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 5 out of the 6 exercises for your exercise grade.

Exercise structure

Introduction

- Learning goals
- Chapter in script
- Resources

Theory section

- Useful theory for the exercise
- Theoretical exercises

Practical exercises

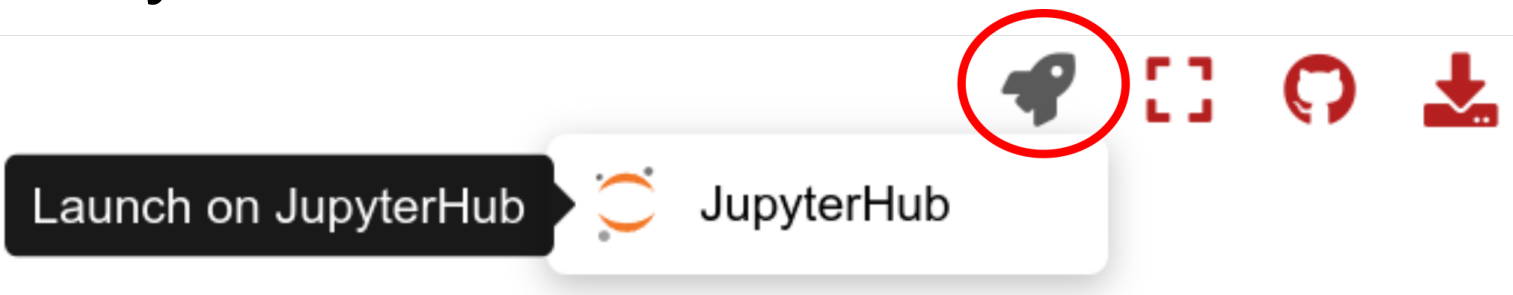
- "Coding" exercises
- Interpretation of results

Resource Platforms

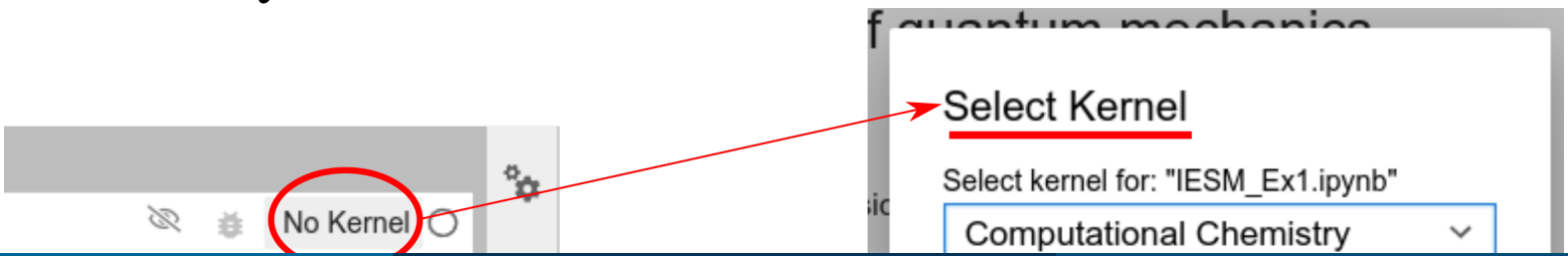
The following resources will be used to access and complete the exercises (more details later): - Moodle page - Access exercise notebook - Turn in reports - Ask questions on the forum - Exercise website: **https://lcbc-epfl.github.io/mdmc-public/** - Access juptyer notebooks on Noto - Access to public 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!**

