Exercise Session 2

MDMC Spring 2025

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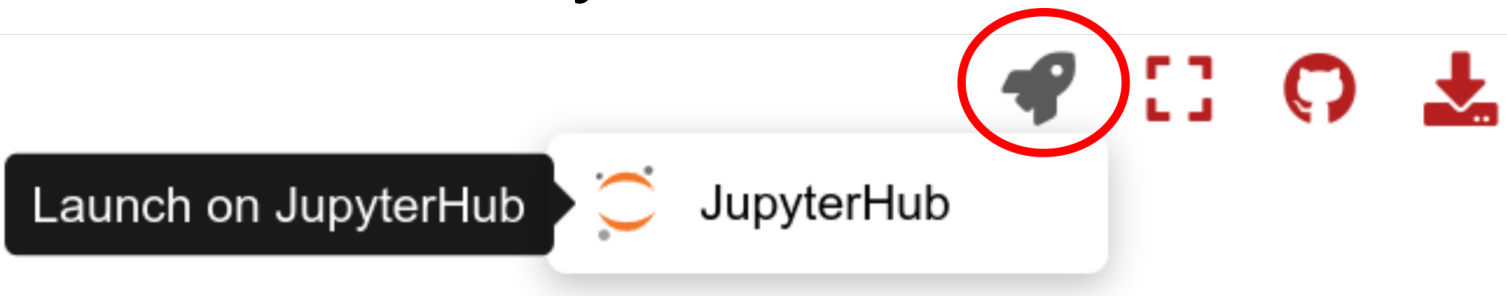
Exercise General Information

- Interviews
  - 10 minutes discussion to test your understanding of the exercise
  - Good occasion to discuss your doubts and questions
- Report feedback
  - After your interview, you will get a detailed feedback via Moodle
    - No grade
    - Overall comment and detailed correction of the exercises

Exercises contribute to 1/2 of final grade! We count the best 5 out of the 6 reports for your exercise grade.

Notebooks Reminder

- Always access the notebooks via the rocket button on the top right of the code files and choose JupyterHub to launch noto.epfl.ch
- **Make sure to access noto this way each time you begin the exercise to ensure you have the latest version!**



Exercise Structure

🎯 Learning goals

Follow a (re)introduction to statistical mechanics

Learn differeces between canonical and microcanonical ensembles

Understand how to calculate the Boltzmann distribution for a harmonic oscillator

📖 Chapter in script

Chapter 2 - Statistical Mechanics in a Nutshell

📚 Resources

Understanding Molecular Simulation, Frenkel & Smit, p.9-17

Exercise 2 - Intro & Tips

Today we'll be building a tool to compute the probability distribution of the energy of a system using Boltzmann statistics. The focus of the exercise is to refresh your notions of statistical mechanics, which is the foundation for all simulation techniques we'll see during the course.

- The theoretical part is about statistical thermodynamics. Be sure to know what we mean by
  - Thermodynamic ensembles
  - Microstate
  - Partition function and why its useful
  - Boltzmann distribution

Exercise 2 - Intro & Tips

- The practical part is about computing the Boltzmann distribution of a fictitious harmonic oscillator.
  For simplicity
  - Boltzmann constant $= 1$
  - Beta $= 1/T$
  - Energies represented as integer values

Exercise 2 - Intro & Tips

- Modify the code below to translate into code concepts from statistical mechanics

```
# MODIFY HERE
# set number of energy levels and temperatures here
n_energy_levels= 0
reducedTemperatures=[0, 0, 0, 0]


def calculateStateOccupancy(T, i):
    # No degeneracy
    return 1  # MODIFY HERE

def calculateStateOccupancy_s1(T, i):
    # Degeneracy s+1
    return 1  # MODIFY HERE

def calculateStateOccupancy_s2(T, i):
    # Degeneracy s+2
    return 1  # MODIFY HERE


functions ={
    "no_degeneracy": calculateStateOccupancy,
    "s+1": calculateStateOccupancy_s1,
    "s+2": calculateStateOccupancy_s2
}

for f in functions.keys():
    fig, ax =plt.subplots(1)
    ax.set_title(f)
    ax.set_xlabel("Energy level")
    ax.set_ylabel("Occupancy")

    calculateOccupancy=functions[f]

    for reducedTemperature in reducedTemperatures:
        distribution = [] # For each state there is one entry
        partition_function=np.float64(0.0)

        for i in range(n_energy_levels):
            stateOccupancy=calculateOccupancy(reducedTemperature, i)
            distribution.append(1.0) # MODIFY HERE
            partition_function+=1.0  # MODIFY HERE

        ax.plot(distribution/partition_function, label=reducedTemperature)

    ax.legend()
    plt.show()
```

Exercise 2 - Intro & Tips

- Remember there is also Exercise 8 (often accidentally skipped in previous years!)

```
# INSERT YOUR WORKING CODE HERE
# ADAPT it for the linear rotor case
# defining a new calculateStateOccupancy_rotor function and a "linear rotor" key

# Then run the following cell (after having edited it where indicated!)
```

```
for f in functions.keys():
    fig, ax =plt.subplots(1)
    ax.set_title(f)
    ax.set_xlabel("Reduced Temperature")
    ax.set_ylabel("Partition Function")

    calculateOccupancy=functions[f]
    Z = []  # This variable will store the partition function
            # for different reduced temperatures

    for reducedTemperature in reducedTemperatures:
        distribution = [] # For each state there is one entry
        partition_function=np.float64(0.0)

        for i in range(n_energy_levels):
            stateOccupancy=calculateOccupancy(reducedTemperature, i)
            distribution.append(1.0) # MODIFY HERE
            partition_function+=1.0  # MODIFY HERE
        Z.append(1.0) # MODIFY HERE
    ax.plot(reducedTemperatures, Z, label="Z Exact")
    ax.plot(reducedTemperatures, Z, label="Z Approximated") # MODIFY HERE
                                                            # insert approximated Z

    ax.legend()
    plt.show()
```