

# Test case: 2D Lennard-Jones fluid versus lammmps output

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## Positions and velocities

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. 1.

Note that the first 100 points represent the  $x$  coordinate of all  $N = 100$  particles, the subsequent 100 points represents 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.

## 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. ??.

## Energies

Total energies calculated deviate from

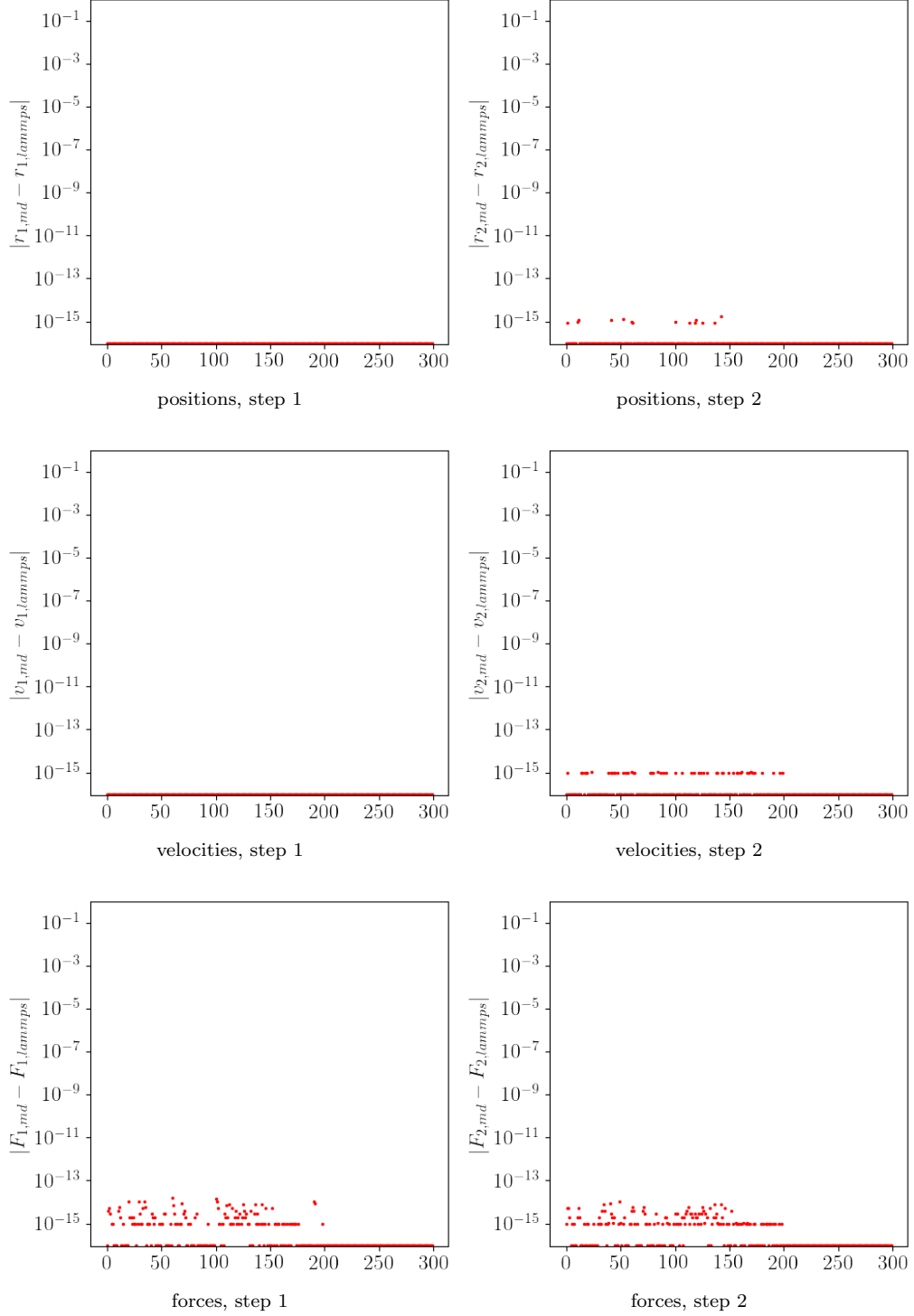


FIG. 1. Positions and velocities read in from LAMMPS data on the left hand side, and comparison with subsequent LAMMPS data after integrating a single time step on the right hand side. The forces are calculated for both time steps, and the comparison with LAMMPS reference data is shown in the bottom two subplots.

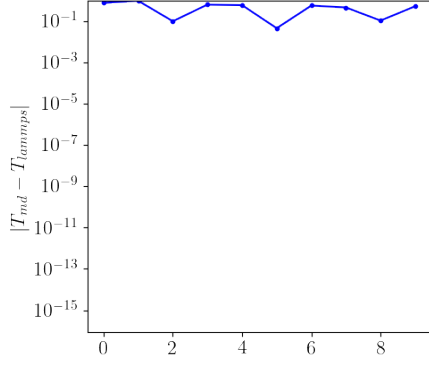


FIG. 2

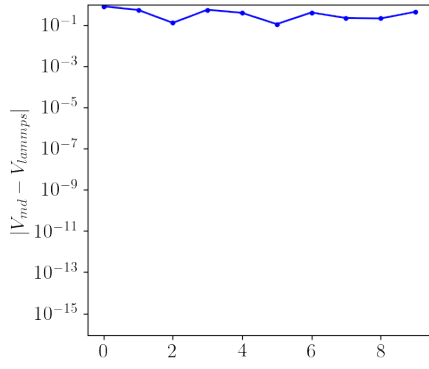


FIG. 3

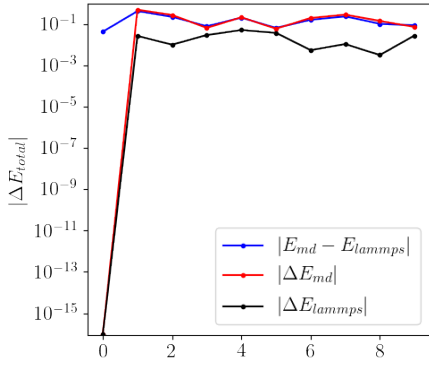


FIG. 4