

Outline

- Intro: Campaign-scale software
- Path sampling and OpenPathSampling
- Alchemical free energy transformations and Open Free Energy
- **Best practices to interface with campaign-scale software**

Have an API

- Have a well-documented API aimed at people using your platform
- Ideally, have bindings to high-level languages (e.g., Python) to facilitate integration with campaign-scale tools in those ecosystems.
 - Running OpenMM: OPS just uses the OpenMM Python API
 - Running GROMACS: OPS launches a gmx subprocess and has to monitor as it writes to a file, and then adapt that into something that works with the simpler API approach.
- Be careful that your bindings give expected behavior in the target language

```
from ████████ import Chem
mol = Chem.MolFromSmiles("CC")
atom = mol.GetAtoms()[0]
atom.GetOwningMol() == mol
# False
```