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Joint Colloquium

GPU implementation of a plane wave pseudopotential density functional theory code: PEtot

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Date: 30 November 2012 (Friday)

Time: 2:30 p.m. – 3:30 p.m.

Venue: RRS638, Sir Run Run Shaw Building
Ho Sin Hang Campus, HKBU, Kowloon Tong

Abstract

One rapidly developing area in scientific computing is the use of general purpose graphic processing units (GPU). In materials science simulations, the plane wave pseudopotential method is the most widely used density functional theory (DFT) simulation method. We have implemented our plane wave pseudopotential code PEtot using GPU. This requires a redesign of the parallelization algorithm. In particular, we calculate the band to band overlapping matrix elements in G-space parallelization, with the wave function to Hamiltonian application in band index parallelization. We found that it is possible to accelerate the original MPI code by a factor of 20 by the GPU code. As a result, in a molecular dynamics (MD) simulation of a 512 atom GaP system, each MD step takes only about 10 seconds using 256 GPUs.

Biography

Dr. Wang has 20 years of experience in large scale electronic structure calculations. He has worked on O(N) electronic structure calculations in the early 1990s. Working with Alex Zunger, he invented the folded spectrum method which pushed the limit of non-self-consistent electronic structure calculations from 100 atoms to thousands of atoms. He developed a linear combination of bulk bands (LCBB) method for semiconductor heterostructure electronic structure calculations, which allows the calculation of million-atom devices. He developed generalized moments method which calculates the density of states and optical absorption spectra of a given system without explicit calculation of its eigenstates. He also developed a popular parallel total energy plane wave pseudopotential program (PEtot). He invented a charge patching method, which enables ab initio accuracy in thousand atom calculations for nanosystems. He has developed a linear scaling three dimensional fragment method (LS3DF), which can be used to self-consistently calculate systems with tens of thousands of atoms. Recently, he developed a non-adiabatic molecular dynamics method which can simulate a 5,000 atom system for 10 picoseconds.

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ALL Interested Are Welcome!