Test case: 2D Lennard-Jones fluid versus lammps output

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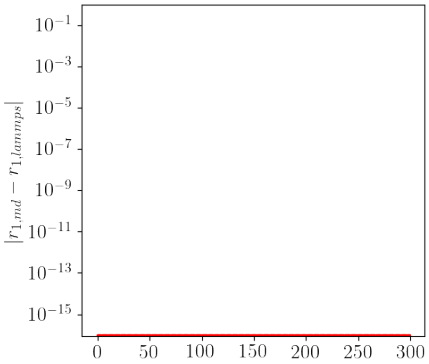

FIG. 1. Positions read in by the subroutine read_state_lammps in the file_writer module, after being dumped by dump (...) x y z (...) in lammps.**in** input script. Difference between LAMMPS output and the imported Fortran positions shown—should be zero to machine precision, which it is.

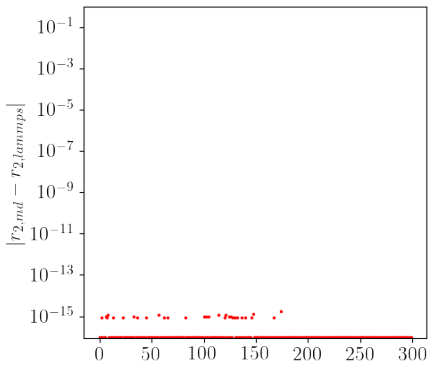

FIG. 2. Positions after a single time step at $\Delta t = 0.001$, as compared to the LAMMPS trajectory positions.

Positions

Loading initial positions from a LAMMPS output file gives equal positions to within machine precision, c.f. Fig. 1. After a single time step at $\Delta t = 0.001$, positions deviate from the LAMMPS trajectories by between 10^{-15} and 10^{-16}, as seen in Fig. 2.

Note that the first 100 points represent the x coordinate of all $N = 100$ particles, the subsequent 100 points reprents the y coordinate, while the last 100 are the z component of the positions. Since we are working in 2D, the positions and forces in the z-direction should always vanish.

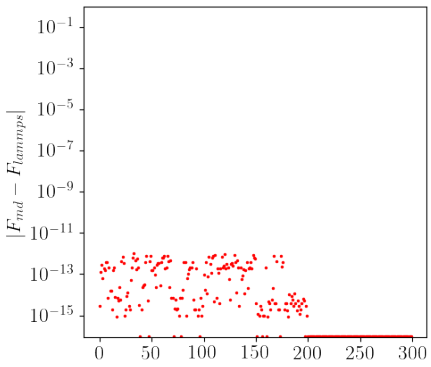

FIG. 3

Forces

The initial forces—calculated at the exact positions of the LAMMPS particles—deviate from the LAMMPS values by up to 10^{-12}, c.f. Fig. 3.

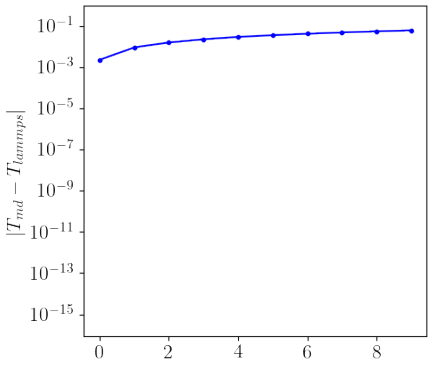

FIG. 4

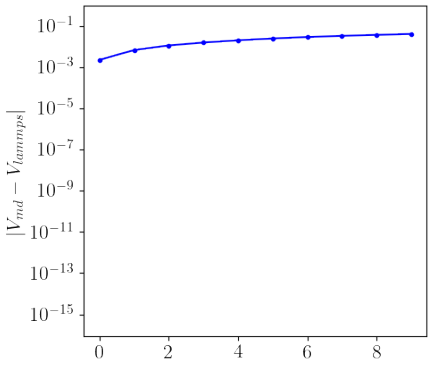

FIG. 5

Energies

Total energies calculated deviate from

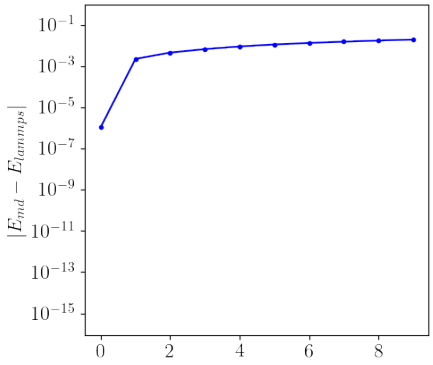

FIG. 6