Exercise Session 4

MDMC Spring 2024

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Reports Reminder

- We encourage you to work together, but the content in your report should be original
- If you use an image or wording from an external source please cite it correctly

Exercise 4 Structure

- Learning goals
  - Derive a time evolution integrator (e.g. Verlet)
  - Understand importance of periodic boundary conditions
  - Run a molecular dynamics simulation for a small molecule (CO_2)
- Chapter in script
  - Chapter 4 - Molecular Dynamics Simulations
- Resources
  - Understanding Molecular Simulation, Frenkel & Smit, 2nd Edition - Chapter 3 & Chapter 5 (extra)
  - Computer Simulation of Liquids, Allen & Tildesley, 2nd Edition - Chapter 4

Exercise 4 - Intro & Tips

Today we will provide you a simple Molecular Dynamics (**Toy MD**) code in python and you will extend it to run a MD simulation.

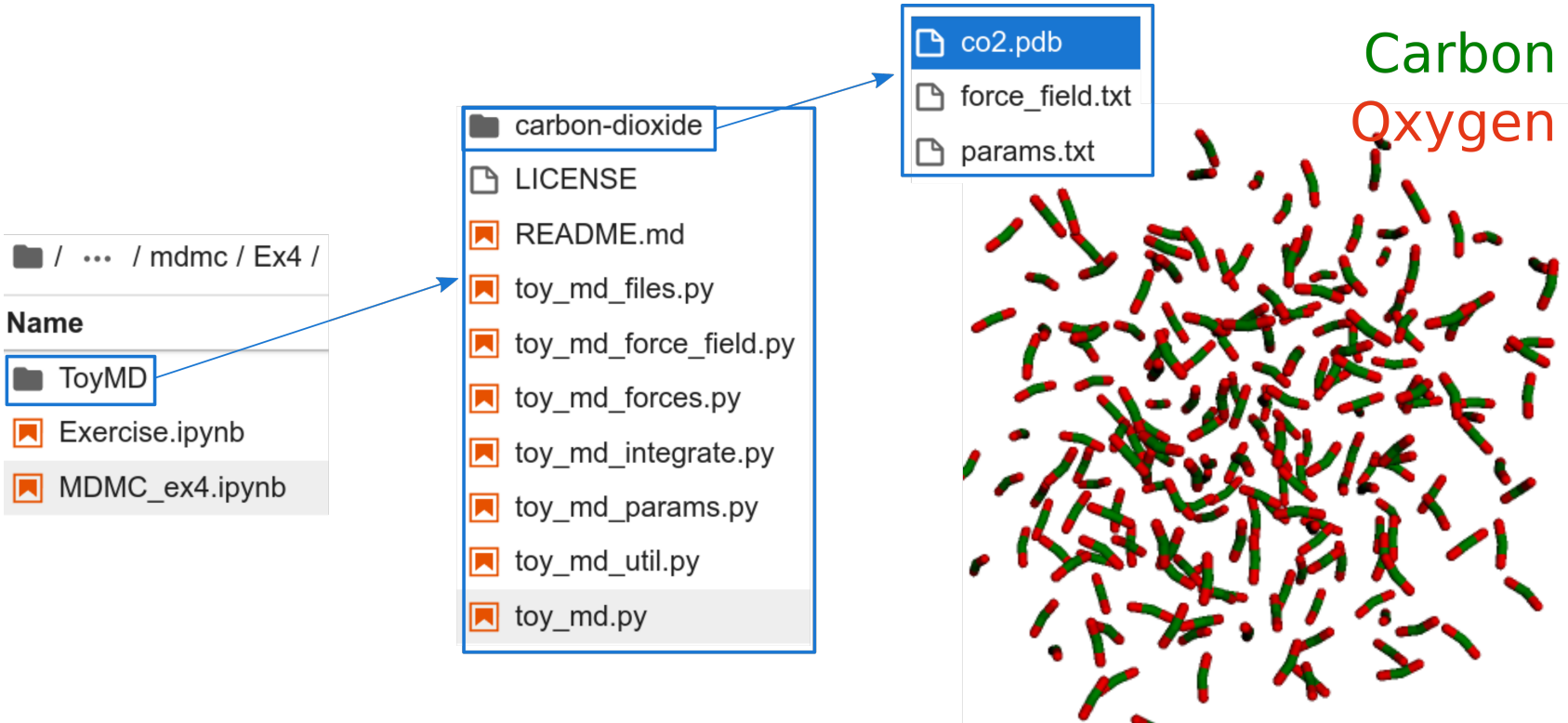
- The theoretical part introduces you to MD
  Be sure to understand what we mean by:
  - ergodicity
  - phase space sampling
  - MD propagation algorithm
  - periodic boundary conditions
- In the practical part you will implement:
  - Velocity verlet algorithm
  - Periodic boundary conditions (PBC)

N.B.: Question 8 is no longer a bonus question in case you worked on Ex4 earlier this semester

Exercise 4 - ToyMD structure

`ToyMD` code 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 4 - Run ToyMD

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

1. via terminal
2. via jupyter notebook

(see instructions in the exercise). In both cases, you will 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
```

If you'd like to re-run the code with different parameters, please delete the previous `traj.pdb` file or rename it