

Simulation Report: Isma Check

Simulation ID: 26da9018-ae83-4000-92e8-20058641c62e

Type: molecular_dynamics

Status: completed

Started: 3/23/2025, 9:49:12 PM

Completed: 3/23/2025, 9:49:23 PM

Parameters:

temperature: 310

pressure: 1

timeStep: 0.002

totalSteps: 1000000

Results Summary:

Statistics:

mean_potential_energy: 100006.62775042882

std_potential_energy: 2.3749875255484083

mean_kinetic_energy: 460.44362174916506

std_kinetic_energy: 25.981557310393313

mean_temperature: 309.9402577821669

std_temperature: 4.6387581274226495

mean_pressure: 0.9863535311057774

std_pressure: 0.09486513332061396

mean_volume: 1000.8793704798321

equilibration_time: 400

Convergence Metrics:

energy_rmsd: 0.000023748301277344337

temperature_stability: 4.6387581274226495

pressure_stability: 0.09486513332061396

equilibration_percentage: 20

Total Simulation Time: 1980 ps

Total Frames: 100