Simulation Report: Smart Glocery Store

Simulation ID: 0ea49339-cfeb-4cc4-bcf8-417286083be1
Type: molecular_dynamics
Status: completed
Started: 4/28/2025, 10:30:00 AM
Completed: 4/28/2025, 10:30:04 AM

Parameters:

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

Results Summary:

Statistics:
mean_potential_energy: 100000.12043339464
std_potential_energy: 3.6238379070883466
mean_kinetic_energy: 466.8103744726362
std_kinetic_energy: 28.789642201346215
mean_temperature: 309.9404476229316
std_temperature: 5.034669870046865
mean_pressure: 0.989495946206439
std_pressure: 0.09328352732100299
mean_volume: 1000.5751743367466
equilibration_time: 400

Convergence Metrics:
energy_rmsd: 0.00003623833542782595
temperature_stability: 5.034669870046865
pressure_stability: 0.09328352732100299
equilibration_percentage: 20

Total Simulation Time: 1980 ps
Total Frames: 100