NNSA HSAP Computational Laboratory 8 - 2026 Update

Goals: Molecular Dynamics in Python: Rocket trajectory code!

```
import matplotlib.pyplot as plt
import numpy as np

dt = float(input('Enter dt: '))
m0 = float(input('Enter mass: '))
y = 0.001
v = float(input('Enter v0: '))
g = -9.8
THR = float(input('Enter thrust: '))
tTHR = float(input('Enter duration of thrust: '))

pm = float(input('Enter propellant mass : '))
b = float(input('Enter air resistance: '))

time = np.array([0.0], dtype=np.float32)
ysave = np.array([y], dtype=np.float32)
vsave = np.array([v], dtype=np.float32)

t = 0.0

while y > 0:
 t = t + dt
 y = y + v *dt
 if (t < tTHR):
  m = m0-pm*t/tTHR
  F = THR + m * g - b*v
  v = v + (F / m) * dt
 else:
  m = m0 - pm
  F = m *g -b*v
  v = v + (F / m) * dt
 if (abs(t - tTHR) < dt / 2):
  print('height when the engine turned off', y)
 time = np.append(time, t)
 ysave = np.append(ysave, y)
 vsave = np.append(vsave, v)


print('time of flight', t)

plt.axvline(x=tTHR, linestyle=":", color = 'black', label='Engine turns off')
plt.axhline(y=0, color='black')
```

```
plt.axvline(x=0, color='black')
plt.scatter(time, ysave, color='r', marker='.', s=1, label='Rocket trajectory')
plt.scatter(time, vsave, color='orange', marker='.', s=1, label='Rocket velocity')
maxheight = np.max(ysave)
timeofmax = time[np.where(ysave == maxheight)[0][0]]
plt.scatter(timeofmax, maxheight, marker='o', color='blue', label=('Max height =' + str(
plt.xlabel('t')
plt.ylabel('y')
plt.legend()
plt.show()
```