Exercise Session 1

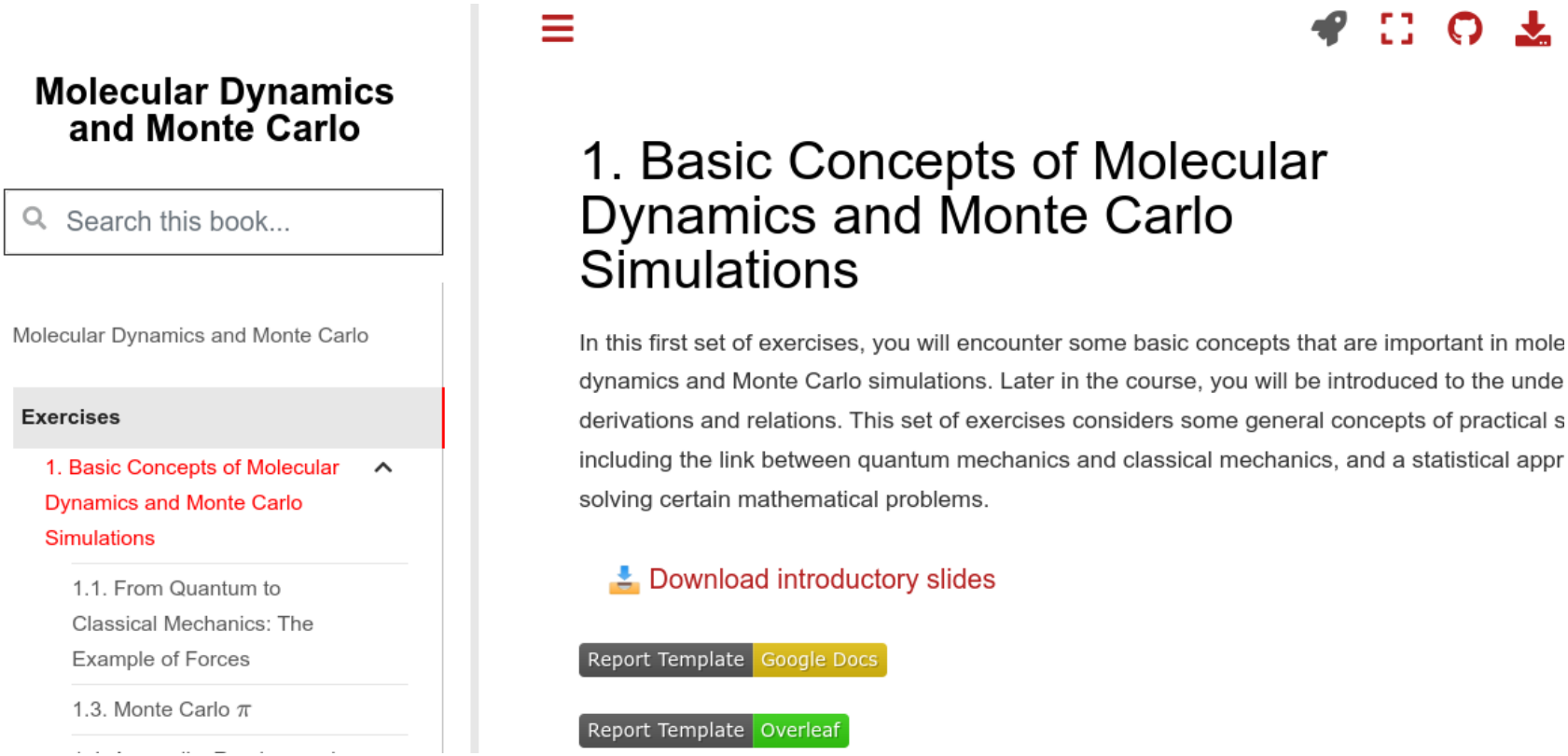
MDMC Spring 2025

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 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

