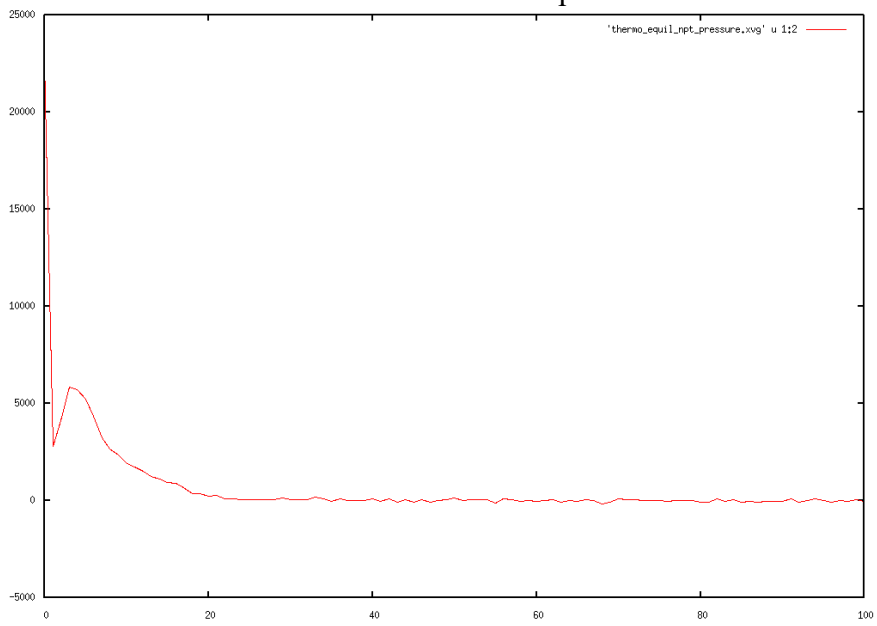
MolSim Homework 5

Kaylyn Torkelson

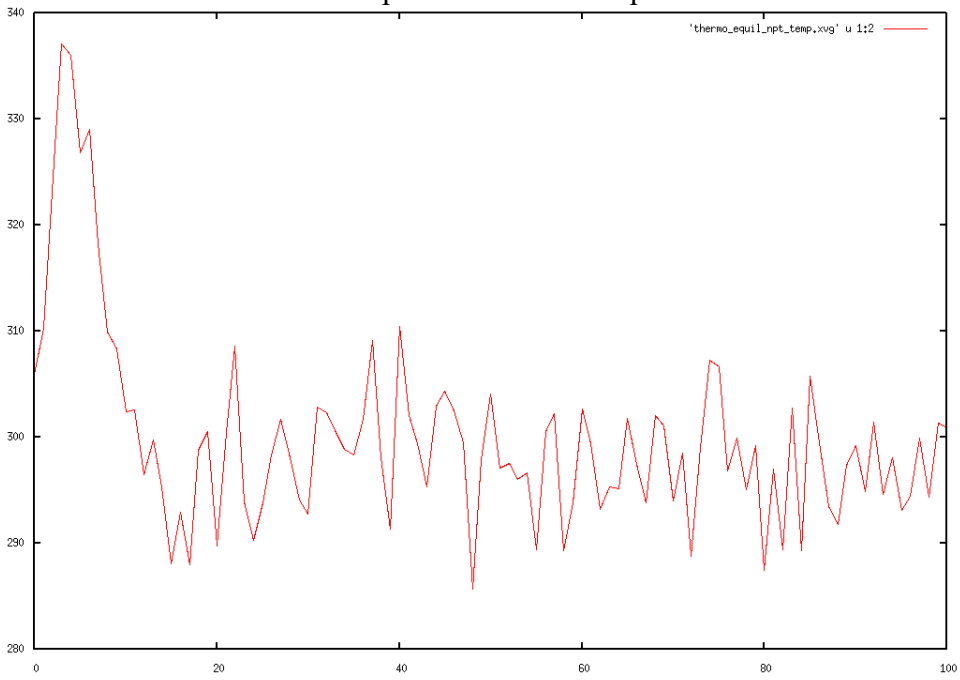
Part One

NPT Equilibration

Pressure v. Timestep

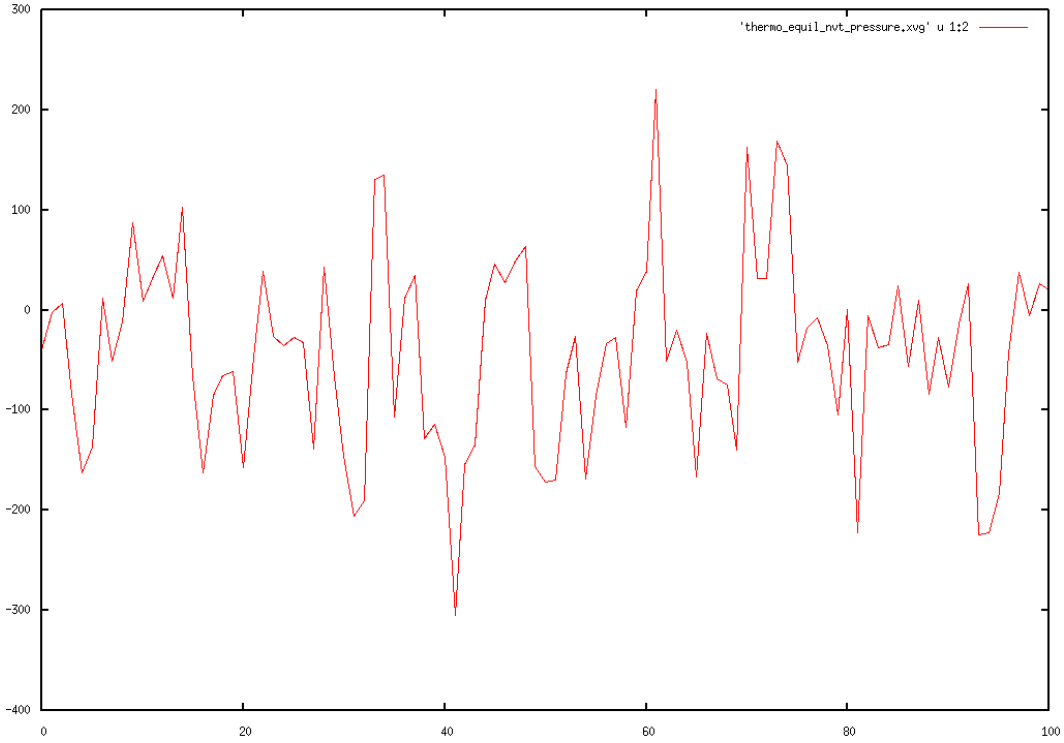


Temperature v. Timestep

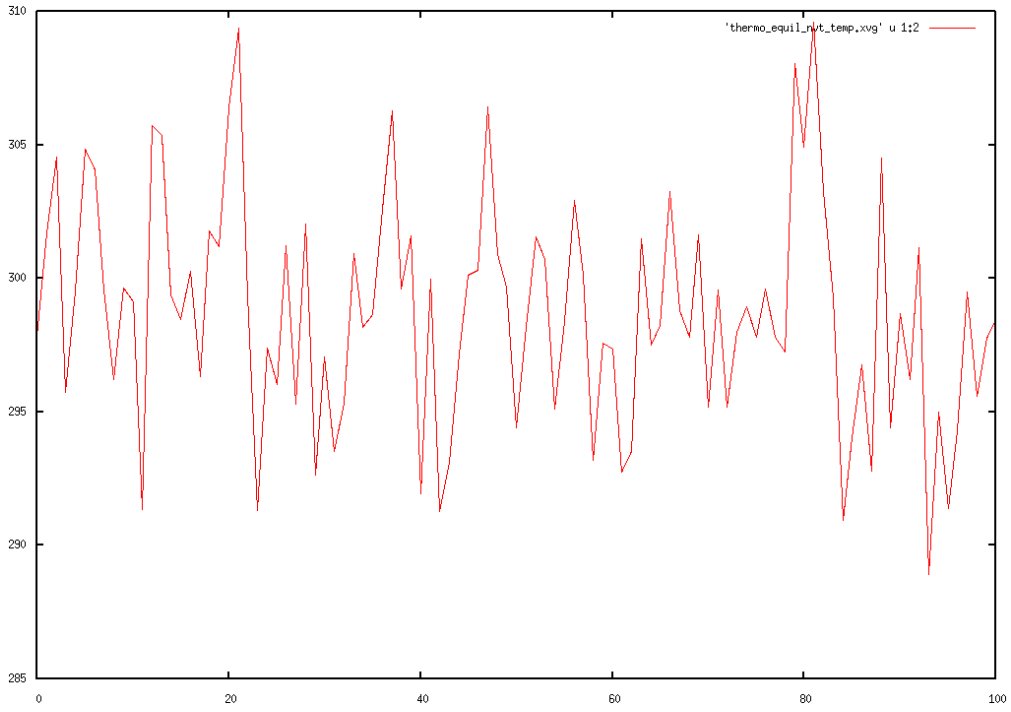


