Simulation Report: Simulation Testing

Simulation ID: cdebb1c3-7fe2-4d66-b0f1-519f213ff601
Type: molecular_dynamics
Status: completed
Started: 3/26/2025, 10:34:58 PM
Completed: 3/26/2025, 10:35:02 PM

Parameters:

temperature: 310
pressure: 1
timeStep: 0.002
totalSteps: 1000000

Results Summary:

Statistics:

mean_potential_energy: 100003.42956343778
std_potential_energy: 4.269185289808289
mean_kinetic_energy: 468.6610553993427
std_kinetic_energy: 35.568381480034226
mean_temperature: 311.14988904794717
std_temperature: 4.758507383727273
mean_pressure: 1.0145590064819097
std_pressure: 0.10031463343399297
mean_volume: 1000.578392288433
equilibration_time: 400

Convergence Metrics:

energy_rmsd: 0.000042690388804117014
temperature_stability: 4.758507383727273
pressure_stability: 0.10031463343399297
equilibration_percentage: 20

Total Simulation Time: 1980 ps
Total Frames: 100