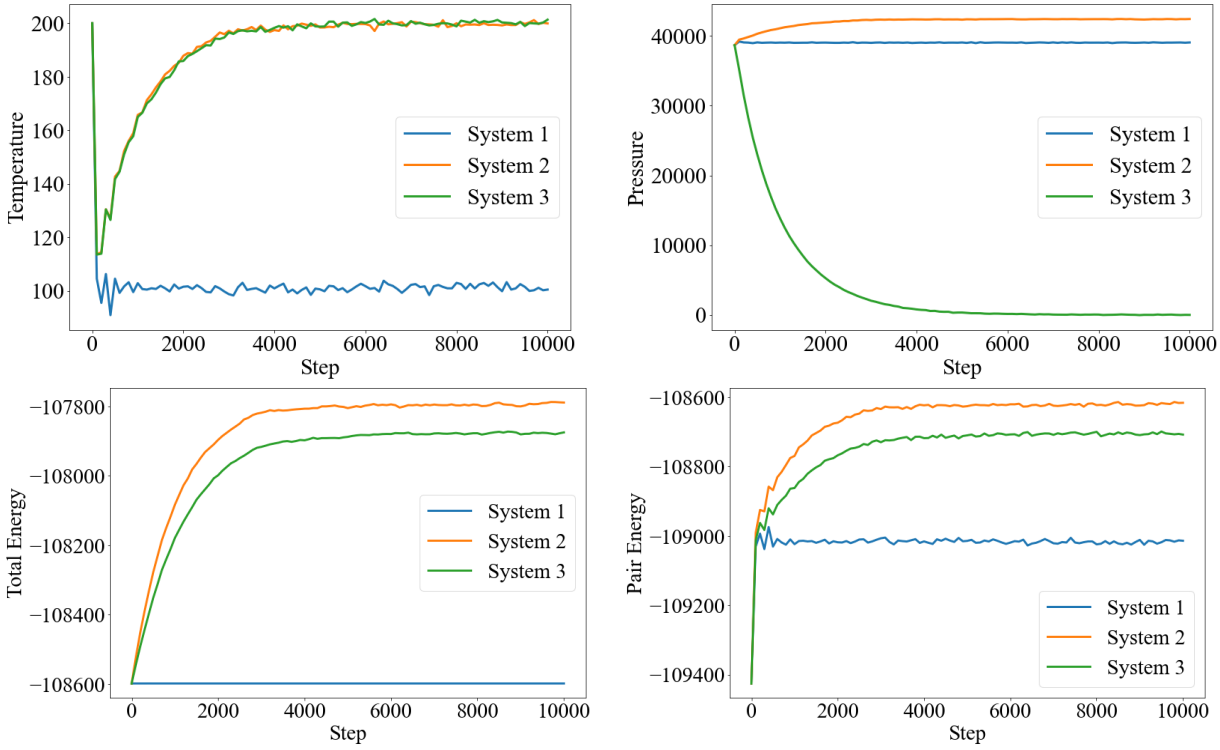
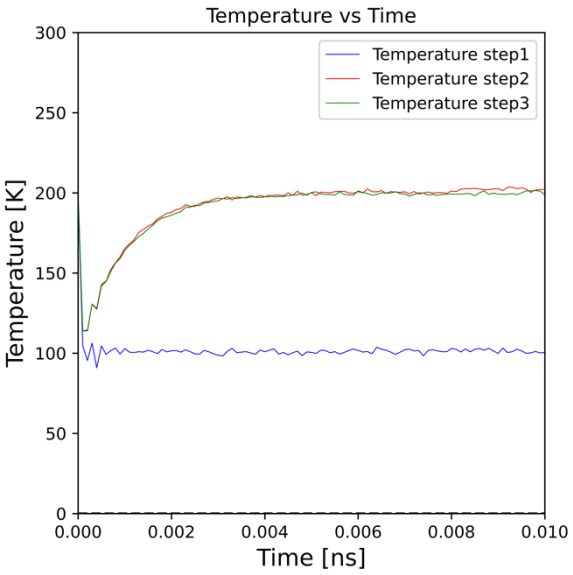
Molecular dynamics with LAMMPS

