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

Jeff Wagner, OpenFF Technical Lead

The Open Force Field Consortium

INDUSTRY

AbbVie
Amgen
AstraZeneca
Bayer
Cresset
Eli Lilly
Janssen
OpenEye
Pfizer
Redesign
Roche
Ventus
Vertex
... and others

Open Molecular Software Foundation

PROJECT STAFF


Jeff Wagner
Technical Lead


Lily Wang
Science Lead

...

ACADEMIC


John Chodera (MSKCC)


Michael Gilson (UC San Diego)


David Mobley (UC Irvine)


Michael Shirts (CU Boulder)

Plus affiliates:

- Danny Cole (Newcastle)
- Lee-Ping Wang (UCD)
- Dennis Della Corte (BYU)
- MolSSI (Virginia Tech)

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

Governing Board


David Mobley
Acting PM

James Eastwood
Acting PM

Lily Wang
Science Lead

Jeff Wagner
Technical Lead


Alexandra McIsaac
Staff scientist

Brent Westbrook
Staff scientist



Matt Thompson
Software scientist

Joshua Mitchell
Sci. Comm.

David Dotson
Software scientist

Org chart

Pavan Behara
OpenFF Alumnus

Joshua Horton
Cole Postdoc

Trevor Gokey
Mobley PhD

Chapin Cavender
Gilson Postdoc

Alexandra McIsaac
Staff scientist

Brent Westbrook
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David Mobley
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Tobias Hufner
OpenFF Alumnus

Jeffry Setiadi
OpenFF Alumnus

Matt Thompson
Software scientist

Joshua Mitchell
Sci. Comm.

