Exercise Session 5

MDMC Spring 2024

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Reminders

- Always access the notebooks via the rocket button on the top right of the code files and choose JupyterHub to launch noto.epfl.ch
- Google Colab: For Ex 6, you need to activate 3rd party permission on your EPFL Google Account. To be able to do that, it is necessary to activate 3rd party permission on your EPFL Google Account at this link https://go.epfl.ch/GoogleColabPermissions. Since the activation can take some time, it is important that you do it well in advance to the last exercise session to be able to run exercise 6 on May 14th! To test if you got access, simply try to log in to colab.research.google.com with your EPFL account after ~24h you asked for permission.

Reminders

- Important Dates:
  - Due date for Ex 5 will be Tuesday May 14th
  - Q&A Session on Tuesday May 21rd in lecture classroom
  - Written exam on Tuesay May 28th in lecure classroom

Exercise 5 Learning Goals

🎯 Learning goals

Review inter- and intramolecular interactions for building a classical force field

Compare common thermostat schemes

Understand how and why we initialize MD simulations

Draw a connection between the pair radial distribution function, the partition function, and ensemble average

📖 Chapter in script

Chapter 5 - Molecular Dynamics Simulations (II)

📚 Resources

Understanding Molecular Simulation, Frenkel & Smit, 2nd Edition - Chapter 6

Exercise 5 - Intro

Today we will re-provide you a simple Molecular Dynamics (**Toy MD**) code in Python and you will edit it to run an MD simulation in the NVT ensemble.

- The theoretical part discusses the practical of relativistic MD systems:
  - describing potential energy via force fields
  - sampling NVT (canonical) ensemble using thermostats
  - understanding pair radial distribution functions
- In the practical part you will implement:
  - system initialization code
  - thermostat schemes
  - trajectory visualizations for small systems
  - RDF plotting for homogeneous and heterogeneous systems

Exercise 5 - Tips

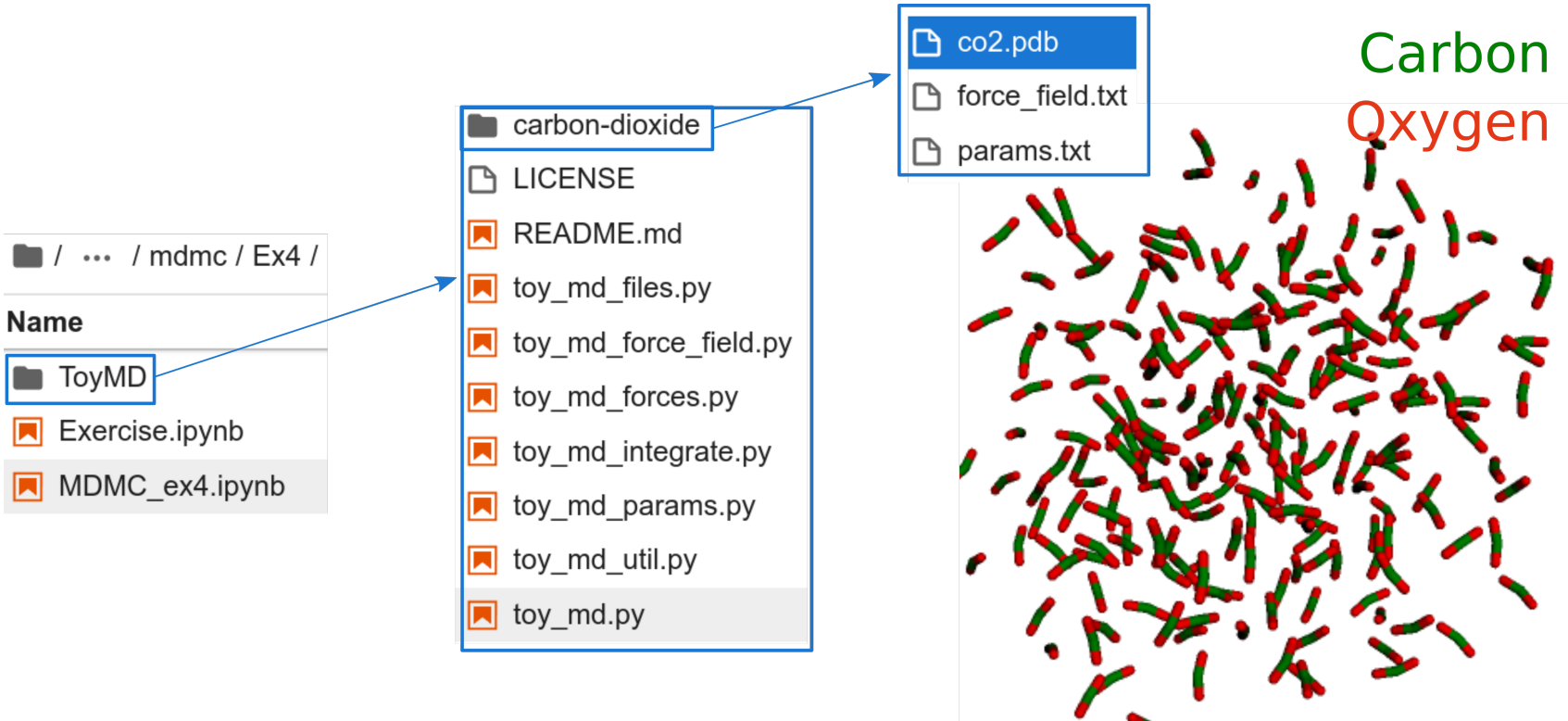
Tips:

- Download and unzip ToyMD directory from Moodle: to make sure nobody starts with a buggy version of the code, we provide the correct version you should have from Ex4. Follow the instructions at the beginning of the Ex5 notebook to use that code!

Exercise 5 - ToyMD structure

`ToyMD` code is the same structure:

- main code (propagation of MD steps) in `toy_md.py` script
- additional code for specific tasks, i.e. `toy_forces.py`
- parameters for the system in separate files (`carbon-dioxide` folder)



Exercise 5 - Run ToyMD

`ToyMD` is a Python script, which can be run

1. via terminal
2. via jupyter notebook

Recall that you can execute a bash command, passing files as arguments to the `toy_md.py` script with the following structure (paths may change):

```
python3 toy_md.py -c co2.pdb -p params.txt -ff
force_field.txt -o traj.pdb -w co2-output.pdb
```

or, alternatively, you can run the same bash command from code cells, starting with an exclamation mark (the cell will be interpreted as a bash command to execute):

```
! ./toy_md.py -c co2.pdb -p params.txt -ff
force_field.txt -o traj.pdb -w co2-output.pdb
```

Exercise 5 - Thermostats

Let's look deeper into different thermostats Simon's Explanation of Thermostats