

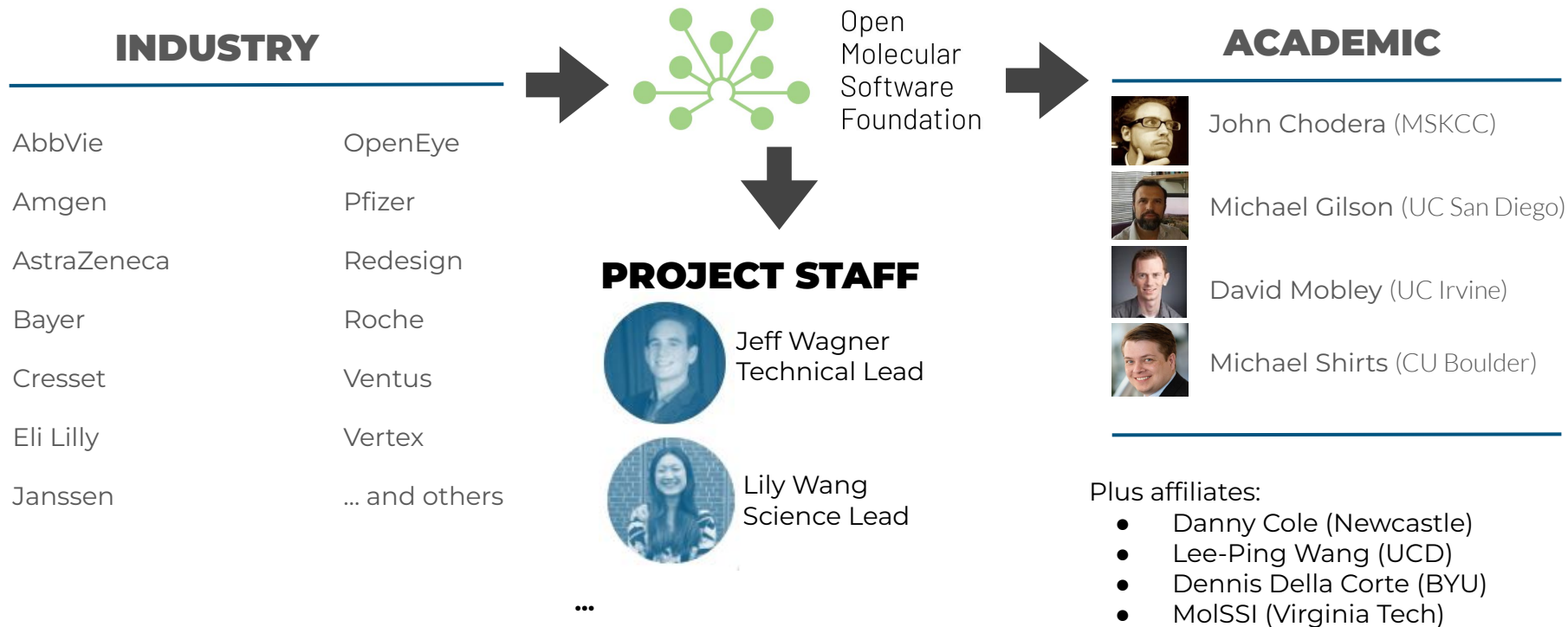


From RDKit to MD simulation in seconds: An introduction to Open Force Field

Jeff Wagner, OpenFF Technical Lead



The Open Force Field Consortium





