OpenMM Workshop July 2023

https://openmm.org

Engineering and Physical Sciences Research Council

THE UNIVERSITY of EDINBURGH

OpenMM Workshop

- 2:00-2:10. Introduction
- 2:10-2:50. Section 1 notebooks (Protein in water + protein-ligand complex)
- 2:50-3:00. Recap
- 3:00-3:15. Break
- 3:15-4:45. Section 2 (Custom forces) and/or section 3 (Machine learning Potentials), or continue section 1
- 4:45-4:55. Recap

Introduction

- What is OpenMM?
- What will we do in this workshop?
- How can I get help after the workshop?

What is OpenMM?

- A high-performance toolkit for molecular simulation
  - Use it as an Application
  - And/or use it as a Library
- Made up of two main parts:
  - Application layer
    - Run simulations with Python scripts.
    - Source code is Python. You use Python code/scripts to use it.
  - OpenMM Library
    - Set of functions for running molecular dynamics, e.g. force evaluation.
    - Source code is C++. API is auto-generated into Python. Youcan use C++ or Python (or C or Fortran) to use it.

What is OpenMM?

- Hardware specific code – ***Platforms***

- **Reference**: Designed to serve as reference code for writing other platforms. Simple and Clear (slow) code.
- **CPU**: High performance on CPUs (Shared memory parallelism using threads).
- **CUDA**: Nvidia GPUs
- **OpenCL**: Other GPUs

- By default OpenMM will run on the fastest platform available.

Workshop

- Set of Jupyter notebooks you can work through that will demonstrate how to use OpenMM.
- Hosted on Github: https://github.com/openmm/openmm_workshop_july2023
- Four notebooks:
  - Beginner:
    - Protein in water
    - Protein-ligand complex
  - More Advanced:
    - Custom forces
    - Machine learning potentials

Workshop notebooks

- You can run them on google Colab or you own machine.
- They have some exercises where you need to add a line of code. The cell will have a `FIXME` that you will need to change before it will run.
- Work through at your own pace and ask us questions.
- Don’t worry if you don’t get through them.
- The workshop will stay up on Github and continue to be available.

Getting help after the workshop

- For workshop specific issues: https://github.com/openmm/openmm_workshop_july2023
- For all OpenMM issues: https://github.com/openmm/openmm/issues
- You can post questions as issues. Don’t be afraid!
- We are currently adding in some issue templates to make this a bit easier to do.