

OpenPathSampling Toolchain

Python:

setuptools: installation tools
nose: unit testing

Scientific Python:

numpy: basic numerics (e.g., math on arrays)
scipy: more advanced numerics (optimization, linear algebra)
pandas: tables, series
matplotlib: visualization
jupyter: interactive notebooks
netcdf4: data storage

Omnia:

openmm: MD simulation
mdtraj: trajectory analysis package
openmmtools: additional OpenMM-based tools

- Overview: What are the steps in path sampling?
- Using OpenPathSampling: A simple example
- Introduction to developing for OpenPathSampling