

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

```
class Model:
    def __init__(self, J: float, h: float, m: int):
        self.J = J
        self.h = h
        self.m = m
        self.energies = []

    def get_energy(self):
        return (np.dot(self.S, np.roll(self.S, -1))) * self.J * (-1) - np.sum(self.S) * self.h # Usin

    def simulate(self, N: int):
        self.S = np.random.choice([1, -1], self.m)

        while (N != 0):
            N -= 1
            old_E = self.get_energy()

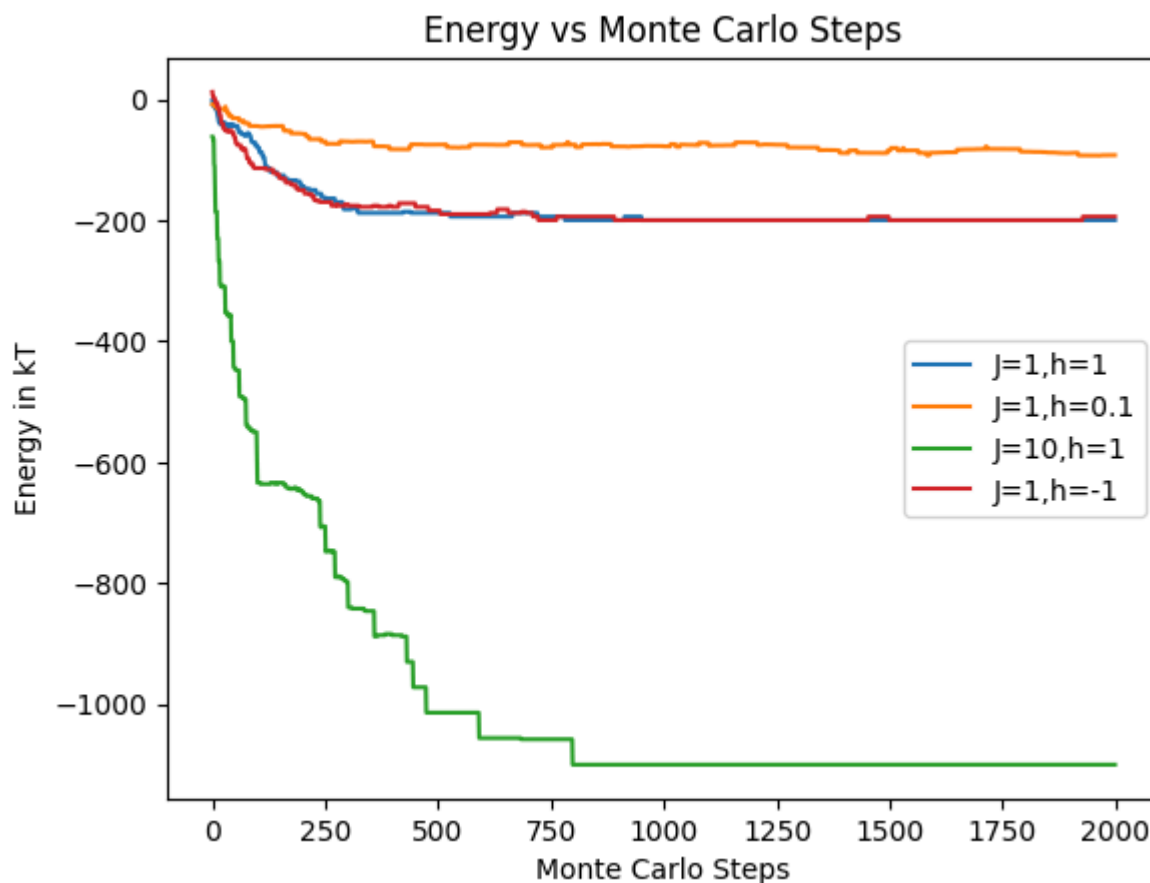
            state = np.random.choice(np.arange(0, self.m))
            self.S[state] *= -1

            new_E = self.get_energy()
            delta_E = new_E - old_E
            if delta_E > 0:
                p = np.exp(-delta_E)
                if np.random.random() > p:
                    self.S[state] *= -1
                    self.energies.append(old_E)
                    continue

            self.energies.append(new_E)

    def plot_graph(self):
        plt.title("Energy vs Monte Carlo Steps")
        plt.plot(self.energies, label=f"J={self.J}, h={self.h}")
        plt.xlabel("Monte Carlo Steps")
        plt.ylabel("Energy in kT")
```

```
for J, h in ((1, 1), (1, 0.1), (10, 1), (1, -1)):
    my_model = Model(J, h, 100)
    my_model.simulate(2000)
    my_model.plot_graph()
