Exercise Session 3

MDMC Spring 2024

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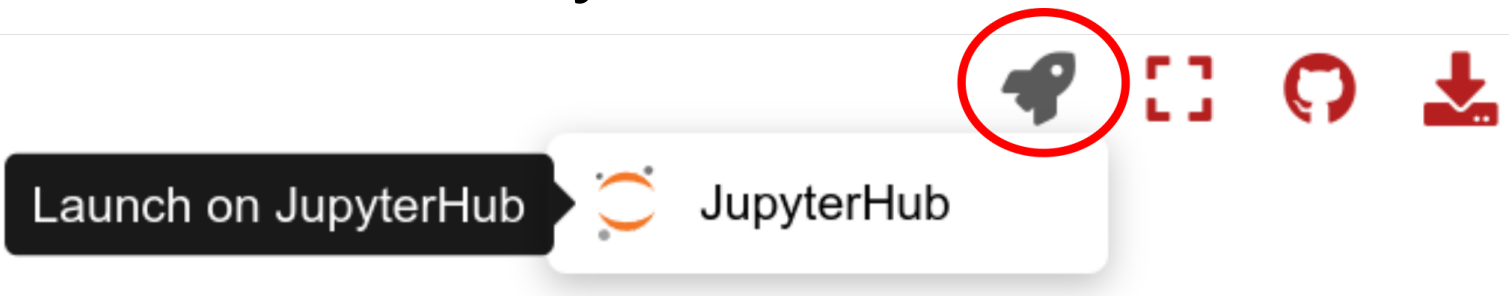
Exercise Check-In

How did you feel during the process of completing, turning in, interviewing, and receiving the comments for Ex 1?

Remember: 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

Understand importance sampling

Learn importance of detailed balance

Apply the Metropolis Monte Carlo algorithm to calculate properties of a model gas

📖 Chapter in script

Chapter 3 - Monte Carlo Simulations

📚 Resources

Understanding Molecular Simulation, Frenkel & Smit, 2nd Edition - Chapter 3 & Chapter 5 (extra)

Computer Simulation of Liquids, Allen & Tildesley, 2nd Edition - Chapter 4

Exercise 3 - Intro & Tips

Today we'll be writing and executing Monte Carlo code.

Tips!

- The theoretical part is about basic Monte Carlo simulations. Be sure to know what we mean by:
  - random sampling vs importance sampling
  - configurational space
  - transition or Markov matrix
  - detailed balance
  - Metropolis algorithm
- In the practical part we will run MC code for two systems:
  - A photon gas in which the energy states are quantized meaning we can calculate the ensemble average of state occupancy analytically
  - A gas in which we test different ensembles (NVT vs NPT) and use the Lennard-Jones potential to describe pairwise interactions

Exercise 3 - Intro & Tips

- Photon Gas
  - You'll need to write a loop of code to define the *estimatedOccupancy* function (read the hints and ask questions)
  - NB: *randint(0,1)* function will generate either 0 or 1. However, in our loop we need either 1 or -1
  - Recall that beta is the inverse of the product of the Boltzmann constant and simulation temperature. Varying beta is a way of varying simulation T

Exercise 3 - Intro & Tips

- LJ Potential
  - Lots of helper functions to import and functions to define. You don't need to modify anything there but it is good to have a look to understand what those functions do!
  - While there is quite a bit of code to execute, the goal is to see how we incorporate the system ensemble and its interactions when generating sample configurations for MC moves

Exercises 3 & 4 - Additional Notes

Due to the Easter Break, report 3 won't be due until Tuesday April 16th when we hold the session for Exercise 4

26.3. Tue	exercise	Ex 3 - LJ gas Monte Carlo
02.4. Tue		Easter Break
09.4. Tue	course	Chapter 4 (MD Simulations 1)
16.4. Tue	exercise	Ex 4 - Molecular Dynamics