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APL3410
ASSIGNMENT - 2

Q1. (a) The particle velocities are initialized randomly from the uniform distribution (0, 1) using the rand() function. The velocities are then scaled to (-1, 1) using $\underset{\sim}{v}_i = -1 + 2\underset{\sim}{v}_i$, $i = 1, \ldots, 256$. Next, the momentum of the system $\underset{\sim}{p}_{net}$ is computed as

$$\underset{\sim}{p}_{net} = \sum_{i=1}^{256} m_i \underset{\sim}{v}_i$$

Finally, to ensure that system has 0 momentum, the individual velocities are adjusted:

$$\underset{\sim}{v}_i = \underset{\sim}{v}_i - \frac{\underset{\sim}{p}_{net}}{\text{mass} \times 256}$$

(b) The Lenard-Jones interatomic potential energy, $V_{int}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$

To incorporate the cutoff scheme, modified V_{int}:

$$V_{int}(r_{ij}) = \begin{cases} V_{int}(r_{ij}) - V_{int}(r_{cut}) - (r_{ij} - r_{cut})(-f(r_{cut})) & , r < r_{cut} \\ 0 & , r \geq r_{cut} \end{cases}$$

where, $f(r_{cut}) = -\frac{dV_{int}}{dr}(r_{cut}) = +\frac{48\varepsilon\sigma^{12}}{r_{cut}^{13}} - \frac{24\varepsilon\sigma^{6}}{r_{cut}^{7}}$

For a continuous force with cutoff scheme,

$$\underset{\sim}{f}_{ij} = \begin{cases} (f_{int}(r_{ij}) - f(r_{cut}))\,\underset{\sim}{r}_{ij}/r_{ij} & , r_{ij} < r_{cut} \\ \underset{\sim}{0} & , r_{ij} \geq r_{cut} \end{cases}$$

where, $f_{int}(r_{ij}) = -\frac{dV_{int}}{dr}(r_{ij}) = \frac{24\varepsilon\sigma^{6}}{r_{ij}^{7}}\left(\frac{2}{r_{ij}^{6}} - 1\right)$

$$\underset{\sim}{r}_{ij} = \underset{\sim}{r}_i - \underset{\sim}{r}_j$$

(c) The instantaneous temperature is found using the instantaneous kinetic energy values:

$$K_{inst} = \sum_{i=1}^{256} \frac{1}{2} m_i |v_i|^2 \,, \quad T_{ins} = \frac{2}{3 \times 256 \times k_B} K_{inst}, \quad k_B = 1.38 \times 10^{-23}\ \text{J K}^{-1}$$

(d) The nearest image convention is used as follows:

$$r_{ij}[k] = r_{ij}[k] - r_j[k]$$

if $r_{ij}[k] > L/2 \Rightarrow r_{ij}[k] = r_{ij}[k] - L$

else if $r_{ij}[k] < -L/2 \Rightarrow r_{ij}[k] = r_{ij}[k] + L$

(e) To determine when the system is equilibrated, we monitor the system's temperature & energy (kinetic, potential, and total energy) over time. When these quantities fluctuate around stable average values, rather than showing a continuous increase/decrease, the system is considered to attain equilibrium.

(i) Track system's kinetic energy and temperature for a few thousand timesteps. When these quantities do not change significantly the system can be considered equilibrated.