NVT Equilibration

Pressure v. Timestep

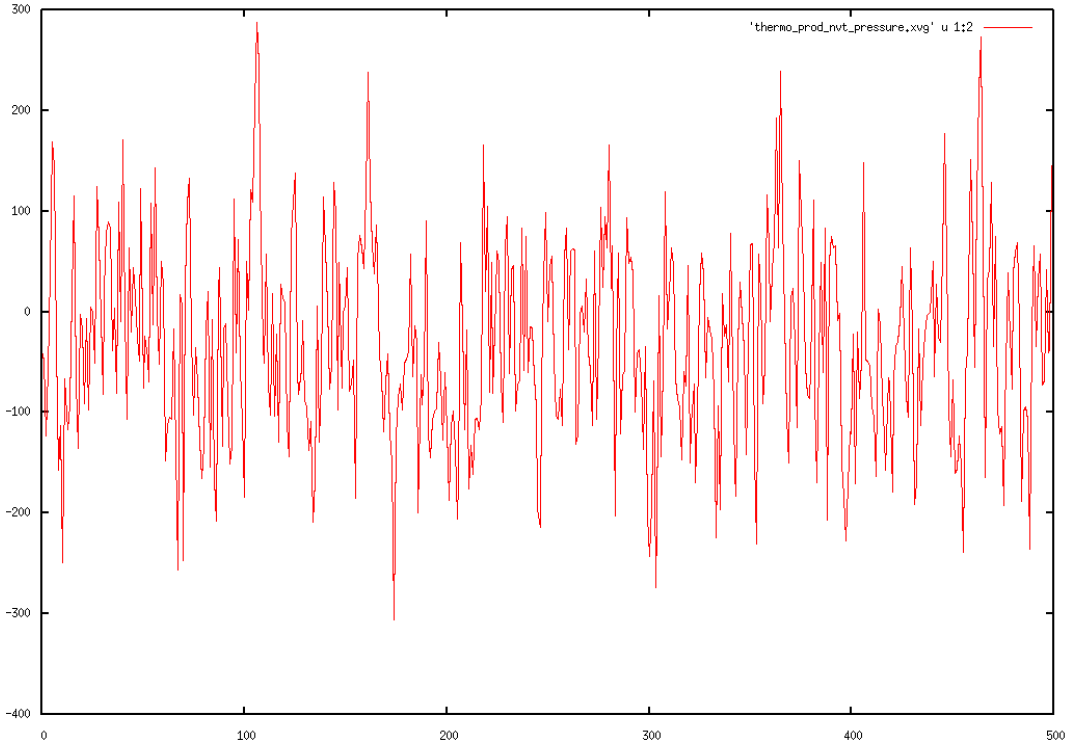


Temperature v. Timestep

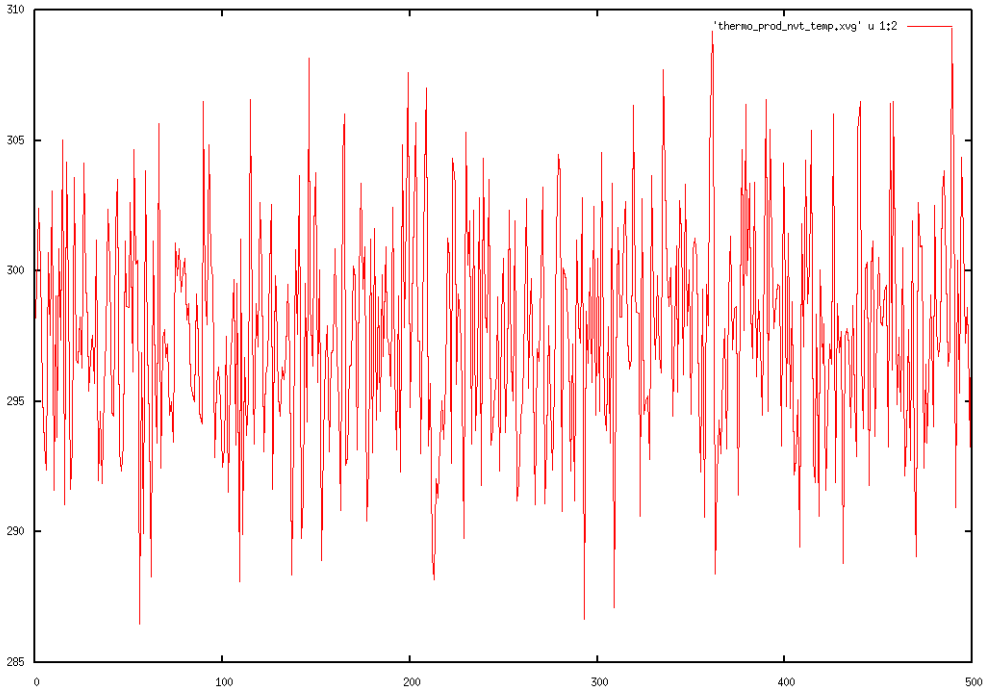


NVT Production

Pressure v. Timestep



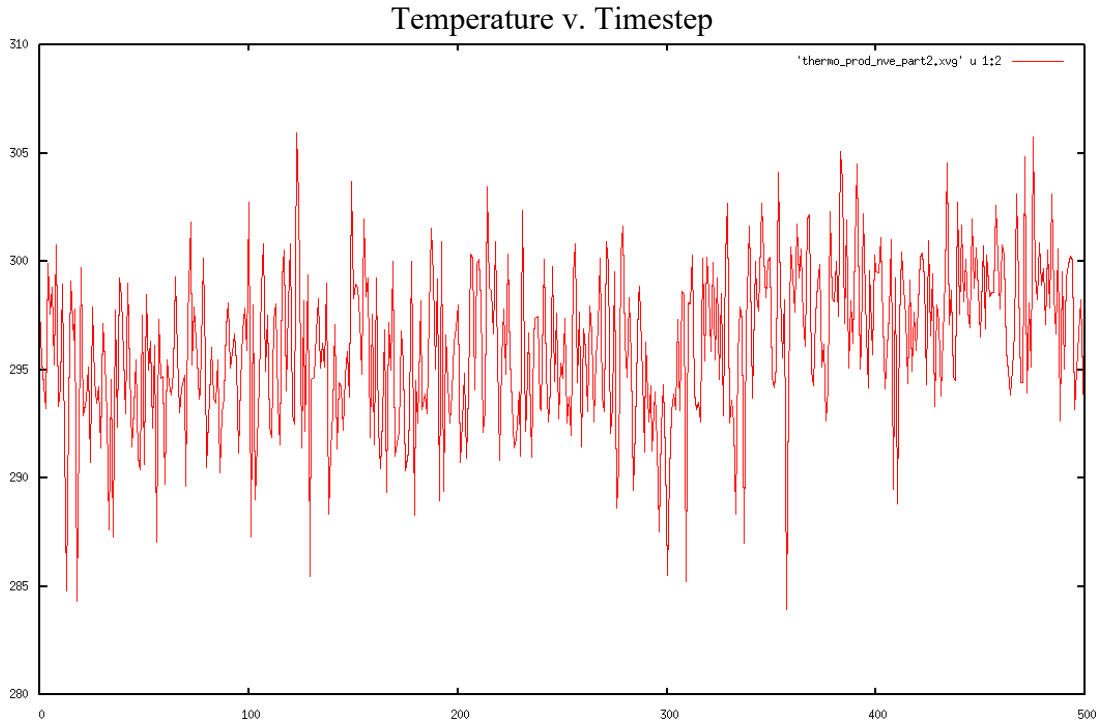
Temperature v. Timestep



