

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Large-Scale First-Principles Molecular Dynamics Simulations on the BlueGene/L Computer FRANCOIS GYGI, University of California Davis, Davis, CA 95616, ERIK W. DRAEGER, Lawrence Livermore National Laboratory, Livermore, CA 94551 — We present the results of large-scale First-Principles Molecular Dynamics (FPMD) simulations performed on the BlueGene/L computer, using up to 65,536 processors. Simulations involving 1000 molybdenum atoms were carried out using the Qbox code with non-local, norm-conserving pseudopotentials. A parallel efficiency of 85% can be attained when solving the same problem on partitions ranging from 512 nodes to 32,768 nodes. When using 65,536 processors, a floating point performance of 64 Tflops is reached. Optimization of the logical-to-physical mapping of tasks is essential in order to achieve this performance on the BlueGene/L torus architecture. We discuss the challenges encountered when implementing FPMD in the plane-wave, pseudopotential formalism on 10,000 processors and beyond. Part of this work was performed under the auspices of the U.S. Dept. of Energy at the University of California/Lawrence Livermore National Laboratory under contract no. W-7405-Eng-48.

Francois Gygi
University of California Davis

Date submitted: 30 Nov 2005

Electronic form version 1.4