

Exercise Session 1

MDMC Spring 2023

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February 28, 2023

Exercise General Information

- Practical exercises every other week in BCH 1113
 - 2 hours to work on your own and with support from TAs
- 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

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

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



Text cell

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

```
[ ]: print(x+y)
```

Jupyter notebooks

- .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 *## 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 Andrea and Sophie)
 - andrea.levy@epfl.ch
 - sophia.johnson@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!