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A hierarchical DPD thermostat to avoid over and/or underdamping at long wavelengths in MD simulations KEVIN GREEN, COLIN DENNISTON, MARTIN MUSER, University of Western Ontario — In this talk, we present a new approach to use dissipative particle dynamics as a thermostat in molecular dynamics simulations. The main idea is to have DPD act on groups of atoms so that damping can be tuned as a function of length scale. This allows one to achieve a quality factor of vibrations, which is barely wavelength dependent. The number of floating point operations per time step is orders of magnitude less for the new approach than for regular DPD or any other thermostat acting on individual particles. In addition, the method avoids both underdamping of natural and/or DPD dynamics at long wavelengths L and overdamping which is unavoidable at large L for Langevin or Nose-Hoover based thermostats. Thus correlation times for observables that live on long wavelengths L, are of order L, rather than of order L^2 as for conventional thermostats.

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