

Campaign-Scale Software

- Difference with “workflow”
 - Campaign is a single scientific result from similar, coordinated, tasks. Details of pipeline may change.
 - Workflow is more general, typically involving different tasks in a relatively constant pipeline
- Examples:
 - Run many loosely-coupled MD runs (we'll see a few specific cases of this!)
 - Hyperparameter optimization

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