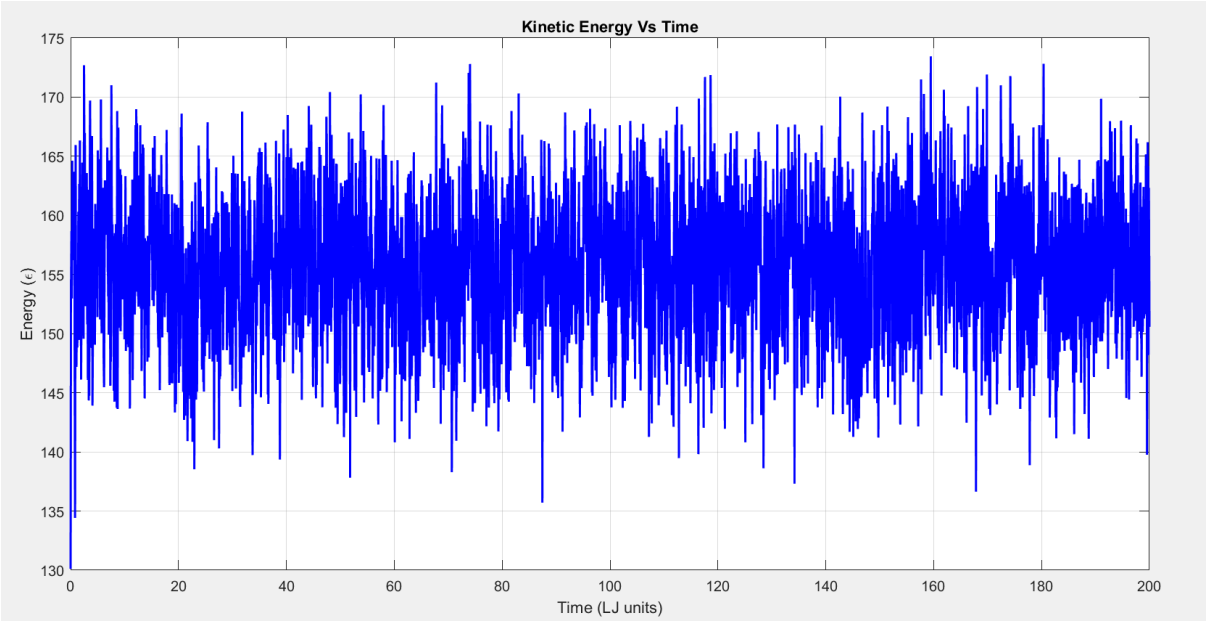
(ii) After running the simulation, we observe that these quantities very quickly start fluctuating around a value of $T = 2.89 \times 10^{22} (\varepsilon/k_B)$ units.

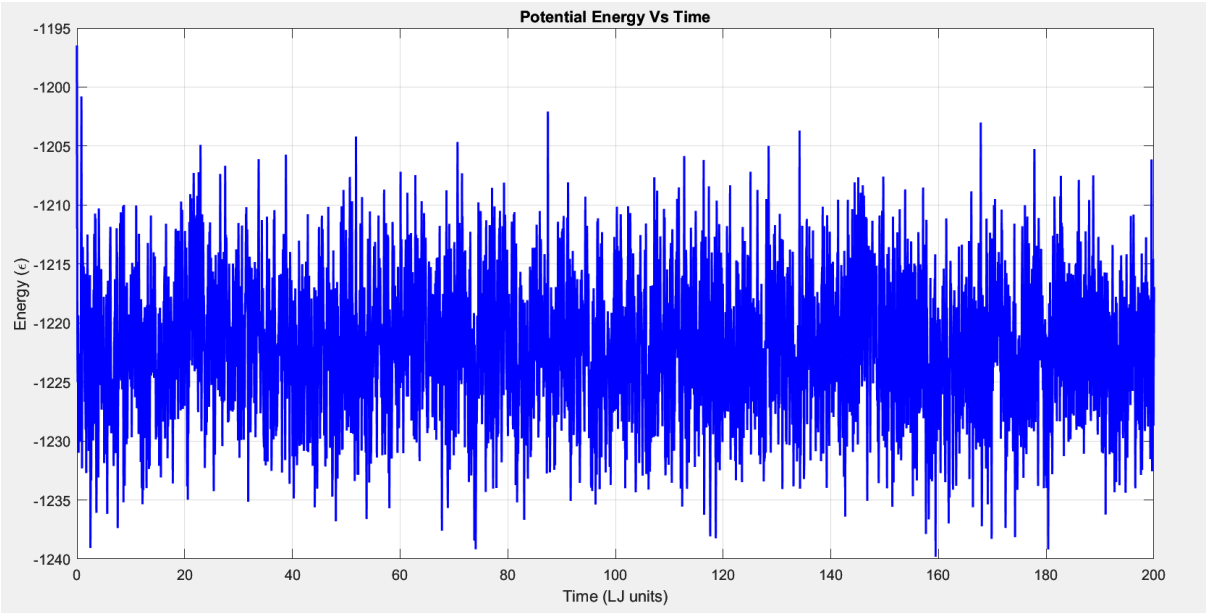
(f) The system's kinetic energy, potential energy, total energy, and instantaneous temperature were stored for every timestep dt; where $dt = \frac{\text{final time}}{\text{No. of steps}}$. & then plotted against time.

