Use Cases Breakout

Jan 7 2019 Open Force Field Workshop
Breakout Session 3

Enumerating and Ranking Use Cases

We don’t currently plan to develop a protein FF. We will develop a non-protein forcefield build to be compatible with a single protein FF.

High

- Binding free energy
- Conformational search
- Mixed solvent MD
- Not docking, but using MD to predict bound poses

Med

- Macrocycle prediction

Low

- Antibody design
- Passive permeability
- Small molecule crystal structure prediction
- Protein stabilization as a result of small molecule binding

Which other polymers will people use? Carbohydrates? Lipids? Nucleic acids?

- We shouldn't go out of our way to do special property calculations for these in the first wave of development, though they would be good for benchmarking when the forcefield is mature.
- The initial molecule dataset will contain nucleoside analogues, things with phosphate groups, linked sugars, etc
    - It would be worth checking that these are present in decent quantity in the training set

Should we make our own water model or train against an existing one? And if so, which one?

Let’s get everyone together to decide this

Are people planning to use explicit solvent only, or is anyone expecting to use vacuum, GB, or PB? (In order)

- Explicit
- GB
- PB
- Vacuum
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If a new feature in the FF broke compatibility with your workflows and favorite simulation engine, would you be willing to switch to a new simulation package to keep getting OFF updates?

It depends on “how much better”

If this happens, we could make a final, maximally optimized release of the previous forcefield form.

Future forcefield updates would assume the new form