

Exercise Session 1 MDMC Spring 2025

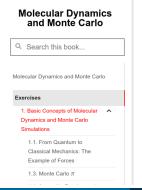
Salomé Guilbert, Qihao Zhang

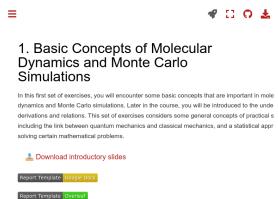
February 25, 2025



Exercise General Information

- Practical exercises every other week in BCH 1113
 - 2 hours to work on your own and with support from TAs
- Reports
 - For each exercise, report answering the questions
 - We provide you templates (google doc/overleaf)







Exercise General Information

- Report Submission
 - pdf document answering the questions and relevant output
 - Due date is usually the next exercise session (check Moodle!)
 - Detailed feedback via Moodle after the interview
 - No grade
 - Overall comment and detailed correction of the exercises
- Interviews during next exercise session are about 10-15 minutes
 - Test your understanding of the exercise
 - Good occasion to discuss your doubts and questions
 - We will release the schedule ahead of the session so you know when and with whom you will interview - you need to email us to reschedule if you can't make it to your allocated time
 - If you don't come to your interview and don't notify us to reschdule, your grade for that report will be 0
 - Exercises contribute to 1/2 of final grade! We count the best 5 out of the 6 reports for your exercise grade.



Exercise structure

@ Learning goals

Follow the link between classical and quantum models

Learn to compute π using a Monte Carlo approach

Understand how to generate randomness on a computer

Chapter in script

Chapter 1 - From Quantum Mechanics to Classical Mechanics Resources

Ab initio molecular dynamics: basic theory and advanced methods, Marx & Hutter, p.11-20

Learn Computer Graphics From Scratch!, Scratchapixel, Monte Carlo Methods in Practice: Generating Random Numbers

Resource Platforms

The following resources will be used to access and complete the exercises (more details later):

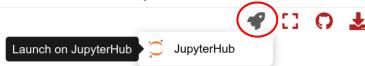
- Moodle page
 - Access exercise notebook
 - Turn in reports
 - Ask questions on the forum
- Exercise website:

https://lcbc-epfl.github.io/mdmc-public/

- Access jupyter notebooks on Noto
- Access to public github repository to raise issues for fixes/improvements to the exercises
- Read theory and questions
- Noto
 - Run and edit code blocks
 - Please note, for the most recent updates to the exercises you must access noto from the exercise website directly

Computer environment

- We will use a virtual environment that you can directly launch from the exercise website
- Click 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!





Computer environment

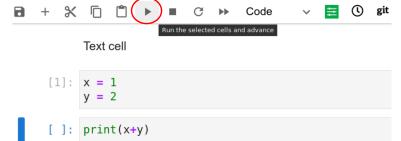
- On noto.epfl.ch your work will be saved on your EPFL storage
- Make sure to always activate (top right) the Computational Chemistry kernel



 Please activate 3rd party permission on your EPFL Google Account using go.epfl.ch/GoogleColabPermissions

Jupyter notebooks

- .iynb files organized in cells
 - Markdown (text)
 - Code
- Run a code cell by pressing Play button (or Ctrl+Enter)



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Jupyter notebooks

- .iynb files organized in cells
 - Markdown (text)
 - Code
- Run a code cell by pressing :arrow_forward: (or Ctrl+Enter)



Text cell

```
[1]: x = 1
```

[3]: print(x+y)

3

Exercise 1 - Intro & Tips

Today we'll be building a tool to estimate the value of π through a random sampling method (akin to Monte Carlo methods). The focus of the exercise is to get a better sense of how we can implement random sampling for numerical integration.

Tips!

- There is a small portion linking quantum ideas to classical mechanics. Please let us know if you need additional support regarding the notation/formalisms here.
- It may be a good idea to start from the practical part, to get familiar with the environment and ask us questions
- Places where you need to modify the code blocks should be noted with comments in the code with something like ## Begin code to modify ##

Questions?

Questions on the exercises (or the theory) outside exercise hours or problems with the reports? You can always contact us

- Moodle Forum, preferred way of communication since everyone can see the questions (and answer!)
- Email us, always better to include multiple of us to get an answer faster (at least always include Salomé, Qihao, and soon Thibault and Evan)
 - salome.guilbert@epfl.ch
 - qihao.zhang@epfl.ch
- At least one of us will always try to be present during lectures, feel free to ask us questions before/after the lecture or during the break!