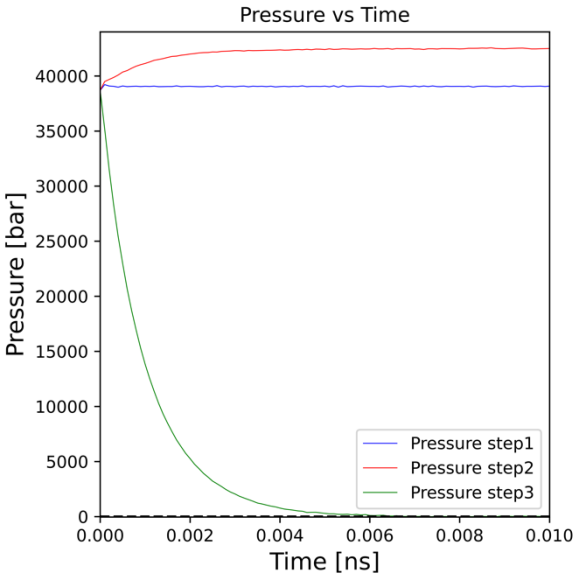
- Calculate the pressure, the temperature, and the energy per particle for the conditions specified above.

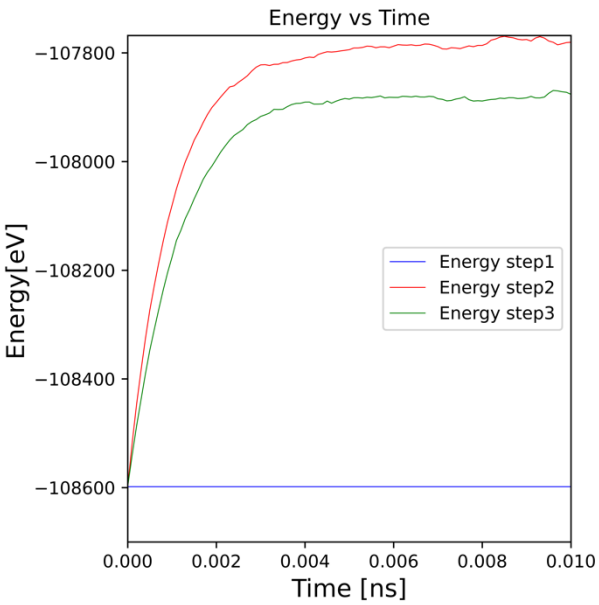
Temperature, pressure, Energy vs time step:

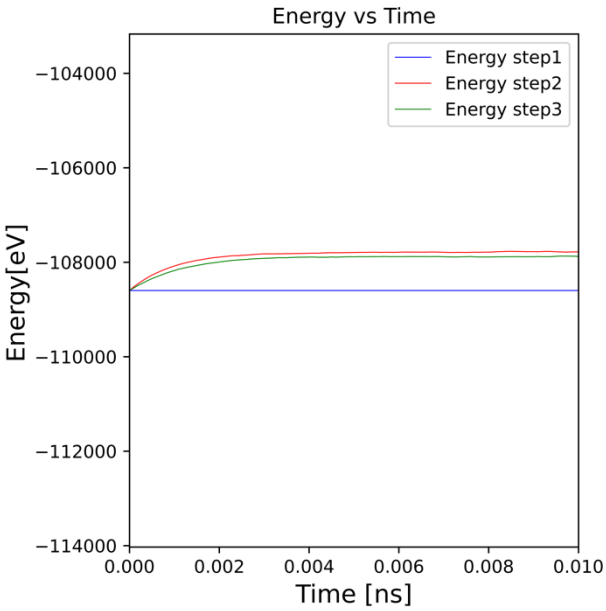


Temperature, pressure, Energy vs time base on ns:









Observations

System 1(step1):

- The temperature drops from 200 K to 100 K due to minimization of energy process. It's tuned to minimize the energy
- The pressure stayed the same.

System 2(step2):

- In the beginning, the temperature decrease to 120 K , the increase to 200 K. the temperature fluctuate at 200 K as a constant value.
- The energy increase gradually.

