

# Exercise Session 1

## MDMC Spring 2023

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## 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  $\pi$  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

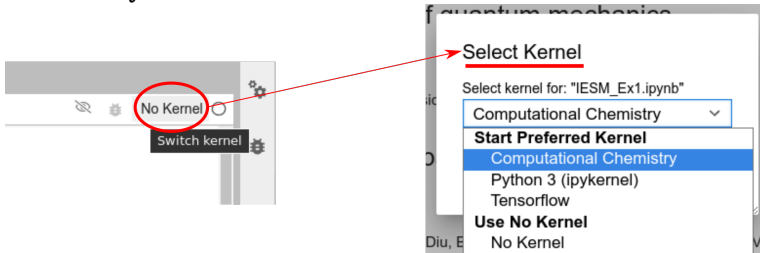
## Computer environment

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



# 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  $\pi$  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 outside on the exercises (or the theory) outside exercise hours? You can always contact us via - **Moodle Forum**, preferred way of communication since everyone can see the answers (and start a conversation!) - 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