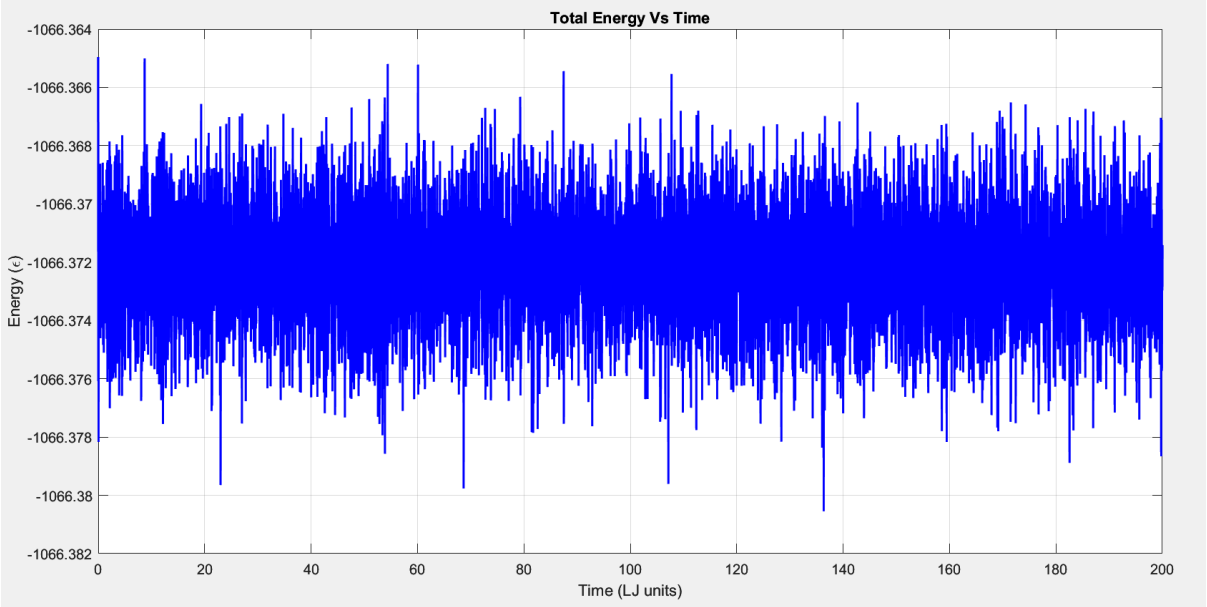
From the plot of total energy, we observe that it fluctuates between $(-1070.114, -1070.038)$ with a maximum percentage variation of 0.015% from the mean. These fluctuations are attributed to machine precision errors and errors due to the discretized numerical integration.

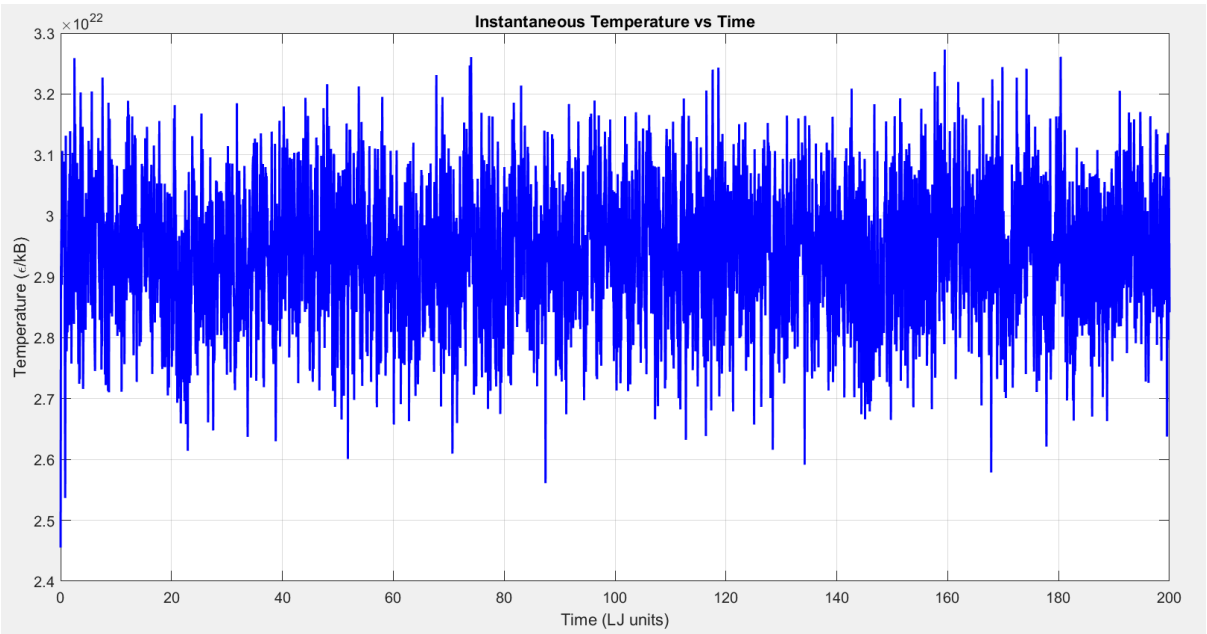
(g) Due to limitations in machine precision, the initial total momentum of the system is non-zero. Thus, it fluctuates and grows slightly with time.