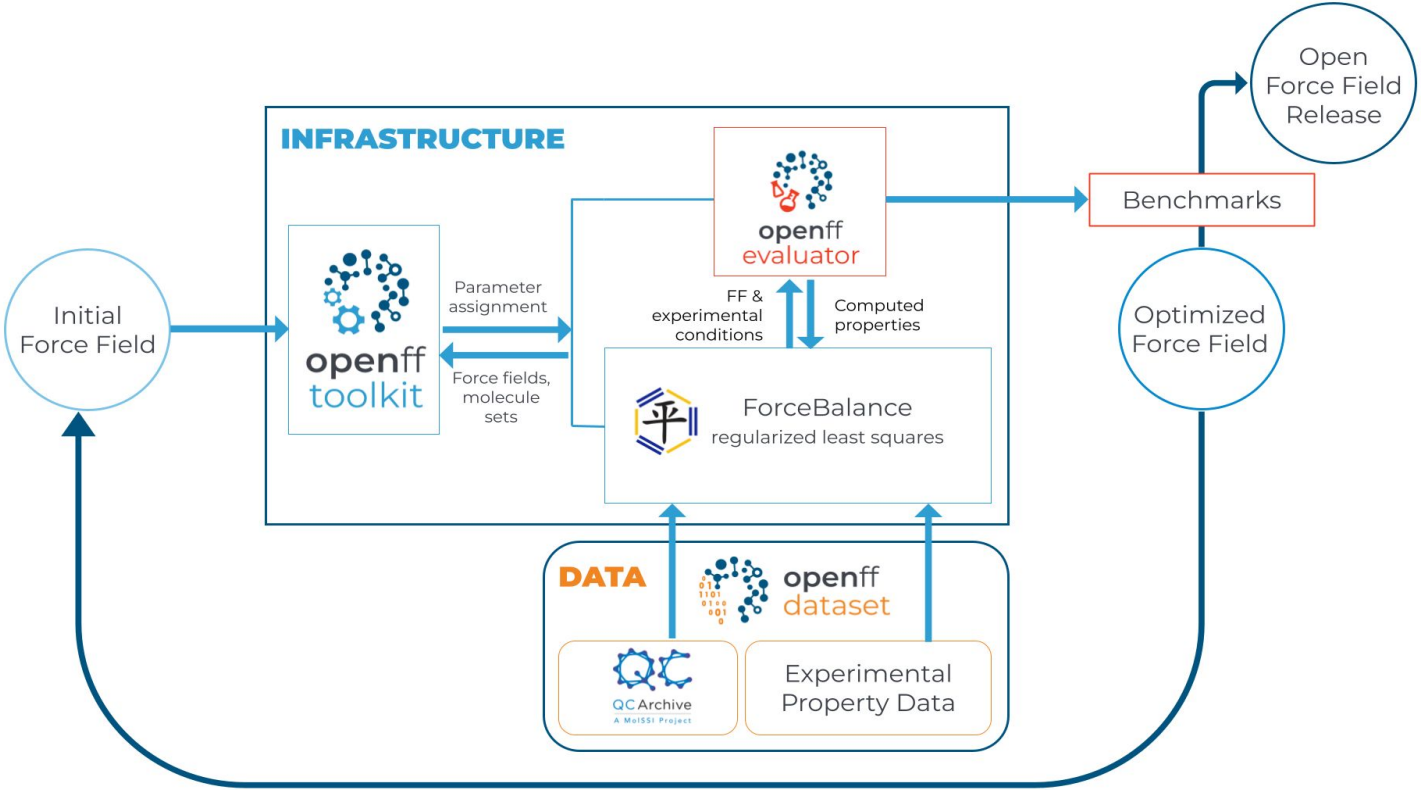
David Dotson
Software scientist

Jeff Wagner
Technical Lead

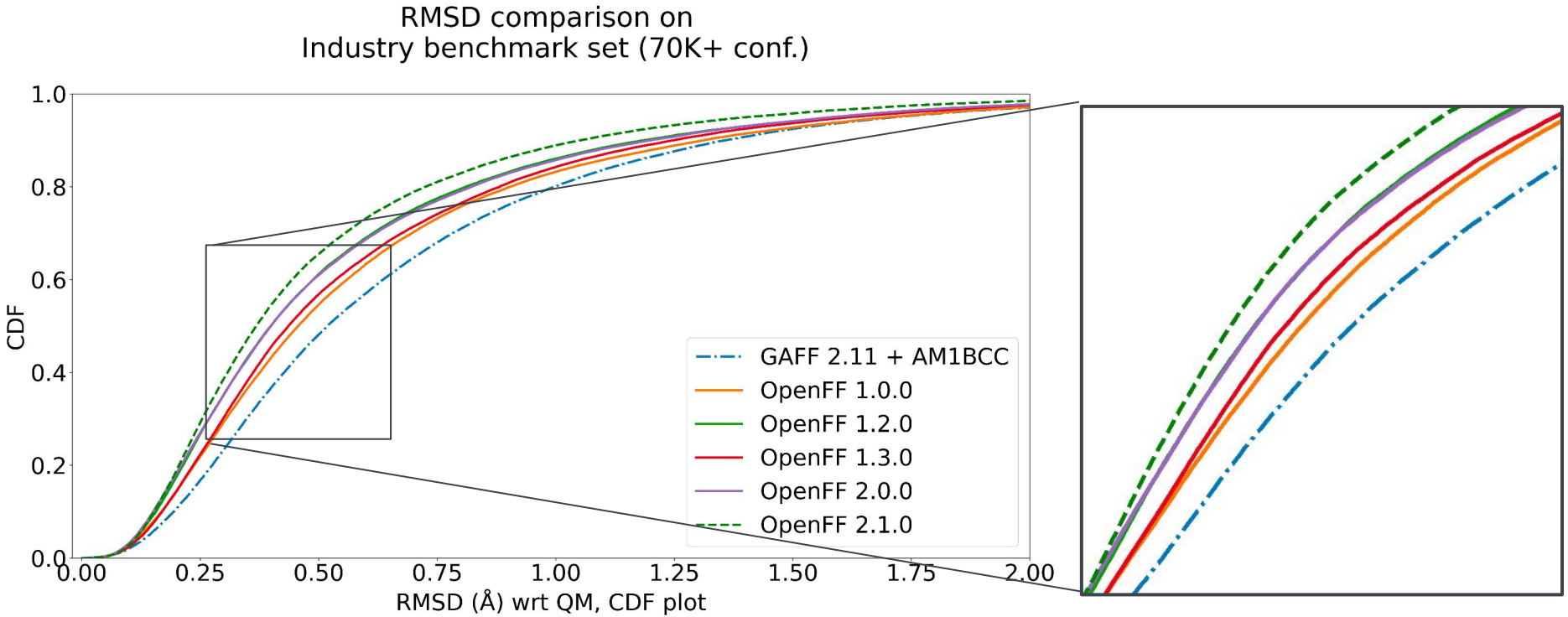
Hannah Turney
Matta PhD

Meghan Osato
Mobley PhD

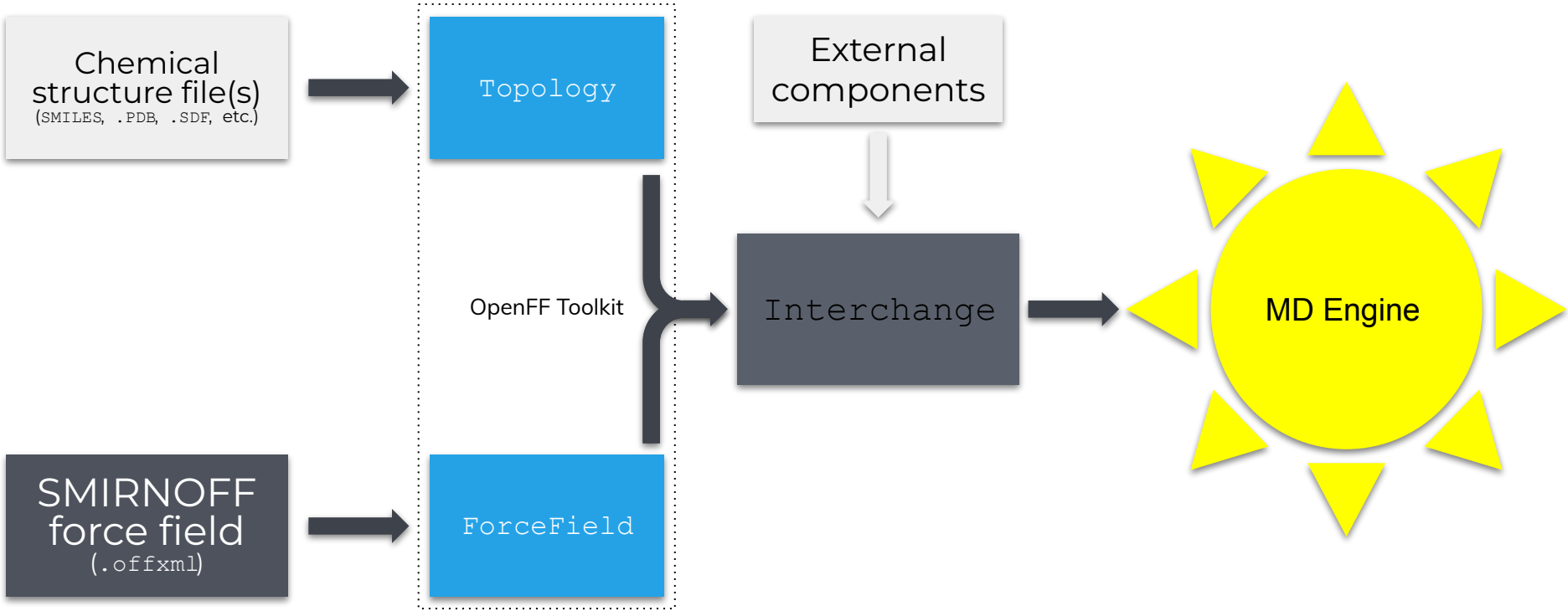
We create new force fields and systematically improve



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



The OpenFF Workflow



And now, for something completely different...

Notebook and input files: https://github.com/openforcefield/rdkit_ugm_2024_demo
Recording of notebook execution (no audio): https://www.youtube.com/watch?v=4F1LWKn2c2s

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!