Abstract

A MPI-friendly density functional theory (DFT) source code was modified within hybrid parallelization including CUDA. The objective is to find out how simple conversions within the hybrid parallelization with mid-range GPUs affect DFT code not originally suitable to CUDA. Several rules of hybrid parallelization for numerical-atomic-orbital (NAO) DFT codes were settled. The test was performed on a magnetite material system with OpenMX code by utilizing a hardware system containing 2 Xeon E5606 CPUs and 2 Quadro 4000 GPUs. 3-way hybrid routines obtained a speedup of 7.55 while 2-way hybrid speedup by 10.94. GPUs with CUDA complement the efficiency of OpenMP and compensate CPUs' excessive competition within MPI.

References

- A. Ghosh, P. R. Taylor, "High-level ab initio calculations on the energetic of low-lying spin states of biologically relevant transition metal complexes: a first progress"

- OpenMX webpage, http://www.openmx-square.org/
- SIESTA webpage, http://www.icmab.es/siesta/
- You can see our patch for OpenMX3. 6 at http://www.eriksevre.com/projects/openmxcuda/

- Netlib website, http://www.netlib.org/

Index Terms

Computer Science
Applied Sciences
Keywords

MPI    CUDA    OpenMP    electronic structure    graphical processing unit
pseudo-atomic-orbital