Exercise Session 1
MDMC Spring 2026

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February 24, 2026

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)

Molecular Dynamics and Monte Carlo

🔍 Search this book...

Molecular Dynamics and Monte Carlo

Exercises

1. Basic Concepts of Molecular Dynamics and Monte Carlo Simulations

1.1. From Quantum to Classical Mechanics: The Example of Forces

1.3. Monte Carlo π

1. Basic Concepts of Molecular Dynamics and Monte Carlo Simulations

In this first set of exercises, you will encounter some basic concepts that are important in mole dynamics and Monte Carlo simulations. Later in the course, you will be introduced to the unde derivations and relations. This set of exercises considers some general concepts of practical s including the link between quantum mechanics and classical mechanics, and a statistical appr solving certain mathematical problems.

📥 Download introductory slides

Report Template Google Docs

Report Template Overleaf

Exercise General Information

- Report Submission
  - `pdf` document answering the questions and relevant output
  - Due date is usually of one week, till the next lecture (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 reschedule, **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
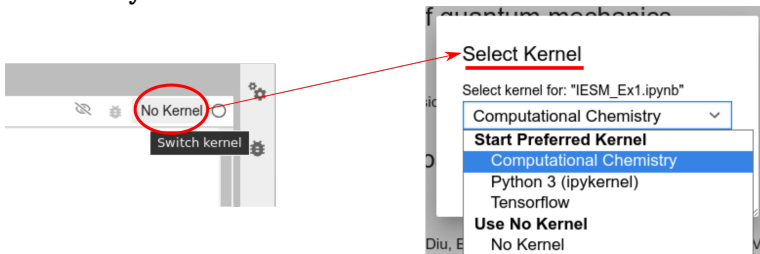 - Please note, for the most recent updates to the exercises you must access noto from the exercise website directly

- 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

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

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

Text cell

```
[1]: x = 1
     y = 2
```

```
[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* $\#\#$

What you should do if Noto doesn't work:

- Most importantly, **do not be a deadline fighter! Do it earlier!**
- Check whether you're working with the correct environment and import the modules correctly
- Try a different browser (Chrome, Firefox recommended)
- Refreshing the page after deleting the browser cache
- Conclude what you have done and what the problem is in detail (don't just mention 'it didn't work') and write to us TAs as soon as possible
- Contact noto support: noto-support@groupes.epfl.ch

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 all TAs)
  - thibault.klay@epfl.ch
  - amina.menhour@epfl.ch
  - alice.piantavigna@epfl.ch
  - evan.vasey@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!