Open source Python Toolkit: use the parameters in most simulation packages



Open curated QM / physical property datasets: build your own force fields

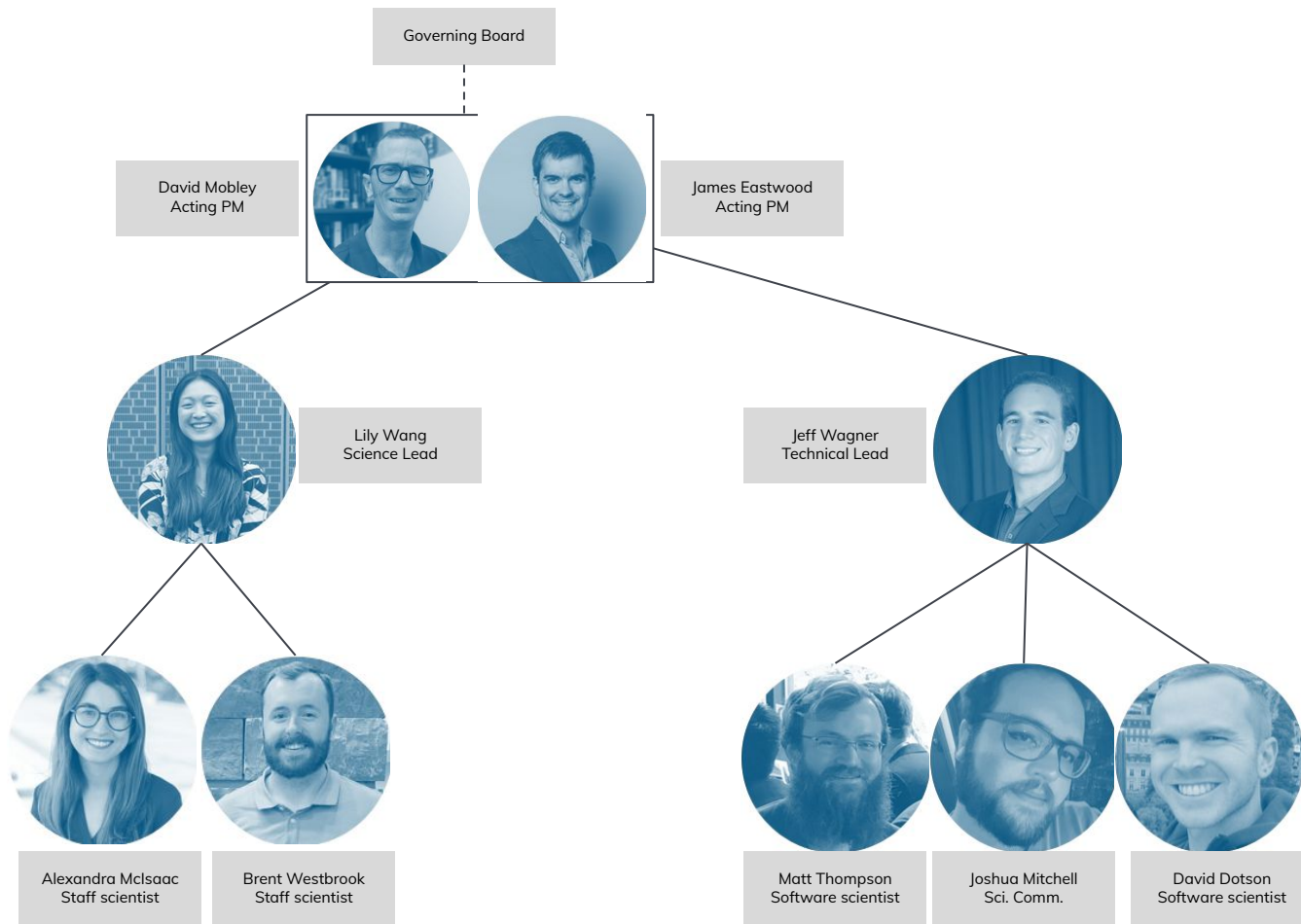


Open infrastructure: Run your own benchmarks; fit your own FFs

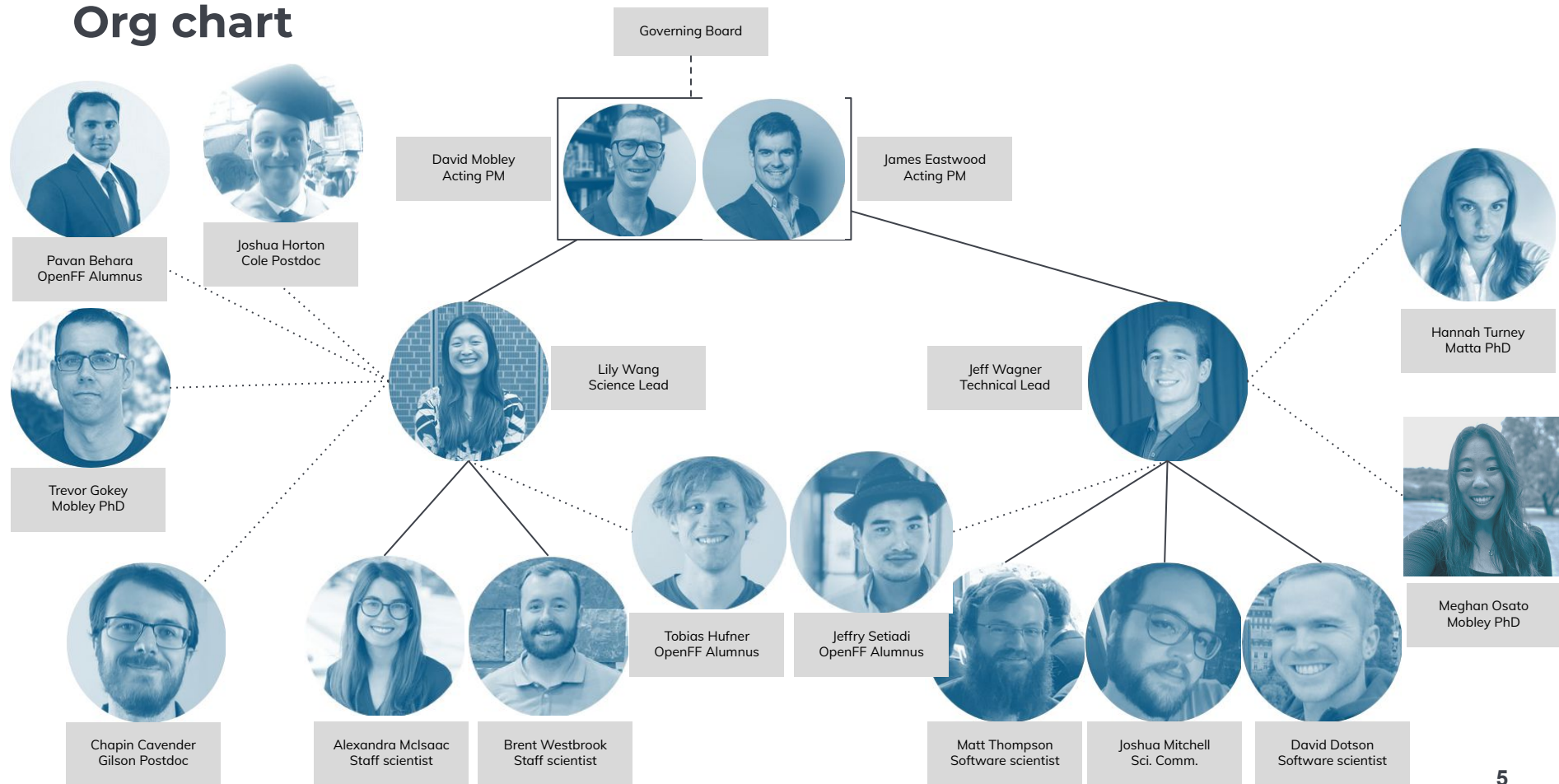


Open science: Everything done in the open/everyone can get involved

