Abstract Submitted
for the SES13 Meeting of
The American Physical Society

Programming Berendsen Thermostat Subroutines for Molecular Dynamics Simulations WARD HOWARD, MICHAEL SALAZAR, BRITTANY HAGLER, Union University — Molecular dynamics (MD) provides a powerful tool for computing the behavior of atoms and molecules using force calculations over all particles in a system. MD simulations are broken up into many time steps. At each step, the quantum mechanical (QM) and molecular mechanical (MM) energy and forces, positions, velocities, and accelerations are recalculated from the values found at the previous time step. These MD basics are nearly always supplemented by other considerations, such as temperature control. We investigated several thermostat variations that provide such functionality to an adaptive, multilevel QM/MM interpolation-based code. The Accelerated Molecular Dynamics with Chemistry (AMolDC) is designed for simulations of large molecular systems that can undergo very complex reactions. Unlike some Berendsen thermostats that act on simple particles in Brownian motion, we created thermostats that control temperature for molecules in several different ways, such as molecular center-of-mass velocity frame transformations, Gaussian thermostat control via system-level velocity scaling of all atoms, and intramolecular- level velocity scaling. This is primarily application-based research that integrates well-known methods into a specific and groundbreaking code. Results are extremely preliminary, but these tests show promise for future enhancements to the capability of AMolDC.

Ward Howard
Union University

Date submitted: 20 Sep 2013 Electronic form version 1.4