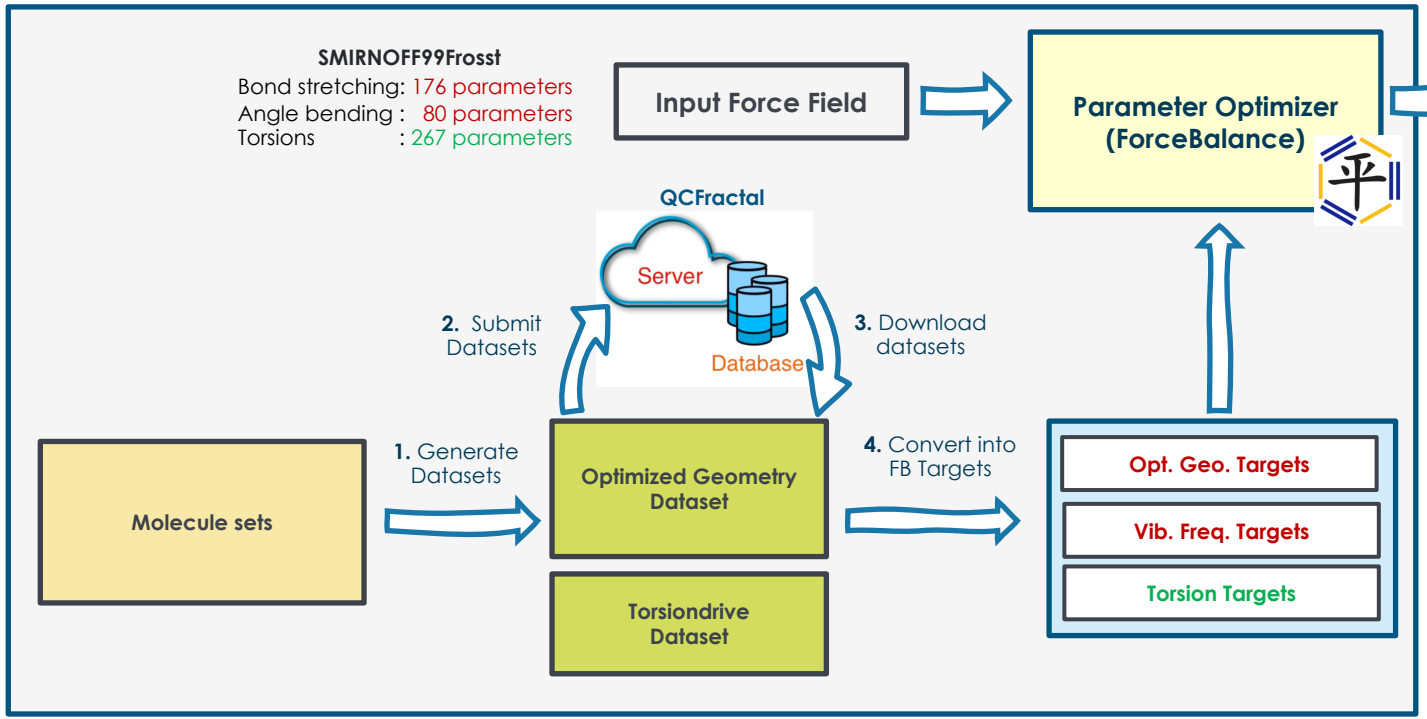
open
forcefield

2020 May OFF meeting

Parsley Minor Releases Update

Presenter: Hyesu Jang

Valence Parameter Optimization Workflow



Parsley	Release Date
v1.0.0	Oct 12, 2019
v1.1.0	Mar 3, 2020
v1.2.0	May 2020 (Anticipated)

v1.1.0 “Parsley”

w/ Modified parameter definitions
and addition of new parameter definitions

1. A fix for tetrazole optimization issue

2. Modification of for N=,:N rotations periodicity

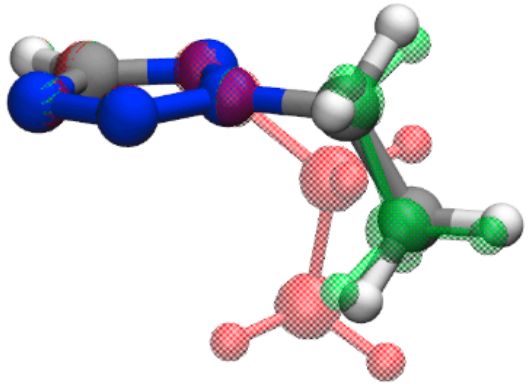
3. Addition of three new bond and angle terms

- Improper torsion for trivalent N center in a 5-membered hetero-aromatic ring

i3b	[*:1]~[#7X3$(*@1-[*]=,:[*][*]=,:[*]@1):2](~[*:3])~[*:4]

- Addition of associated torsion for sp3 C and trivalent N bond connected to a 5-membered hetero-aromatic ring