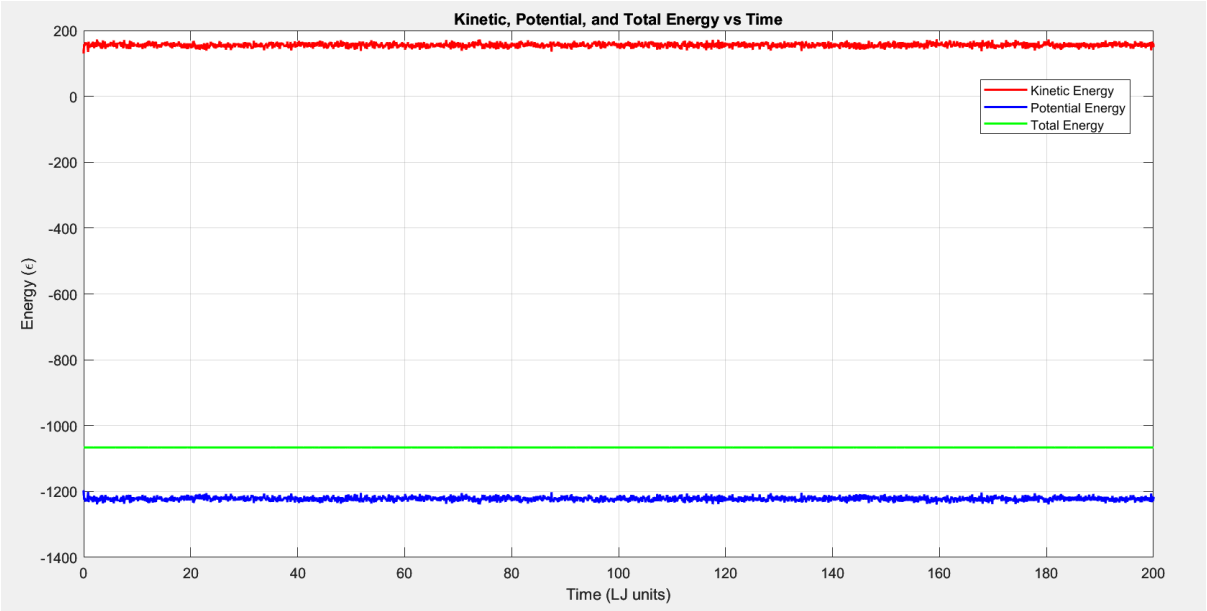
(f)


Kinetic Energy Vs Time
Energy (ϵ)
Time (LJ units)
175
170
165
160
155
150
145
140
135
130
0
20
40
60
80
100
120
140
160
180
200

