high-performance computing. On the other hand, graphics processing units (GPU's) were designed to accelerate graphic applications in 1978. NVIDIA Co. began to provide CUDA for C-language users to manipulate the GPU's in 2007. They applied it to computational fluid dynamics, medical real time simulation and astronomical N-body problem among others. This is the GPGPU (general-purpose computation on GPU's), which is faster in operation than CPU in the fields of linear algebras, FFT, and others. We have experienced that one- dimensional CUFFT ver1.1 (GPU-FFT) is eight times faster than FFTW for single-precision case. We implement the GPU-FFT into our in-house first principles planewave code, in which the hot spot is the FFT routine. We will present the performance of the implementation.

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