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
- 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 Tuesday May 28th in lecture classroom

Reminders

Google Colab: For Ex 6, we will use GoogleColab instead of Noto

- 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!
- Add yourself to the GoogleColab user group at this link https://groups.epfl.ch/#/home/S29748
- 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.

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 realistic 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

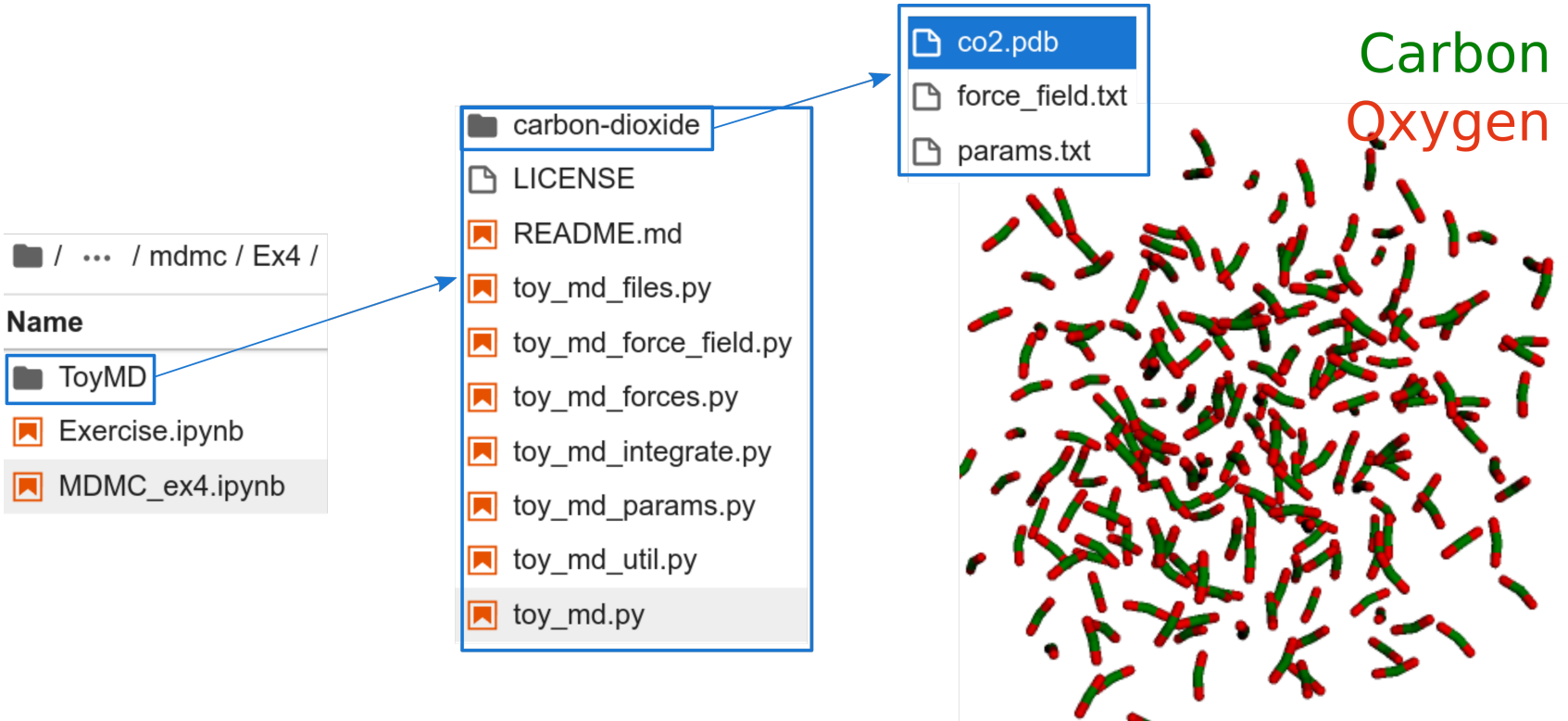
Tips:

- 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