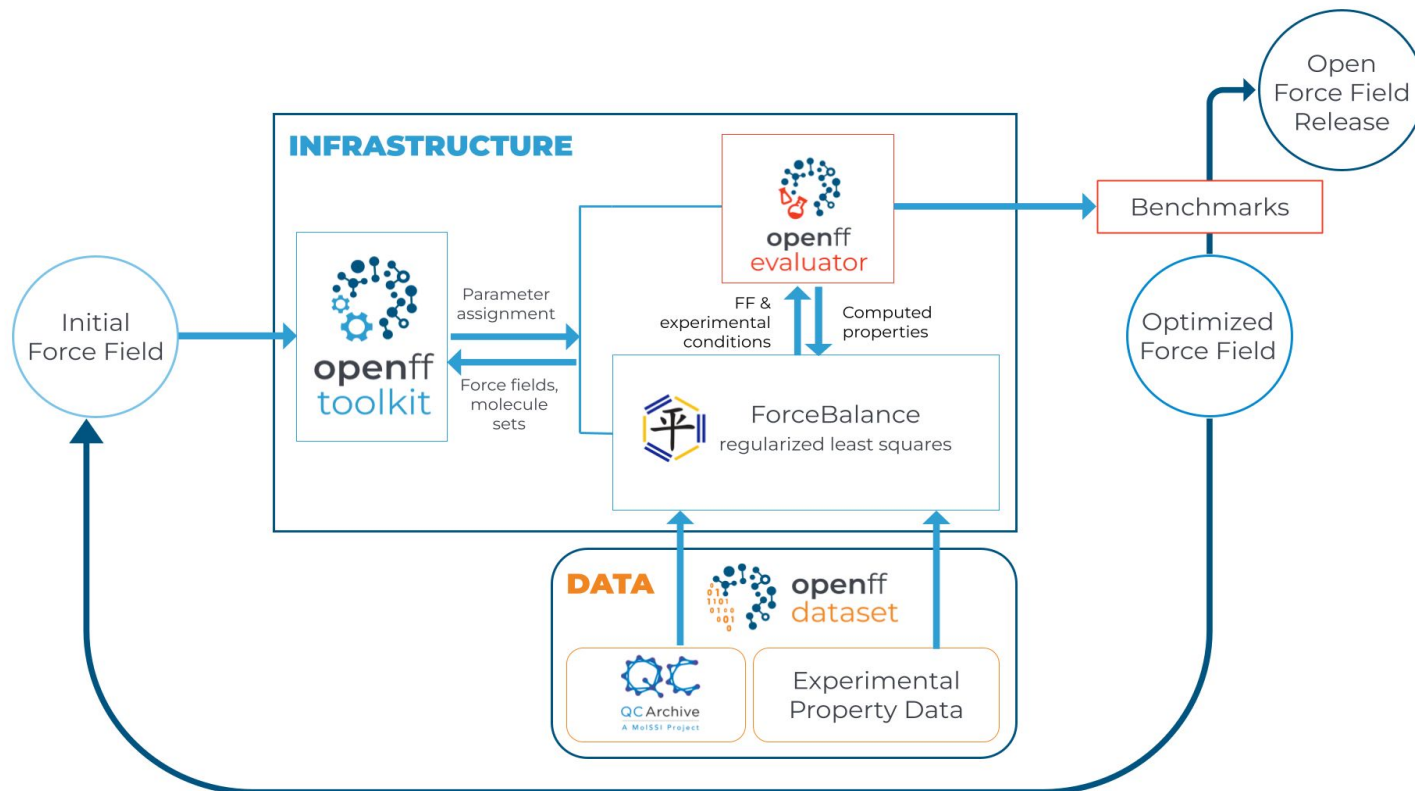
Org chart



Org chart



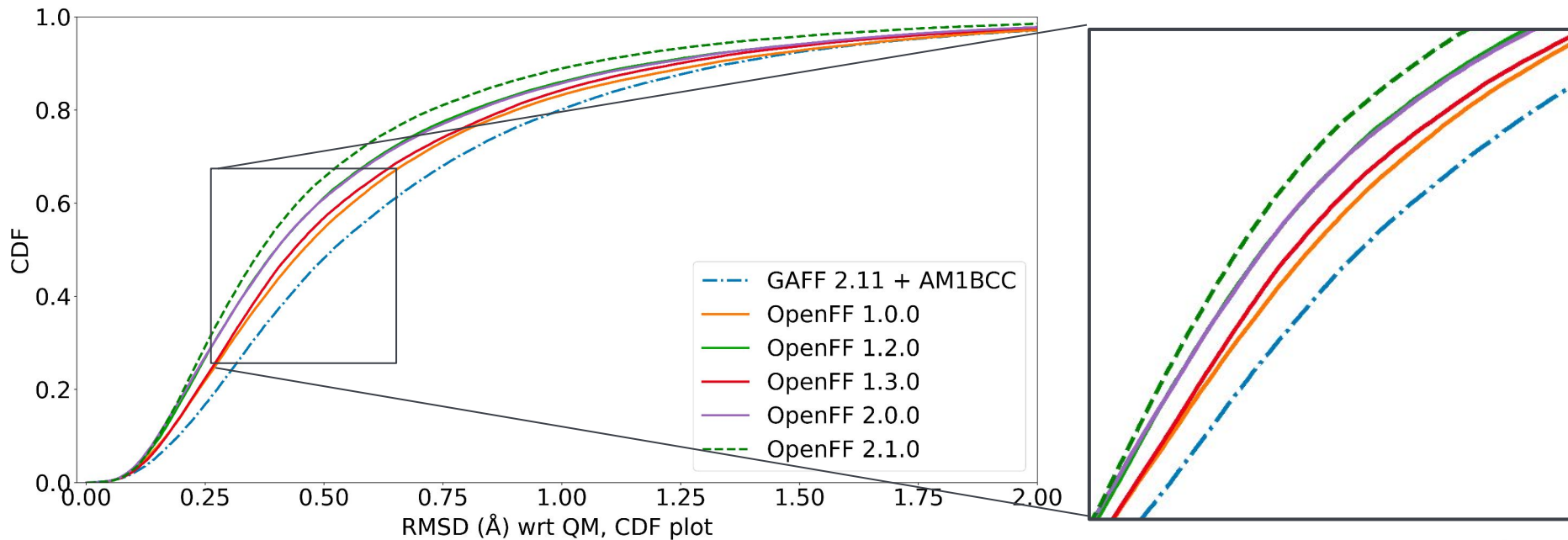
We create new force fields and systematically improve



