OpenMM Workshop

CCPBioSim Training Week, September 2024

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OpenMM Workshop

- **9:30-9:40** | **Introduction**
  Overview of the workshop and introduction to OpenMM.
- **9:40-10:45** | **Section 1: Notebooks**
  - Protein in water
  - Protein-ligand complex
- **10:45-11:00** | **Recap**
  Review of key points from Section 1.
- **11:00-11:15** | **Break**
  Refreshments available outside the room.
- **11:15-12:15** | **Section 2: Custom Forces and/or Section 3: Machine Learning Potentials**
  Continue with Section 1, or move on to explore custom forces or machine learning potentials.
- **12:15-12:30** | **Recap and Final Remarks**
  Summarize key learnings and conclude the workshop

Introduction

1. What is OpenMM?
2. What will we do in this workshop?
3. 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.
    - 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
  - **HIP:** AMD GPUs (coming soon in version 8.2)
  - **OpenCL**: Other GPUs
- By default, OpenMM runs 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_workshops
- Four notebooks:
  - **Beginner:**
    - **Protein in water:** learn the basics of simulating a protein in an aqueous environment.
    - **Protein-ligand complex:** learn how to set up a protein-ligand complex simulation.
  - **More advanced:**
    - **Custom forces:** explore the creation and use of custom forces in your simulations.
    - **Machine learning potentials:** integrate machine learning models in MD simulations

Workshop Notebooks

- You can run them on Google Colab or on your own machine.
- The notebooks 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.
- No need to worry if you don't complete everything.
- The workshop will remain available on GitHub for future reference.

Getting Help After the Workshop

- For workshop specific issues: https://github.com/openmm/openmm_workshops
- Check the documentation: http://docs.openmm.org/latest/userguide/
- For all OpenMM issues:
  - https://github.com/openmm/openmm/issues
  - You can also use the issues pages of other packages from the OpenMM ecosystem (*e.g*, OpenMM-ML, OpenMM-Torch, etc.)
- You can post questions as issues. Don't be afraid!