

Exercise Session 5

MDMC Spring 2025

Evan Vasey, Thibault Kläy, Qihao Zhang, Salomé Gilbert, Sophia Johnson, Andrea Levy

April 29, 2025

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 13th
 - Q&A Session on Tuesday May 20th in lecture classroom
 - Written exam on Tuesday May 27th in lecture 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 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](#)