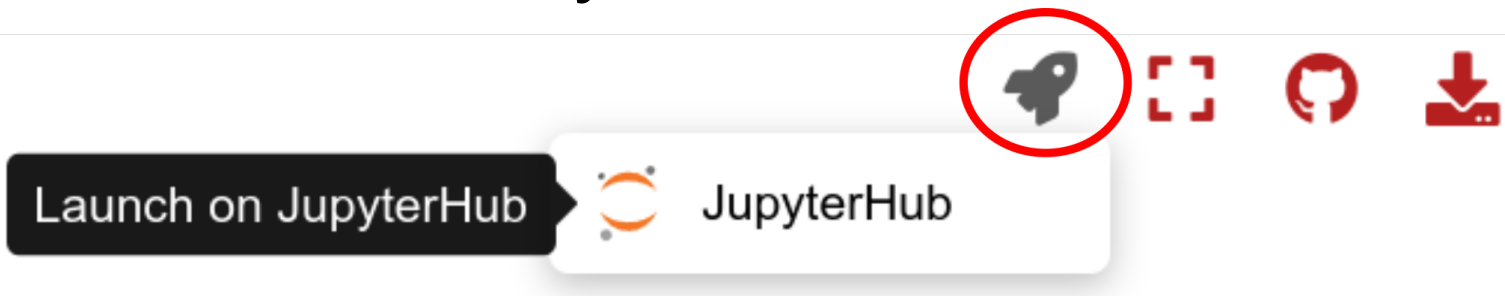
Resource Platforms

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

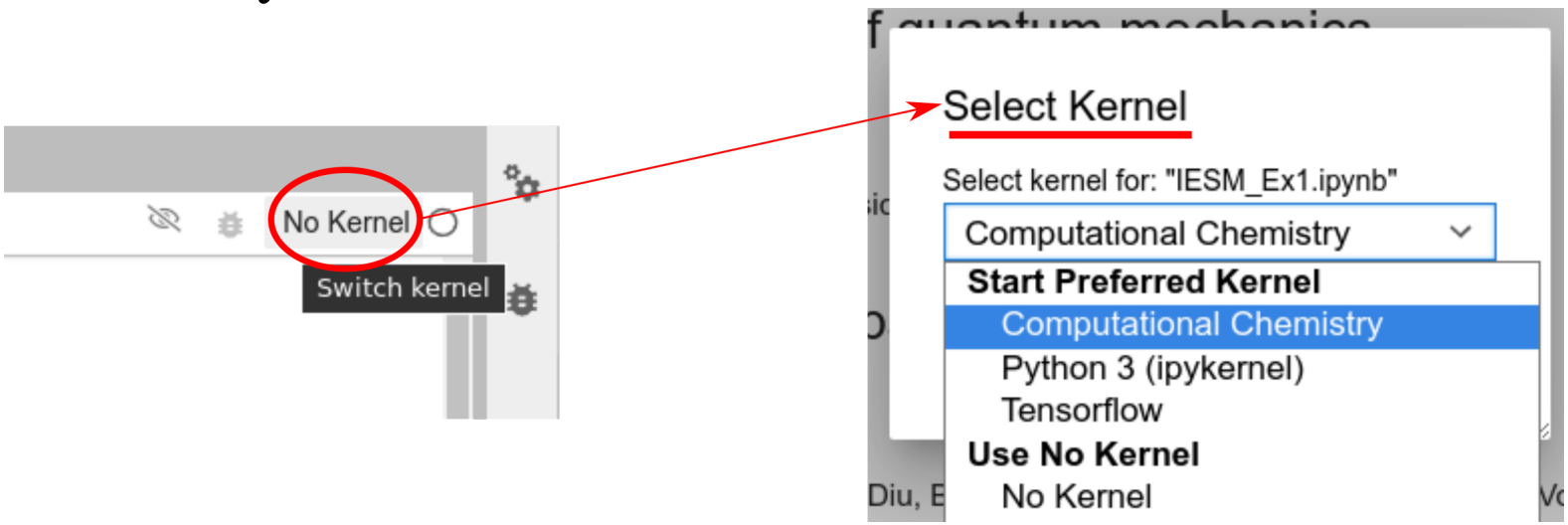
Computer environment

- 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

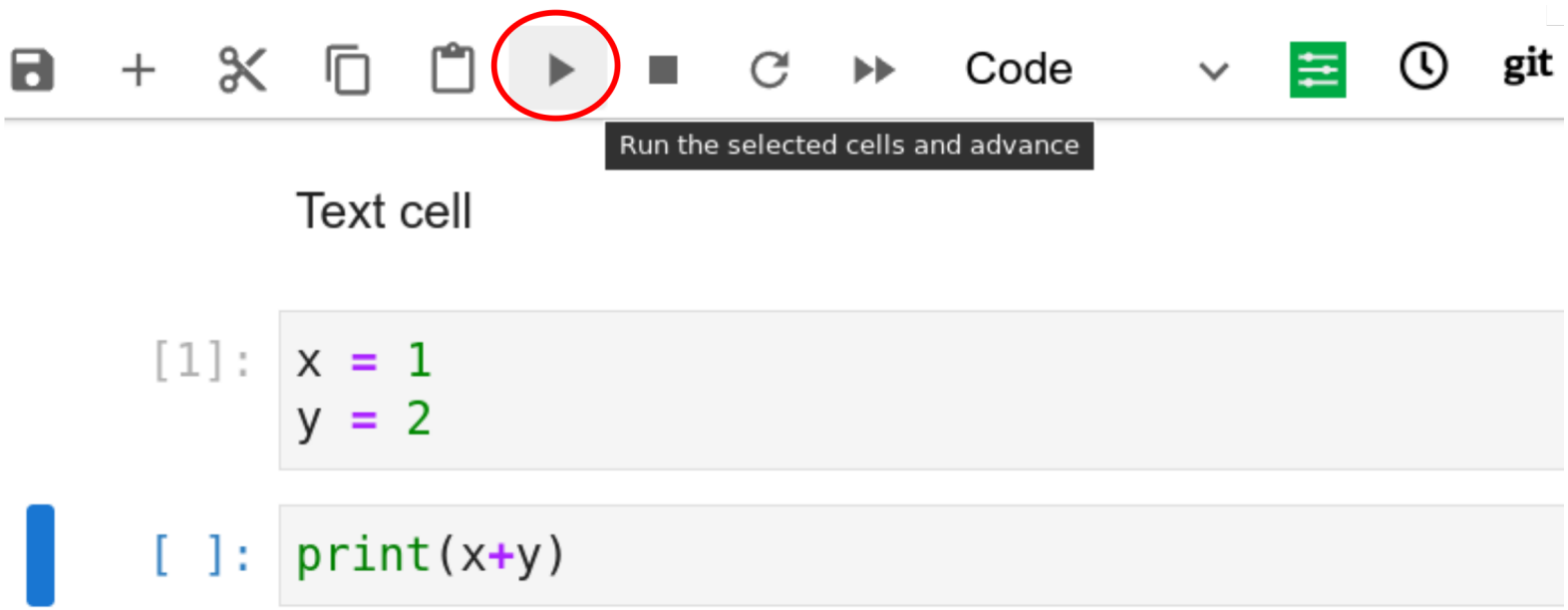
- On noto.epfl.ch your work will be saved on your EPFL storage
- Make sure to always activate (top right) the `Computational Chemistry` kernel