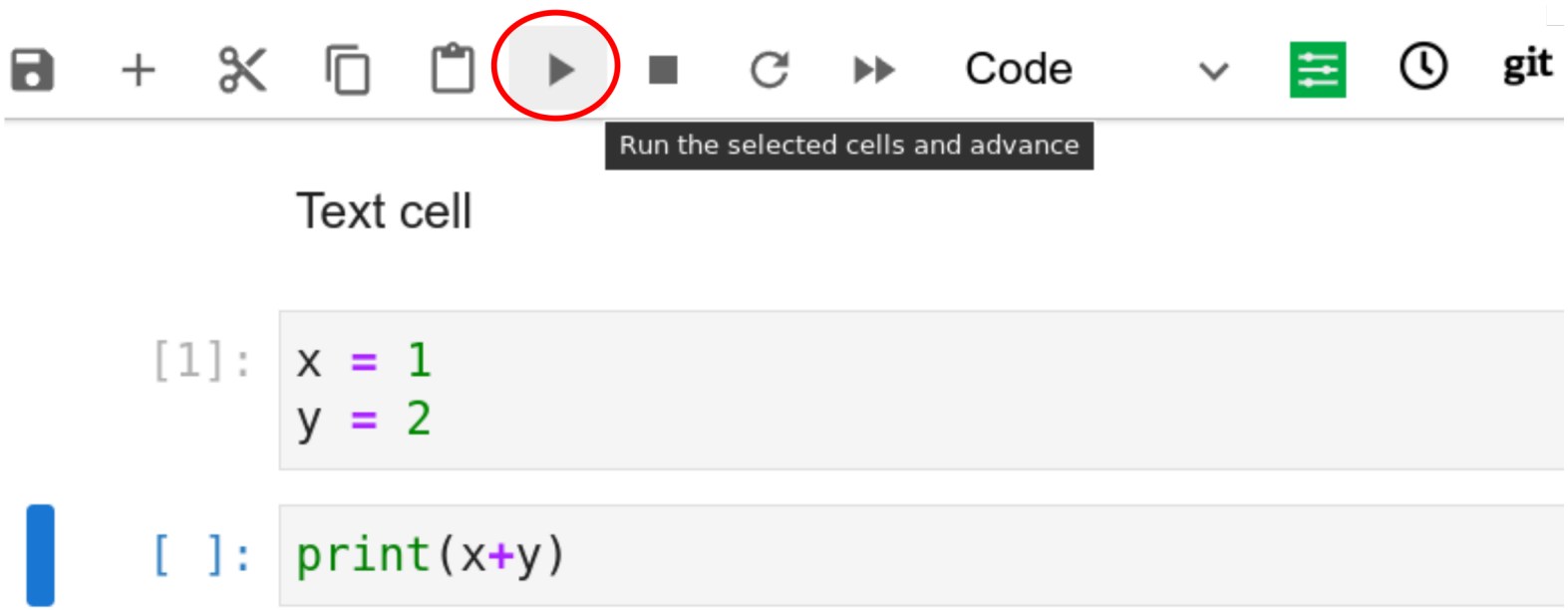


- On noto.epfl.ch your work will be saved on your EPFL storage
- Make sure to always activate (top right) the `Computational Chemistry` kernel



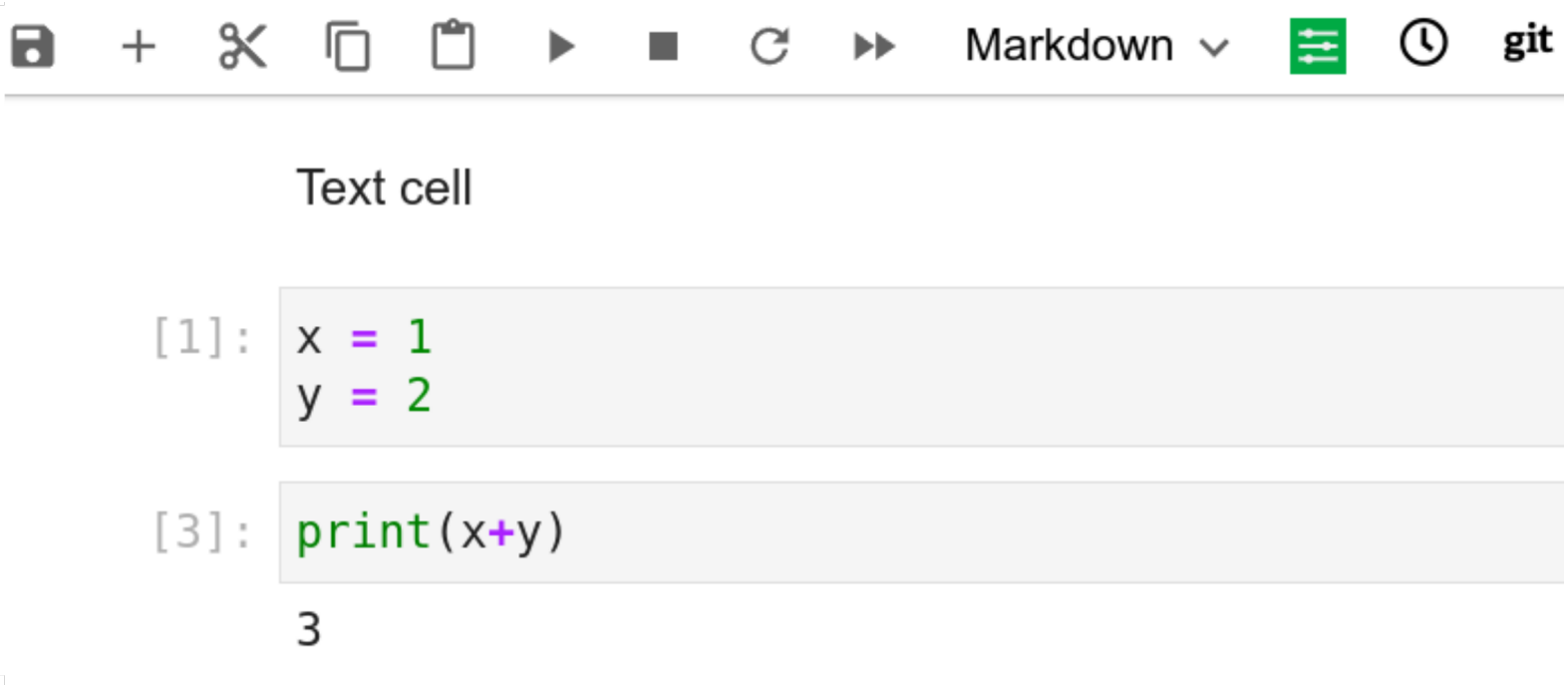
Jupyter notebooks

- `.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 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. - Places where you need to modify the code blocks should be noted with comments in the code "## Begin code to modify ##"