



Open Force Field Consortium Workshop

January 7-8, 2019

University of California San Diego, La Jolla, CA

Workshop Goals

Gather project participants to meet and interact in person

Discuss science with pharma partners, answer questions and collect feedback

Discuss plans for the first year of the effort (2019) and beyond

Provide first opportunity for hands-on use of the developing OpenFF toolkit

Agenda -- Day 1

<https://openforcefield.org/news/jan-2019-meeting-agenda>

Roadmap overview (Michael Shirts)

Short-term parameter optimization strategy: ForceBalance (Lee-Ping Wang)

Break

Long-term parameter optimization strategy: Bayesian fitting (John Chodera)

Chemical perception and SMIRNOFF typing (David Mobley and Caitlin Bannan)

Torsion fitting and fragmentation (John Chodera and Lee-Ping Wang)

Lunch

Afternoon of discussion

- Group discussion to decide breakout topics

- Breakouts (two rounds of two breakouts each → 4 total)

- Reconvene for general discussion

Agenda -- Day 2

<https://openforcefield.org/news/jan-2019-meeting-agenda>

Charge models (Michael Schauperl)

Fitting non-torsion valence terms (David Mobley, Victoria Lim and Lee-Ping Wang)

Break

Software architecture and infrastructure (Jeff Wagner and John Chodera)

Fitting condensed-phase properties (John Chodera and Michael Shirts)

Lunch

Afternoon discussion/hands-on exercise

- Group discussion to decide breakout topics

- Breakouts (two rounds of two breakouts each → 4 total)

- Reconvene for general discussion

Guided Hands-On with the OpenFF Toolkit

optional activity for afternoon Day 2

Led by Jeffrey Wagner, OFF Software Scientist

Installation of software on your personal laptop or remote system

Assignment of parameters to a molecule and running a simulation

Requirement: a computer running Linux or MacOS

Q/A and Discussion

There will be discussion time for each talk

Please post additional questions and discussion topics on the appropriate Slack channels (see agenda)

There will be further time for extended discussion during the afternoons

Participants

Total registrants: 44

34 in-person, 10 virtual

17 industrial, 27 academic

Name tags and pens are on the tables in back

Practicalities

Venue and video

Venue – only this room

WiFi: use UCSD Guest network. No password is needed.

Zoom virtual meeting

Only pre-lunch

Will attempt to record for internal use of consortium members– *please state if you are not in agreement*

Day 2 meeting ID: 342-960-011

Slides will be made available on openforcefield.org

Food

Breakfast, lunch, and snacks in this room both days

Dinner this evening: Rock Bottom Brewery (see address in printed agenda)

Choice of main dish: salmon, veggie tacos, or jambalaya

Should be about \$40/person + any drinks

Tell me if you have changed your plans relative to your registration

Assistance During the Workshop

Mike Gilson, mgilson@ucsd.edu, 301-910-3848

Gilson lab postdocs

Ido Ben Shalom

Katy Kellett

Michael Schauperl

David Slochower