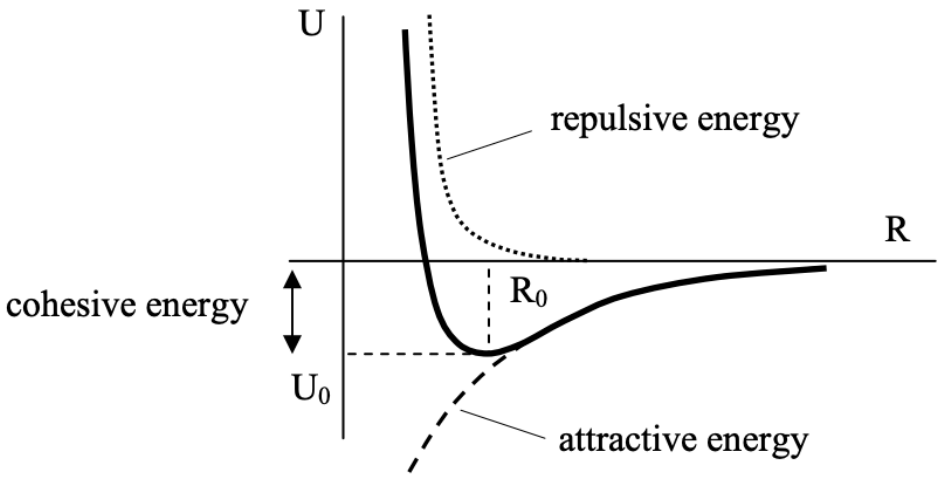
System 3(step3):

- In the beginning, the temperature decrease to 120 K , the increase to 200 K. the temperature fluctuate at 200 K as a constant value.
- The pressure decreases to reach 0 and it fluctuate around the zero value.
- The energy increase gradually, and it fluctuate around a constant value.

System(step1): with thermo100
System(step2): with fix LGV all langevin 200 200 1 7956823
System(step2): fix PRESS all press/berendsen aniso 0 0 1 modulus 1400000

- Is the energy negative? If so, why?

Yes , we know that The amount of energy which is required to pull the crystal apart into a set of free atoms is called the cohesive energy of the crystal.
A typical curve for the potential energy representing the interaction between two atoms. Since the system tends to have the lowest possible energy, it is most stable at R=R0, which is the equilibrium interatomic distance. The corresponding energy U0 is the cohesive energy



The interatomic force is determined by the gradient of the potential energy, so that

$$F(R) = -\frac{\partial U}{\partial R}$$

This means that for large separations the force is attractive, tending to pull the atoms together, On the other hand, the force becomes repulsive at small separations of the atoms, and tends to push the atoms apart. The repulsive and attractive forces cancel each other exactly at the point R0, which is the point of equilibrium.
The negative energy refers to attractive interaction which means that the system is stable. (it has local minima or global minima)

- Did the temperature change with respect to the one you had chosen? If so, why?

In the first system, yes, it changes because in the first system, the NVE ensemble is applied, which means the temperature is not fixed and it will be tuned to minimize the energy but it fix the energy, volume and the number of the particle.

Using Langevin thermostat, Langevin dynamics allows temperature to be controlled like with a thermostat, thus approximating the canonical ensemble. Apply a Langevin thermostat as described to a group of atoms which models an interaction with a background implicit solvent. It performs Brownian dynamics (BD),

$$F = F_c + F_f + F_r$$
$$F_f = -\frac{m}{\text{damp}} v$$
$$F_r \propto \sqrt{\frac{k_B T m}{dt\ \text{damp}}}$$

Where;
Fc is the conservative force
Ff is a frictional drag or viscous damping term proportional to the particle's velocity
Fr is a force due to solvent atoms at a temperature *T* randomly bumping into the particle.

-Is it possible to obtain as a value for the temperature the one you wanted initially?

Yes it can be done by using NPT or NVT ensemble to fix the temperature.

Another way to control the temperature and minimize the pressure is by using Langevin thermostat and press/Berendsen commands which allow the system to get back to the wanted temperature initially.

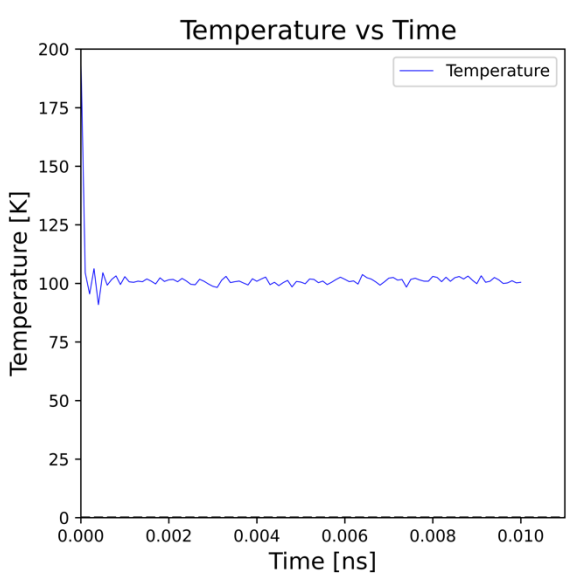
General description:

