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