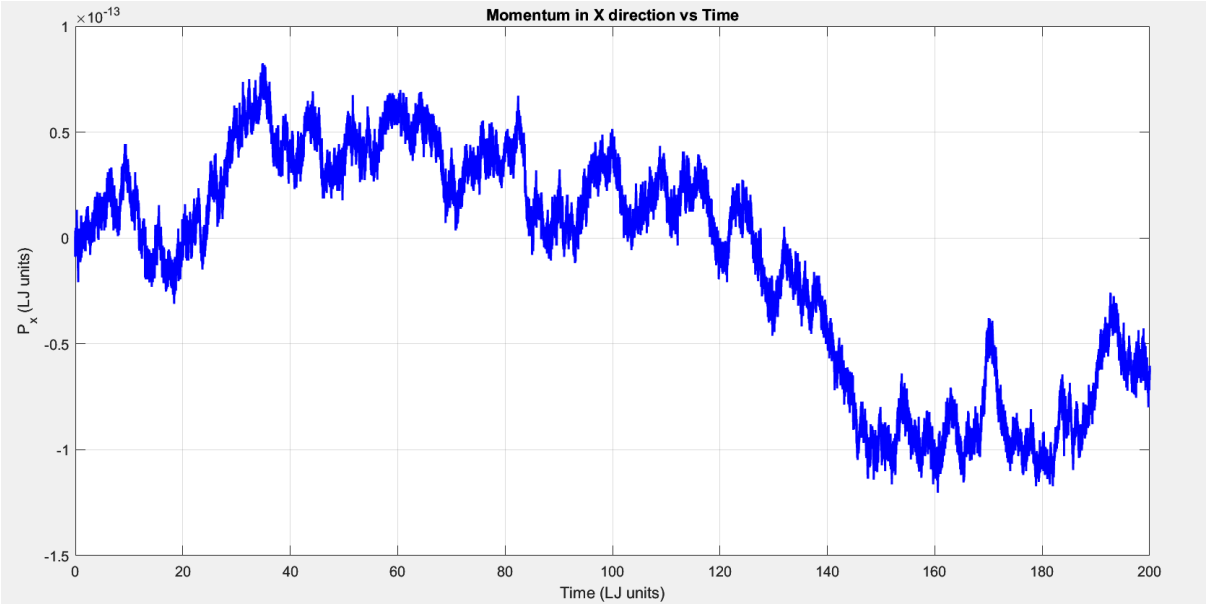

Potential Energy Vs Time
Energy (ϵ)
Time (LJ units)
-1195
-1200
-1205
-1210
-1215
-1220
-1225
-1230
-1235
-1240
0
20
40
60
80
100
120
140
160
180
200

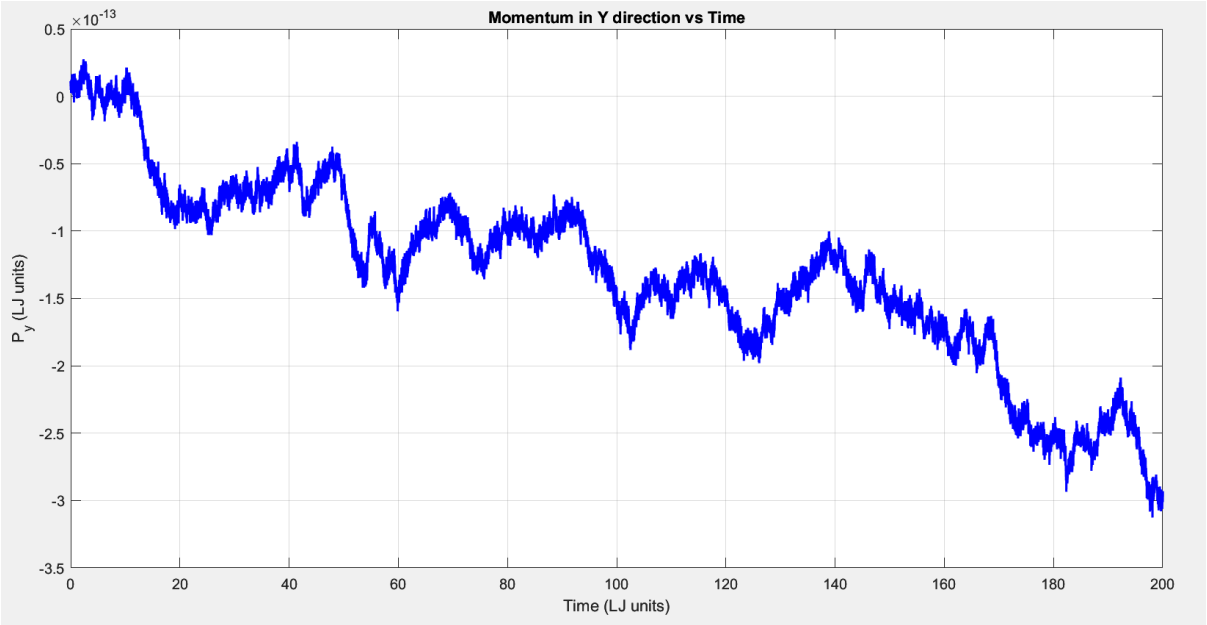

Total Energy Vs Time
-1066.364
-1066.366
-1066.368
-1066.37
-1066.372
-1066.374
-1066.376
-1066.378
-1066.38
-1066.382
Energy (ϵ)
0
20
40
60
80
100
120
140
160
180
200
Time (LJ units)