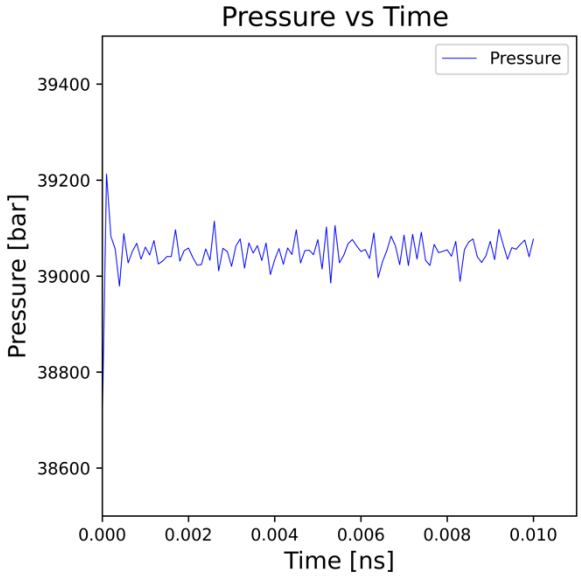
This system sets the units to "metal" and defines the atom style as "atomic". It creates a face-centered cubic (FCC) lattice with a lattice constant of 3.6100. It initializes the velocities of all atoms with a magnitude of 200.0 and a seed value of 232345.
According to question, I set thermos 100, It specifies that thermo output should be printed every 100 timesteps.
In molecular dynamics simulations, the temperature of the system is typically controlled using a thermostat, which adjusts the velocities of the atoms to maintain a desired temperature. The NVE (Newtonian Varlet with constant Energy) integrator used in the script does not include any temperature coupling, which means that the system is not explicitly coupled to a thermostat to control its temperature. As a result, the initial velocity distribution of the atoms could cause the system to rapidly heat up or cool down, leading to temperature fluctuations. Additionally, the potential energy landscape of the system, as determined by the choice of the potential (EAM_Dynano_Mendelev_King_Cu_Mo_748636486270_001), can also affect the temperature fluctuations. If the potential has steep energy barriers or energy wells, it can cause the atoms to undergo rapid changes in kinetic energy, leading to temperature fluctuations. The time step used in the simulation can also impact the temperature fluctuations. A larger time step may result in less accurate integration of the equations of motion and can lead to larger temperature fluctuations. It's possible that the time step used in the simulation is not optimal for the system being simulated, leading to temperature fluctuations.
The values (temperature, potential energy, total energy, pressure) of these quantities change over time as the particles in the system interact with each other and exchange energy through collisions and interactions, providing insights into the system's thermodynamic properties and behavior during the simulation. Total energy after a specific time step remains constant, it indicates that the system has reached an equilibrium state where the energy is conserved. In an NVE ensemble simulation, where the number of particles, volume, and energy are kept constant, the total energy of the system should be conserved over time, it means that no external energy is being added or removed from the system.
Here, by adding fix LGV all langevin 200 200 1 7956823, specifies that the Langevin thermostat will be applied to all particles. The damping constant is set to 200, which determines the strength of the frictional force applied to the particles to dampen their velocities. A higher value of the

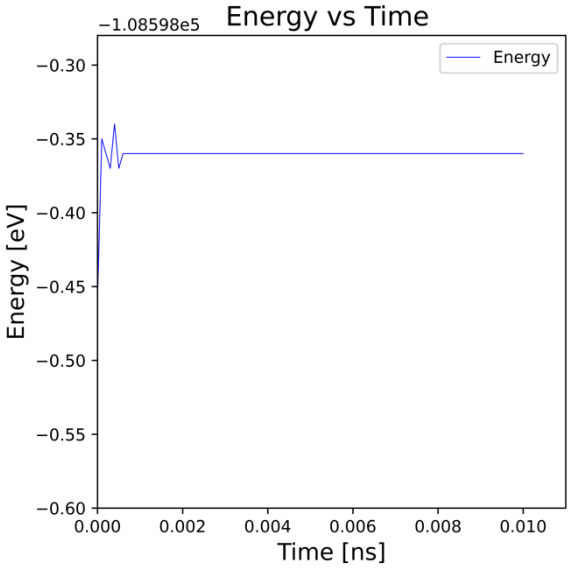
damping constant leads to faster equilibration to the desired temperature. The last parameter, 7956823, is the random seed used for generating the random forces applied to the particles. This seed value is used to ensure reproducibility of the simulation results.

