Things I maybe should have talked about (but won't)

- **Sustainability models** (and OMSF)

- **Serialization and reproducibility** (you'll get some of that)

- **Interfacing MD engines with OpenPathSampling**

Happy to answer questions about any of these, either after talk or over coffee!

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