Next Steps for OpenFF Development

Potential Rationales for Prioritization

Easy to implement
High anticipated improvement in accuracy
Infrastructure that will enable strong later progress
Makes case for continued funding

Aims for...

Next major OpenFF release (Sage)

(likely interim releases as we make improvements)

Software development

Scientific advances

Aims for Next OpenFF Release (Sage)

- Target release date
- Priorities for advances; e.g.,
  - Low-hanging
    - Keep pushing on torsions (technology, chemical space)
    - Electrostatics model (partial charges, etc.);
      - Improved charge model
      - BCC fitting
    - Automated selection of fitting data (can easily generate far more than we need, but selecting the best/most informative?)
    - Dataset (QC and condensed phase) expansion
  - Improved chemical perception
    - Semi-manual
    - Automated
  - High-interest but more difficult?
    - Wiberg bond order parameter interpolation
    - Consistent water model(s)
  - QC method benchmark/selection?

Aims for Software Development

- Toolkit; e.g.,
  - New capabilities
  - Simulation package compatibility
  - Support for future science:
    - Wiberg bond orders
    - Off-site charges (probably implement in spec, then work with other devs to get support into other packages before building into FF)
    - Library charges
    - BCC (& BCC fitting)
- Infrastructure; e.g.,
  - Property calculator: performance advances, new properties, ...
  - Force Balance
  - Bayesian
  - Bespoke torsion/charging tool
  - Datasets/databases (not exactly software, but…)
  - Automated dataset submission to QC pipeline

Potential Scientific Aims

- Keep pushing on torsions- improvements and extensions to wider chemistry
- Electrostatic models (charges, off-site, polarizability…)
- Lennard-Jones parameters
- Expanding the usable dataset for parameterization and benchmarking
- Chemical perception
- Taking advantage of deep learning