

Simulation Report: Check check

Simulation ID: 766947fb-e755-448c-b0c3-7f307bd63af8

Type: molecular_dynamics

Status: completed

Started: 4/28/2025, 9:19:09 AM

Completed: 4/28/2025, 9:19:19 AM

Parameters:

temperature: 310

pressure: 1

timeStep: 0.002

totalSteps: 1000000

Results Summary:

Statistics:

mean_potential_energy: 99998.97729141

std_potential_energy: 1.4886842384417038

mean_kinetic_energy: 472.1529581428871

std_kinetic_energy: 30.46423491067831

mean_temperature: 310.27267144453964

std_temperature: 4.956178756516819

mean_pressure: 0.9806868862196104

std_pressure: 0.10158676106877096

mean_volume: 1000.4331682346904

equilibration_time: 400

Convergence Metrics:

energy_rmsd: 0.000014886994634989964

temperature_stability: 4.956178756516819

pressure_stability: 0.10158676106877096

equilibration_percentage: 20

Total Simulation Time: 1980 ps

Total Frames: 100