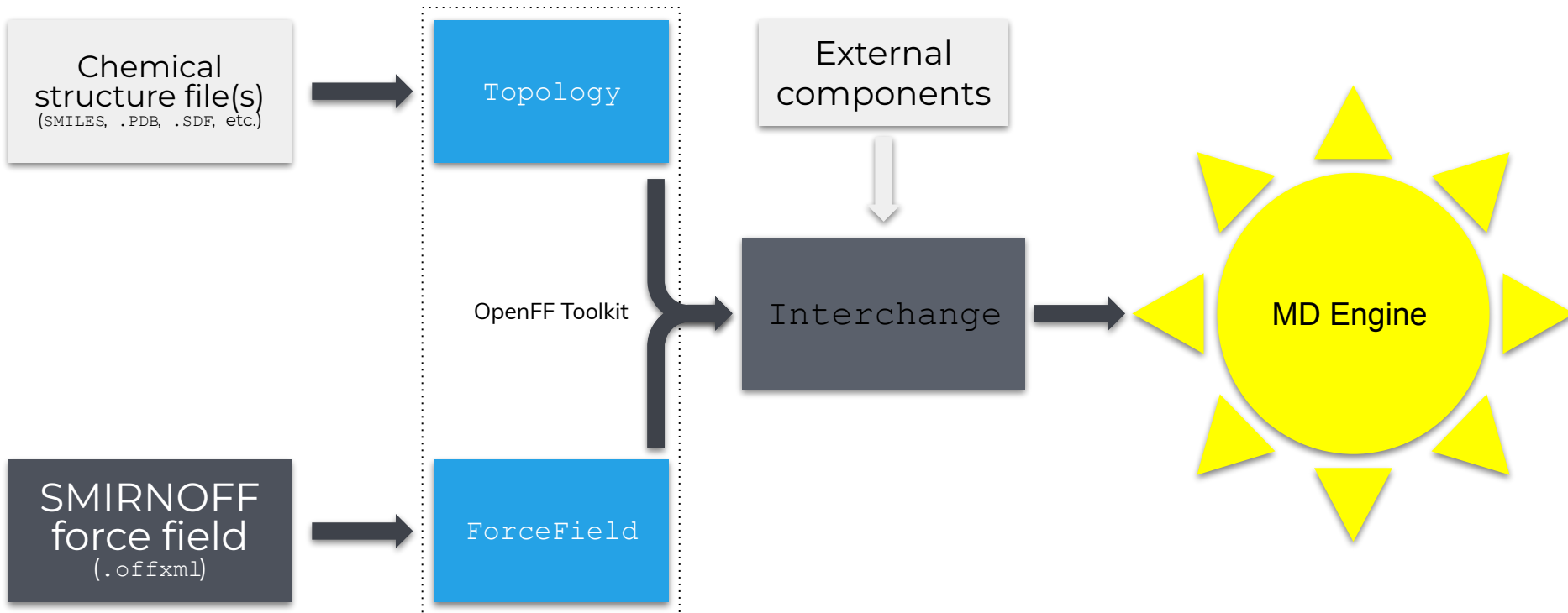
OpenFF already makes one of the best modern public small molecule force fields



