Physics > Computational Physics

GPGPU for orbital function evaluation with a new updating scheme

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We accelerated an {\it ab-initio} QMC electronic structure calculation by using GPGPU. The bottleneck of the calculation for extended solid systems is replaced by CUDA-GPGPU subroutine kernels which build up spline basis set expansions of electronic orbital functions at each Monte Carlo step. We achieved 30.8 times faster evaluation for the bottleneck, confirmed on the simulation of TiO$_2$ solid with 1,536 electrons. To achieve better performance in GPGPU we propose a new updating scheme for Monte Carlo sampling, quasi-simultaneous updating, which is in between the configuration-by-configuration updating and the widely-used particle-by-particle one. The energy deviation caused both by the single precision treatment and the new updating scheme is found to be within the accuracy required in the calculation, $\sim 10^{-3}$ hartree per primitive cell.

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