Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Large scale ab initio molecular dynamics using the OpenAtom software[1] SOHRAB ISMAIL-BEIGI, SUBHASISH MANDAL, MINJUNG KIM, Yale University, ERIC MIKIDA, ERIC BOHM, PRATEEK JINDAL, University of Illinois at Urbana Champaign, NIKHIL JAIN, Lawrence Livermore National Laboratory, LAXMIKANT KALE, University of Illinois at Urbana Champaign, GLENN MARTYNA, IBM T. J. Watson Research Center — First principles molecular dynamics approaches permit one to simulate dynamic and time-dependent phenomena in physics, chemistry, and materials science without the use of empirical potentials or ad hoc assumptions about the interatomic interactions since they describe electrons, nuclei and their interactions explicitly. We describe our collaborative efforts in developing and enhancing the OpenAtom open source ab initio density functional software package based on plane waves and pseudopotentials (http://charm.cs.uiuc.edu/OpenAtom/). OpenAtom takes advantage of the Charm++ parallel framework. We present parallel scaling results on a large metal organic framework (MOF) material of scientific and potential technological interest for hydrogen storage. In the process, we highlight the capabilities of the software which include molecular dynamics (Car-Parrinello or Born-Oppenheimer), k-points, spin, path integral beads for quantum nuclear effects, and parallel tempering for exploration of complex phase spaces. Particular efforts have been made to ensure that the different capabilities interoperate in various combinations with high performance and scaling. Comparison to other available open source software will also be assessed.

[1]This collaboration is supported NSF SI2-SSI grant ACI-1339804.

Sohrab Ismail-Beigi
Yale University

Date submitted: 11 Nov 2016 Electronic form version 1.4