Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

GPU speedup of the plane wave pseudopotential density functional theory calculations[1] LIN-WANG WANG, Material Science Division, Lawrence Berkeley National Lab, Berkeley, CA, 94720, WEILE JIA, ZONGYAN CAO, LONG WANG, XUEBIN CHI, Supercomputing Center, Computer Network Information Center, Chinese Academy of Sciences, Beijing, China, WEIGUO GAO, School of Mathematical Sciences, Fudan University, Shanghai, China — Plane wave (PW) pseudopotential density functional theory (DFT) calculation is the most widely used method for computational design of new materials. In this talk, we will present our recent work in using the graphics processing unit (GPU) to accelerate the PW-DFT calculations. Compared with the pure CPU calculation, the GPU machine with CUDA coding can speed up the calculation by 20 times for systems with a few hundred atoms, while still being able to scale to hundreds of CPU/GPU units. However, to reach this speedup, some algorithm changes are necessary. We will discuss these algorithm changes, and various computational kernels in a PW-DFT code, and their speedups in the GPU code. These include the FFT, the nonlocal projector, the orthogonalization and the diagonalization. We will also discuss the computational times for MPI communication, CPU/GPU memory copy, and floating point operation. We will present the hardware and library requirement to further speed up the calculations. Finally, the implication of the GPU speed up for new material design will be discussed.

[1]This work is supported by SC/BES of U.S. Department of Energy under Contract No. DE-AC02-05CH11231, and DMSE of China.

Lin-Wang Wang
Materials Science Division, Lawrence Berkeley National Lab,
Berkeley, CA, 94720

Date submitted: 17 Nov 2011 Electronic form version 1.4