Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Vectorization for Molecular Dynamics on Intel Xeon Phi Corpocessors HONGSUK YI, kisti — Many modern processors are capable of exploiting data-level parallelism through the use of single instruction multiple data (SIMD) execution. The new Intel Xeon Phi coprocessor supports 512 bit vector registers for the high performance computing. In this paper, we have developed a hierarchical parallelization scheme for accelerated molecular dynamics simulations with the Terfoff potentials for covalent bond solid crystals on Intel Xeon Phi coprocessor systems. The scheme exploits multi-level parallelism computing. We combine thread-level parallelism using a tightly coupled thread-level and task-level parallelism with 512-bit vector register. The simulation results show that the parallel performance of SIMD implementations on Xeon Phi is apparently superior to their x86 CPU architecture.

Hongsuk Yi
kisti

Date submitted: 10 Jan 2014 Electronic form version 1.4