

OpenMM Workshop July 2023

Stephen Farr

Contact: <https://github.com/sef43> || stephen.farr@ed.ac.uk

Helpers: Julien Michel, Will Poole



<https://openmm.org>



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OpenMM Workshop

- 2:00-2:10. Introduction
- 2:10-2:50. Section 1 notebooks (Protein in water + protein-ligand complex)
- 2:45 Refreshments available outside the room
- 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?



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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. You can 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



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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.



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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.
- Join the Discord channel: <https://discord.gg/fFM9hDdA>



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