plt.legend()
plt.show()
```



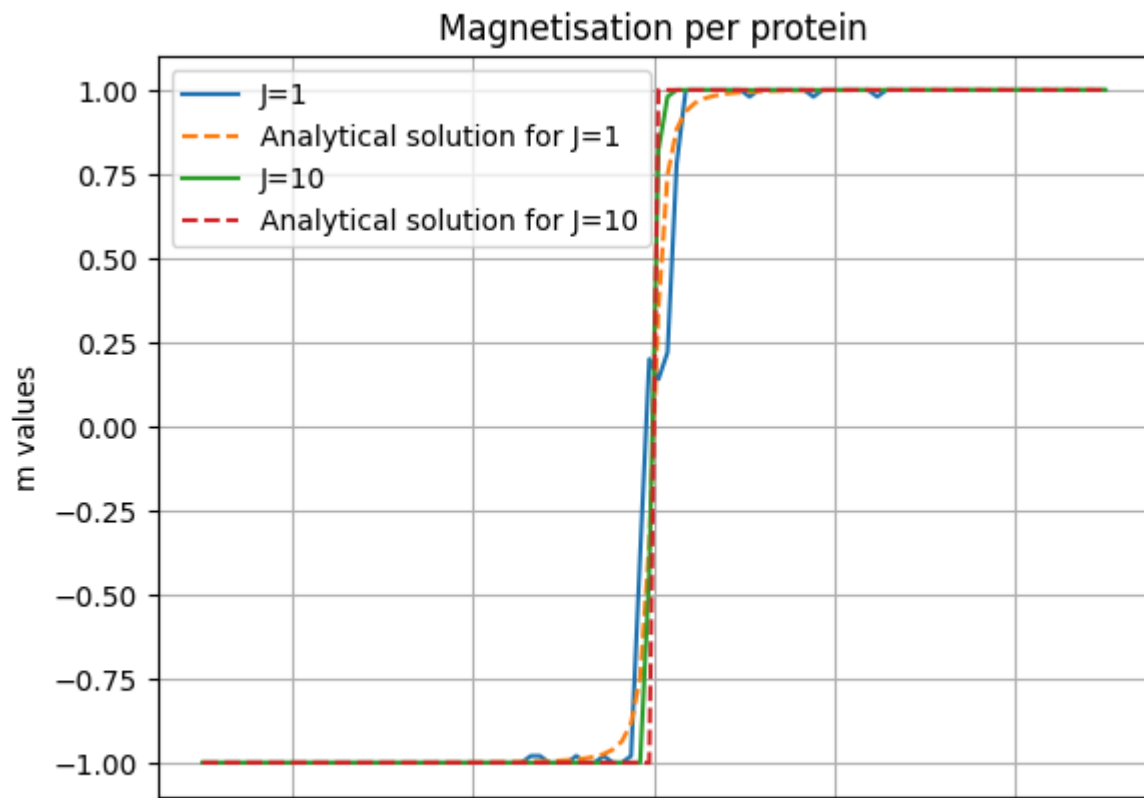
After simulation with 2000 steps, models have reached a steady state

```
def anal(J,h):
    return np.sinh(h)/np.sqrt(np.cosh(h)*np.cosh(h) - 2*np.exp(-2*J)*np.sinh(2*J))

h_values = np.linspace(-5,5,100)
for J in (1,10):
    m_values = []
    for h in h_values:
        mag_model = Model(J,h,100)
        mag_model.simulate(4000)
        M = np.sum(mag_model.S)
        m = M/100
        m_values.append(m)

plt.title("Magnetisation per protein")
plt.plot(h_values,m_values,'-',label=f"J={J}")
plt.plot(h_values,anal(J,h_values),'--',label=f"Analytical solution for J={J}")

plt.xlabel("h values")
plt.ylabel("m values")
plt.legend()
plt.grid()
plt.show()
```



```
for J,h in ((1,1),(1,0.1),(10,1),(1,-1)):
    my_model = Model(J,h,100)
    my_model.simulate(6000)
    eq_energies = my_model.energies[3000:] # Energies after equilibrium attained
    avg_energy = np.average(eq_energies)
    avg_sq_energy = np.average(np.array(eq_energies)**2)
    # print(avg_energy)
    # print(avg_sq_energy)
    print(f"Specific Heat for J={J} and h={h} is: {avg_sq_energy - avg_energy**2:.4f}")
```



```
Specific Heat for J=1 and h=1 is: 4.3967
Specific Heat for J=1 and h=0.1 is: 42.2328
Specific Heat for J=10 and h=1 is: 0.0000
Specific Heat for J=1 and h=-1 is: 2.9287
```