Part Two

NVE Production Run with NPT Equilibration

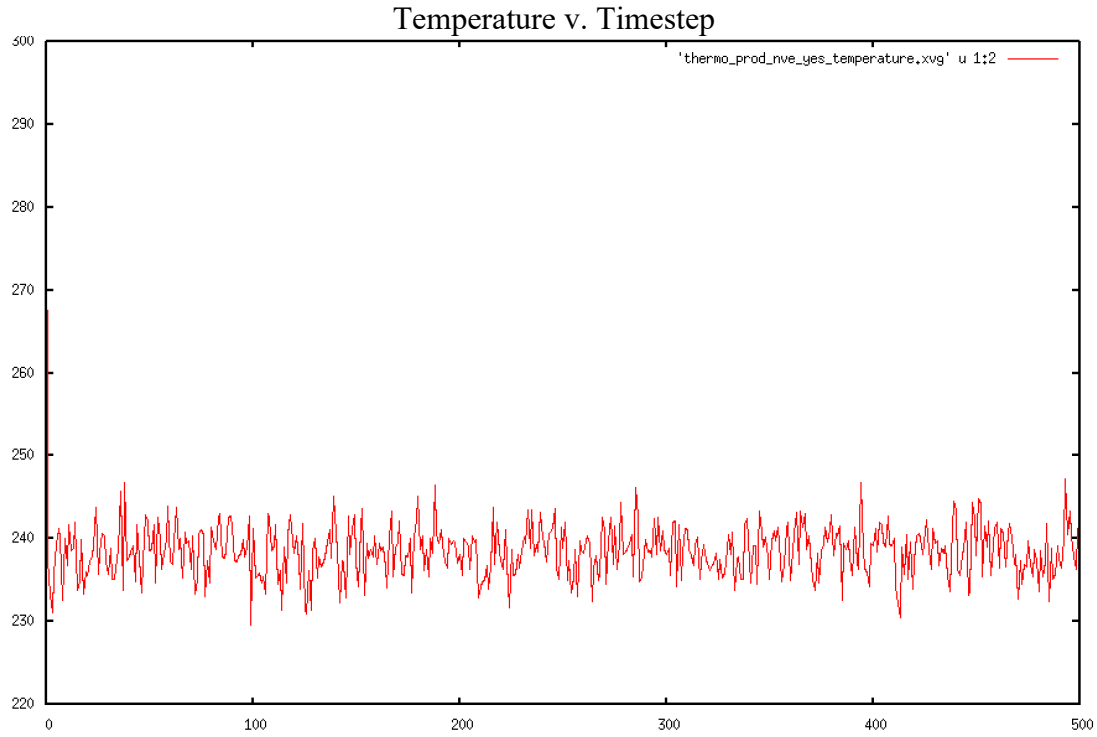
Without the thermostat in use, temperature fluctuates between 295 and 305 K throughout the simulation.



Part Three

The two following runs have similar set-ups except for that one involves setting an initial velocity at 298 K and the other doesn't. The NVE run with initial velocity starts at a higher temperature and quickly drops temperature to around 240 K and hovers around there. The NVE run without an initial velocity starts at a lower temperature and quickly rises in temperature to around 120 K and hovers around there. The NVE ensemble eventually reaches a consistent temperature but the two temperatures are very different.

NVE Production Run with Initial Velocity



NVE Production Run without Initial Velocity