Introduction to OpenPathSampling:
Overview and Usage

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E-CAM Extended Software Development Workshop
Traunkirchen, Austria; 17 November 2016

Tools from the talk: https://gitlab.e-cam2020.eu/dwhswenson/esdw_1_materials

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