Separated figures:

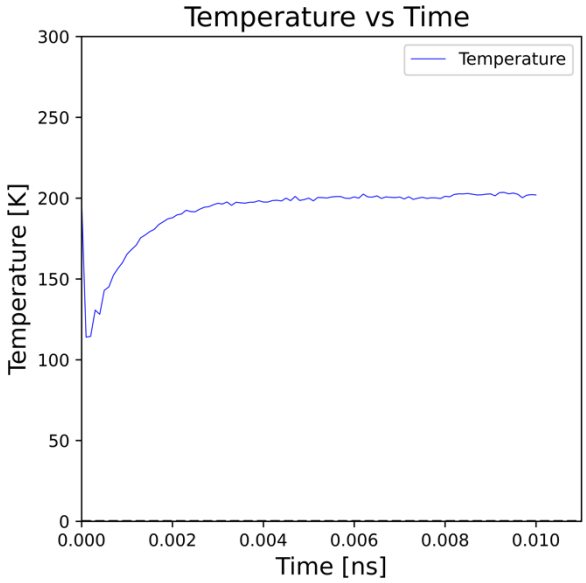
Step1:

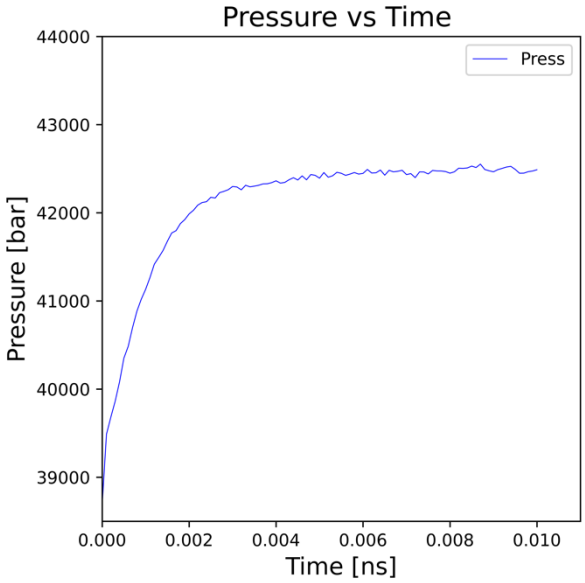






Step2:


Temperature vs Time
Temperature
Temperature [K]
Time [ns]
300
250
200
150
100
50
0
0.000
0.002
0.004
0.006
0.008
0.010


