OpenFE Acknowledgments



Richard Gowers
Project Lead



Diego Nolasco Project Manager



David W.H. Swenson Infrastructure Lead



Benjamin Ries Scientific Software Developer



Irfan Alibay Scientific Lead



Mike Henry Software Scientist

OMSF founders:

- Karmen Čondić-Jurkić
- David Mobley
- Michael Gilson

Chodera Lab:

- John Chodera
- Melissa Boby
- David Dotson
- Ivan Pulido
- Ivy Zhang

OpenForceField Team:

- Jeff Wagner
- Matt Thompson

Technical Advisory Committee:

- Alberto Gobbi
- Antonia SJS Mey
- Ben Cossins
- Ben Sellers
- Bharath Ramsundar
- Charles Hutchins
- Clara Crist
- David Mobley
- David Rooklin
- Demetri Moustakas
- Gard Nelson
- Gavin Bascom
- John Chodera
- Jonah Vilseck
- Julien Michel
- Kaushik Lakkaraju
- Mario Cardozo
- Michael Shirts
- Oliver Beckstein
- Peter Eastman
- Phil Biggin
- Yourong Zhao
- Zoe Cournia

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