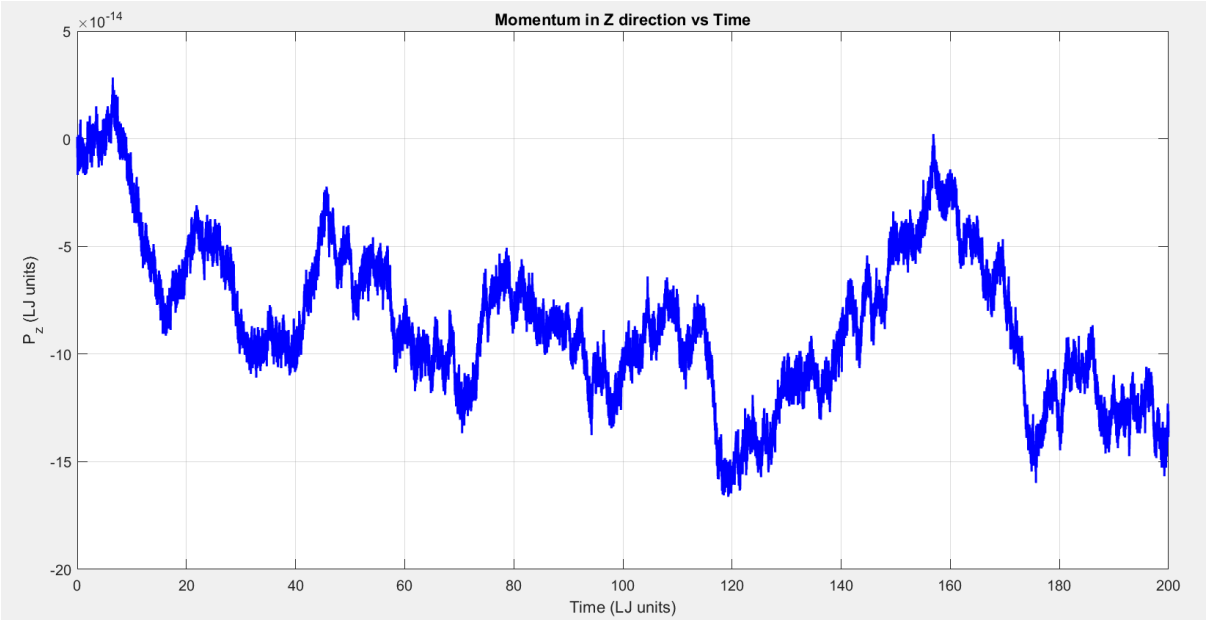

Instantaneous Temperature vs Time
×10^22
3.3
3.2
3.1
3
2.9
2.8
2.7
2.6
2.5
2.4
Temperature (ϵ/kB)
0
20
40
60
80
100
120
140
160
180
200
Time (LJ units)


Kinetic, Potential, and Total Energy vs Time
Kinetic Energy
Potential Energy
Total Energy
Energy (ϵ)
Time (LJ units)
200
0
-200
-400
-600
-800
-1000
-1200
-1400
0
20
40
60
80
100
120
140
160
180
200

(g)


Momentum in X direction vs Time
×10^-13
P_x (LJ units)
Time (LJ units)
1
0.5
0
-0.5
-1
-1.5
0
20
40
60
80
100
120
140
160
180
200


Momentum in Y direction vs Time
×10^-13
0.5
0
-0.5
-1
-1.5
-2
-2.5
-3
-3.5
P_y (LJ units)
0
20
40
60
80
100
120
140
160
180
200
Time (LJ units)


Momentum in Z direction vs Time
×10^-14
5
0
-5
-10
-15
-20
P_z (LJ units)
0
20
40
60
80
100
120
140
160
180
200
Time (LJ units)