**Pressure results**

NPT step

![A close up of a map

Description automatically generated]()

NVT step

![A close up of a antenna

Description automatically generated]()

Prod run

**![A close up of a map

Description automatically generated]()**

**Temperature results**

NPT step

**![A close up of text on a white background

Description automatically generated]()**

NVT step

![A close up of a logo

Description automatically generated]()

Prod run

![A screenshot of a cell phone

Description automatically generated]()

NVE with random velocities

![A close up of a logo

Description automatically generated]()

NVE with no initial velocities

![A close up of a plant

Description automatically generated]()

**Comments:**

The results of the two NVE runs seemed nearly the same, but with one difference. Since temperature was not being held (NVE keeps volume and energy constant), in the run where the initial velocities were not set to correspond to 298K, the steady state temperature was less.

Pressure was steady at 1 in the NPT step, which makes sense as NPT holds pressure constant, it jumped around about a constant value. I did notice that in NPT step, both temperature and pressure spiked initially. I think this is because it takes a bit for the system to change the volume and equilibrate pressure to the desired value.