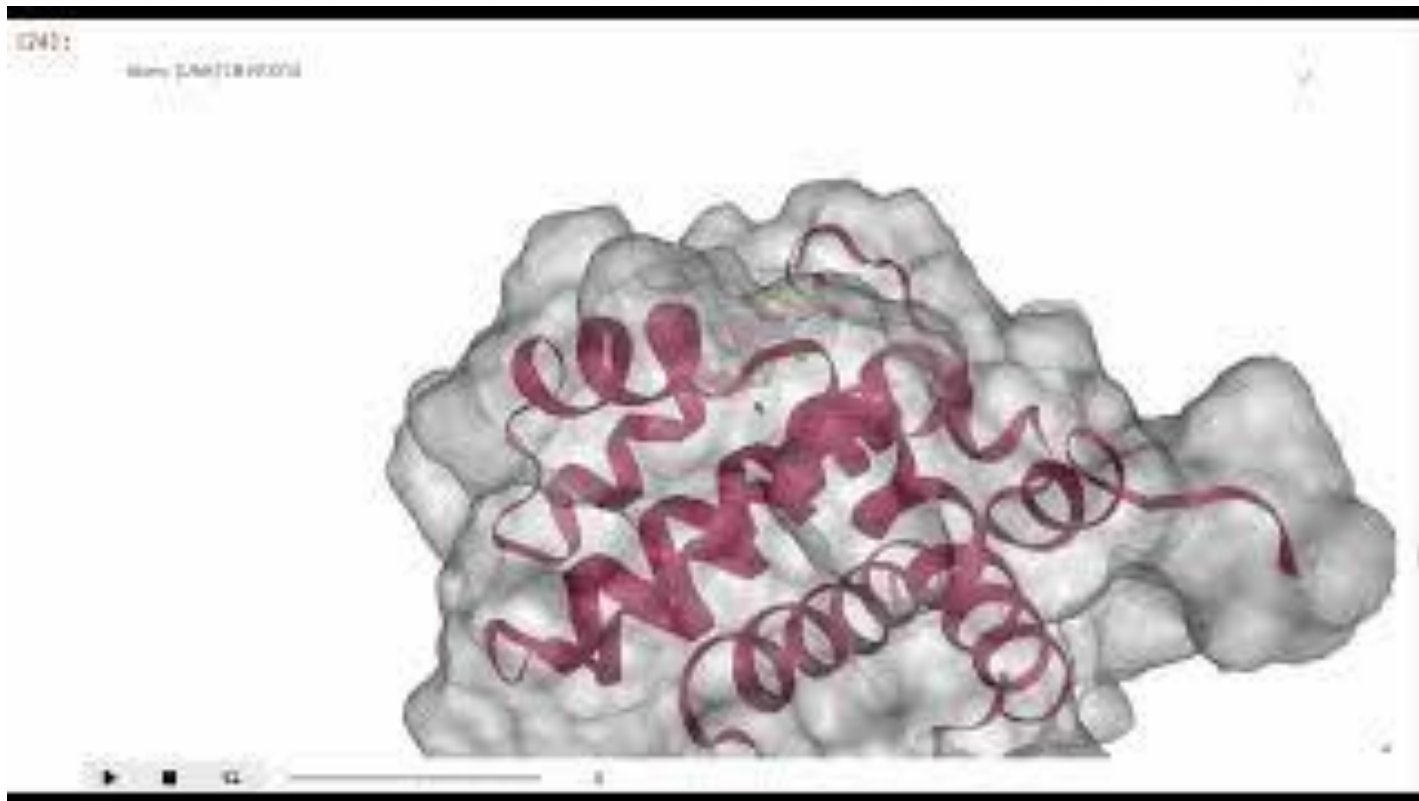
RMSD comparison on
Industry benchmark set (70K+ conf.)



The OpenFF Workflow



And now, for something completely different...



Acknowledgments



- Greg and the RDKit community
- All our partners, past and present (see openforcefield.org)
- Our team and alumni
- The OpenFF Initiative and community
- Virginia Tech for initial hosting
- OMSF for current hosting
- OpenFE for collaboration, and testing
- The AMBER community and AMBER-family force fields (OpenFF began as a sibling)



Get started at docs.openforcefield.org!