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

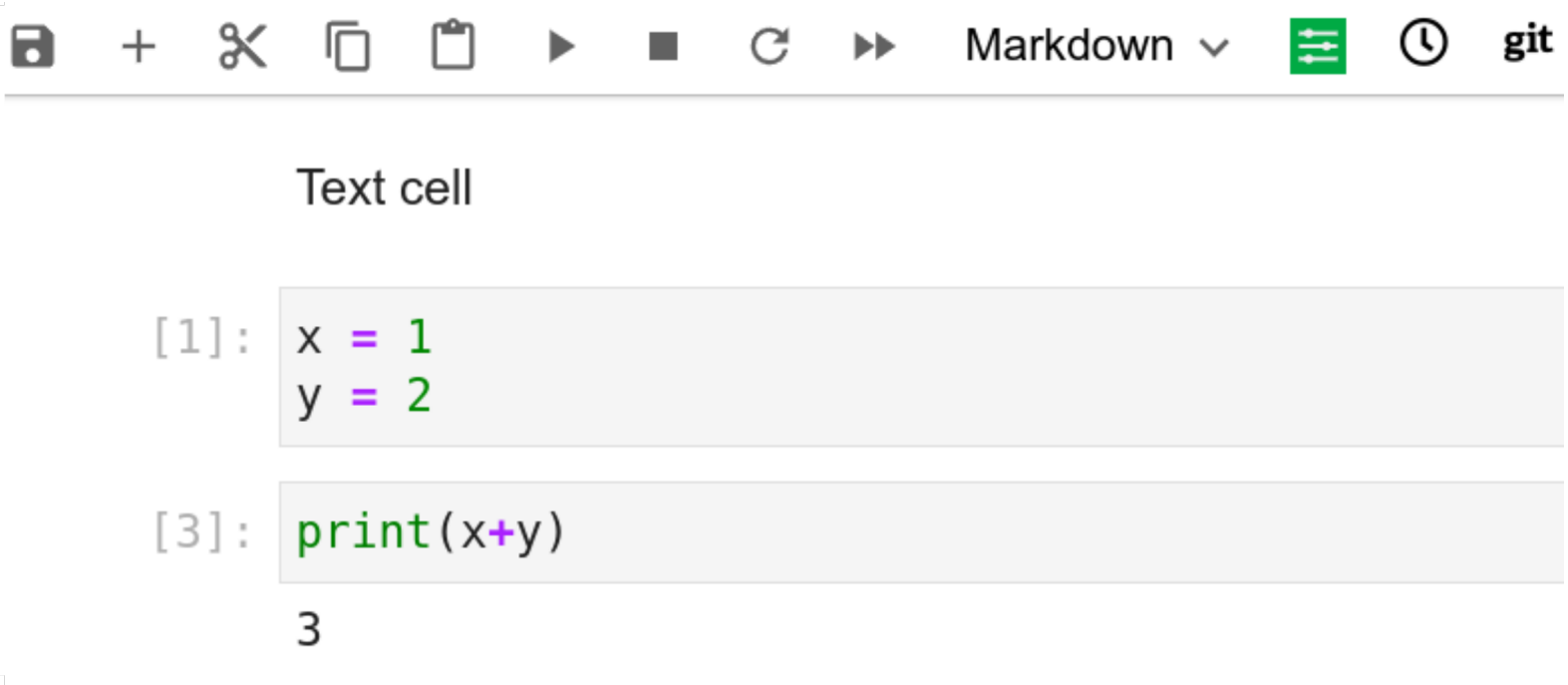
Jupyter notebooks

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



Jupyter notebooks

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



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!