

# Exercise Session 5

## MDMC Spring 2025

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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](https://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](#)