Pressure vs Time
Press
Pressure [bar]
Time [ns]
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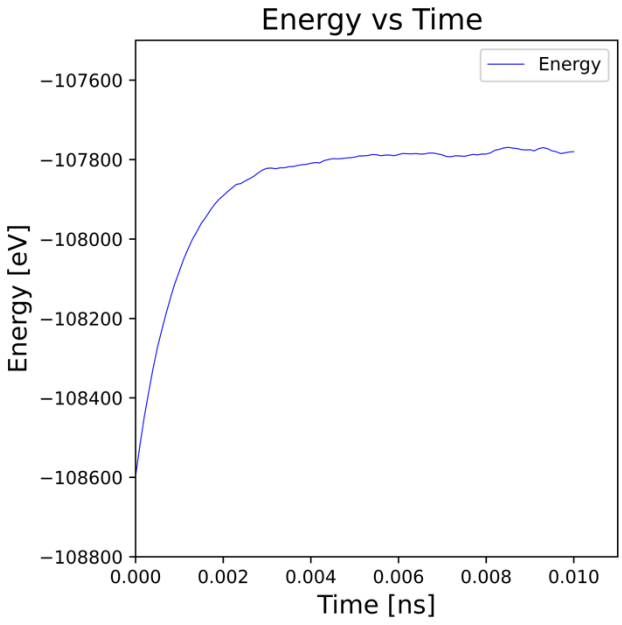
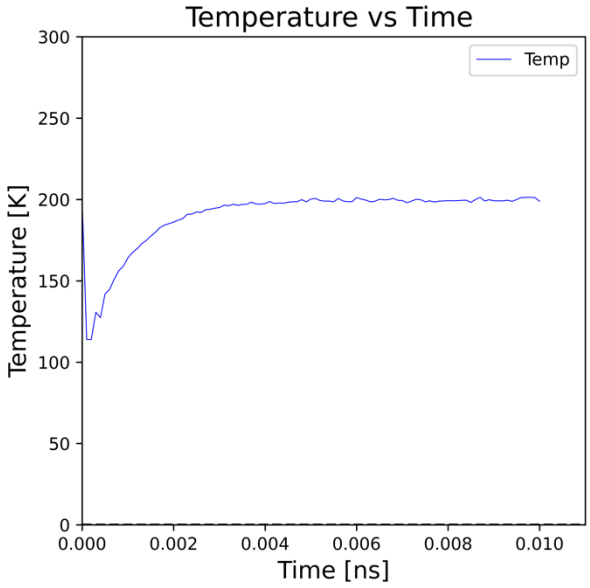
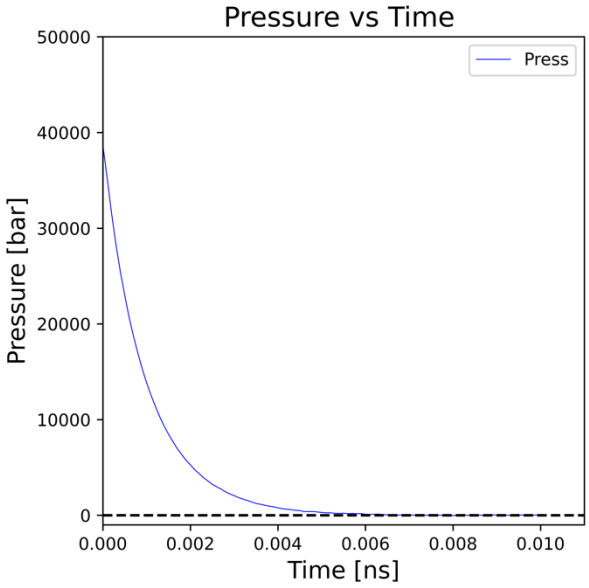
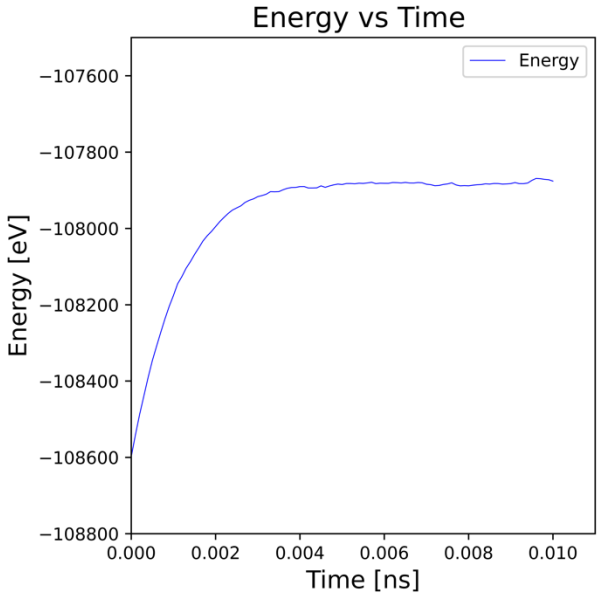
43000
42000
41000
40000
39000
0.000
0.002
0.004
0.006
0.008
0.010


Energy vs Time
Energy
Energy [eV]
Time [ns]
−107600
−107800
−108000
−108200
−108400
−108600
−108800
0.000
0.002
0.004
0.006
0.008
0.010

Step3:


Temperature vs Time
Temp
Temperature [K]
Time [ns]
300
250
200
150
100
50
0
0.000
0.002
0.004
0.006
0.008
0.010


Pressure vs Time
Press
Pressure [bar]
Time [ns]
50000
40000
30000
20000
10000
0
0.000
0.002
0.004
0.006
0.008
0.010


Energy vs Time
Energy
Energy [eV]
Time [ns]
−107600
−107800
−108000
−108200
−108400
−108600
−108800
0.000
0.002
0.004
0.006
0.008
0.010