Simulation Report: Molecular Dynamics Simulation

Simulation ID: 92443f41-7fe1-4e59-ae6c-d20151e70087
Type: molecular_dynamics
Status: completed
Started: 3/11/2025, 9:33:28 PM
Completed: 3/11/2025, 9:33:37 PM

Parameters:

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

Results Summary:

Statistics:

mean_potential_energy: 100004.26227410007
std_potential_energy: 4.656696078816473
mean_kinetic_energy: 459.5940101896687
std_kinetic_energy: 29.845355018097116
mean_temperature: 310.0266295285943
std_temperature: 5.114284294761235
mean_pressure: 1.0145030865360942
std_pressure: 0.0990517091241185
mean_volume: 999.3073386899105
equilibration_time: 400

Convergence Metrics:

energy_rmsd: 0.00004656497606125037
temperature_stability: 5.114284294761235
pressure_stability: 0.0990517091241185
equilibration_percentage: 20

Total Simulation Time: 1980 ps
Total Frames: 100