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# Lab - 4 : Thermodynamic Properties and Ensemble Averages

**Aim :-** Given time evolution of volume and energy at 6 pressure values. Evaluate compressibility and specific heat as function of pressure.

**Theory :-**

Compressibility, $K_P = \frac{\langle (\Delta V)^2 \rangle}{\langle \Delta V \rangle^2 K_B T} = \frac{\langle (V - \langle \Delta V \rangle)^2 \rangle}{\langle \Delta V \rangle^2 K_B T}$

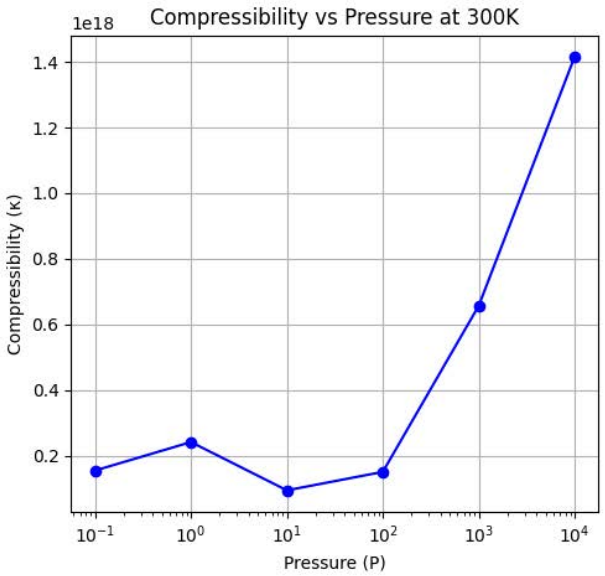
Specific Heat, $C_V = \frac{\langle (\Delta E)^2 \rangle}{K_B T^2} = \frac{\langle (E - \Delta E)^2 \rangle}{K_B T^2}$

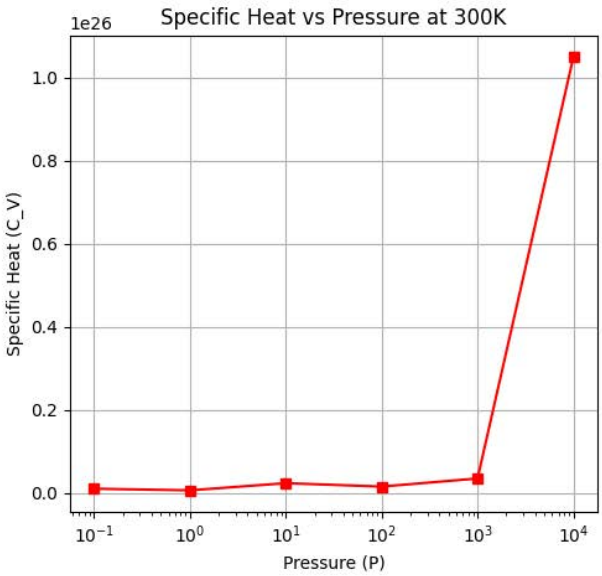
$$\langle \Delta x \rangle = \frac{1}{N} \sum_{i=1}^{N} x_i$$

**Lab4-Fluctuations.py**

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

def read_xvg_file(file_path):
    data = np.loadtxt(file_path, comments=['#', '@'])
    return data[:, 1]

T = 300
k_B = 1.380649e-23

Ps = [0.1, 1, 10, 100, 1000, 10000]
Kps = []
Cvs = []

for P in Ps:
    volume_data = read_xvg_file(f'npt_fluctuations/npt{P}/volume.xvg')
    energy_data = read_xvg_file(f'npt_fluctuations/npt{P}/energy.xvg')

    avg_volume = np.mean(volume_data)
    avg_volume_2 = np.mean((volume_data-avg_volume)**2)

    avg_energy = np.mean(energy_data)
    avg_energy_2 = np.mean((energy_data-avg_energy)**2)

    Kp = avg_volume_2/((avg_volume**2) * k_B * T)
    Cv = avg_energy_2 / (k_B * (T**2))

    Kps.append(Kp)
    Cvs.append(Cv)

# Plot Compressibility vs Pressure
plt.figure(figsize=(10, 5))
plt.subplot(1, 2, 1)
plt.plot(Ps, Kps, label='Compressibility (κ)', marker='o', color='b')
plt.xscale('log')  # Log scale for pressure
plt.xlabel('Pressure (P)')
plt.ylabel('Compressibility (κ)')
plt.title(f'Compressibility vs Pressure at {T}K')
plt.grid(True)

# Plot Specific Heat vs Pressure
plt.subplot(1, 2, 2)
plt.plot(Ps, Cvs, label='Specific Heat (C_V)', marker='s', color='r')
plt.xscale('log')  # Log scale for pressure
plt.xlabel('Pressure (P)')
plt.ylabel('Specific Heat (C_V)')
plt.title(f'Specific Heat vs Pressure at {T}K')
plt.grid(True)

# Show the plots
plt.tight_layout()
```

```
52 plt.show()
```


Compressibility vs Pressure at 300K
1e18
Compressibility (κ)
Pressure (P)


Specific Heat vs Pressure at 300K
1e26
Specific Heat (C_V)
Pressure (P)