

# Exercise Session 1

## MDMC Spring 2024

Simon Dürr, Sophia Johnson, Nikolaos Lempesis, Andrea Levy, Vladislav Slama

February 27, 2023

# 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)

The screenshot displays the interface of the book "Molecular Dynamics and Monte Carlo". On the left, there is a sidebar with a search bar labeled "Search this book..." and a table of contents. The table of contents lists "Exercises" and "1. Basic Concepts of Molecular Dynamics and Monte Carlo Simulations", with sub-items "1.1. From Quantum to Classical Mechanics: The Example of Forces" and "1.3. Monte Carlo  $\pi$ ". The main content area shows the title "1. Basic Concepts of Molecular Dynamics and Monte Carlo Simulations" and a paragraph of introductory text. Below the text, there are links to "Download introductory slides", "Report Template Google Docs", and "Report Template 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  $\pi$

## 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 molecular dynamics and Monte Carlo simulations. Later in the course, you will be introduced to the underlying derivations and relations. This set of exercises considers some general concepts of practical simulations including the link between quantum mechanics and classical mechanics, and a statistical approach 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 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



- Please activate 3rd party permission on your EPFL Google Account using [go.epfl.ch/GoogleColabPermissions](https://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  $\pi$  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 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 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!