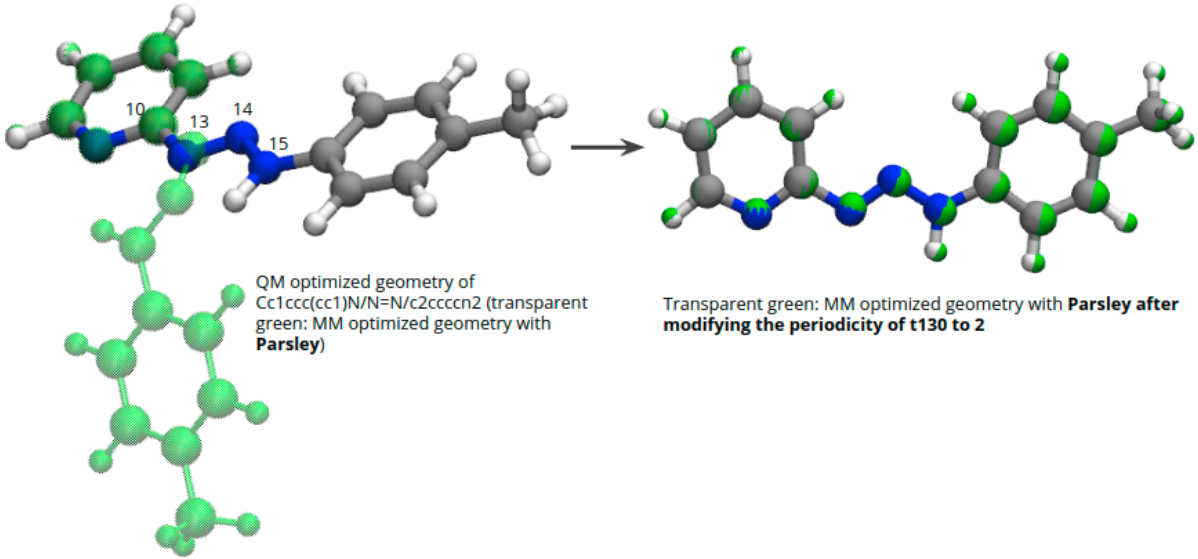
t51c	[*:1]-[#6X4:2]-[#7X3$(*@1-[*]=,:[*][*]=,:[*]@1):3]-[*:4]
t51ch	[#1:1]-[#6X4:2]-[#7X3$(*@1-[*]=,:[*][*]=,:[*]@1):3]-[*:4]



QM optimized geometry of Net-tetrazole.
(transparent red: MM opt. geometry with v1.0.0 Parsley,
transparent green: v1.1.0 Parsley)

2. Modification of for N=,:N rotations

t130	[*:1]~[#7X2:2]=,:[#7X2:3]~[*:4]	Periodicity: 1 ->2



QM optimized geometry of Cc1ccc(cc1)N/N=N/c2ccccn2 (transparent green: MM optimized geometry with **Parsley**)

Transparent green: MM optimized geometry with **Parsley after modifying the periodicity of t130 to 2**

v1.1.0 “Parsley”

3. Addition of three new bond and angle terms

(1) Addition of a22a: conjugation effect from N=C=S;

a22	[*:1]~[#7X2+0:2]~[*:3]
a22a	[*:1]~[#7X2+0:2]~[#6X2:3](~[#16X1])

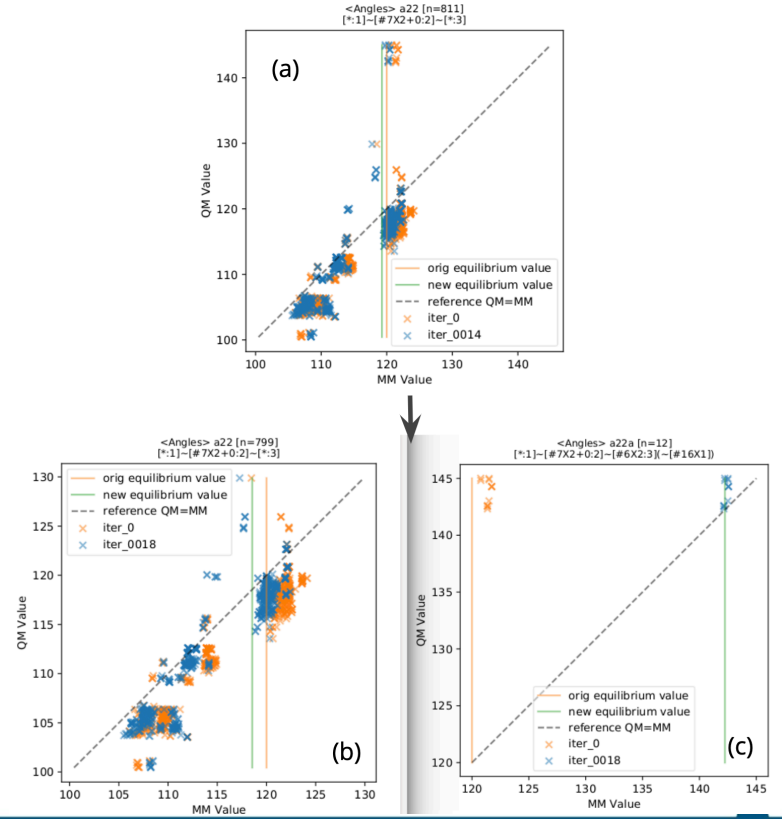
- The result equilibrium angle values are quite different between a22 and a22a. (118, 142 degree each) which validates the separation.

(2) Addition of b14a: Single bond between sp2 C and O^-;

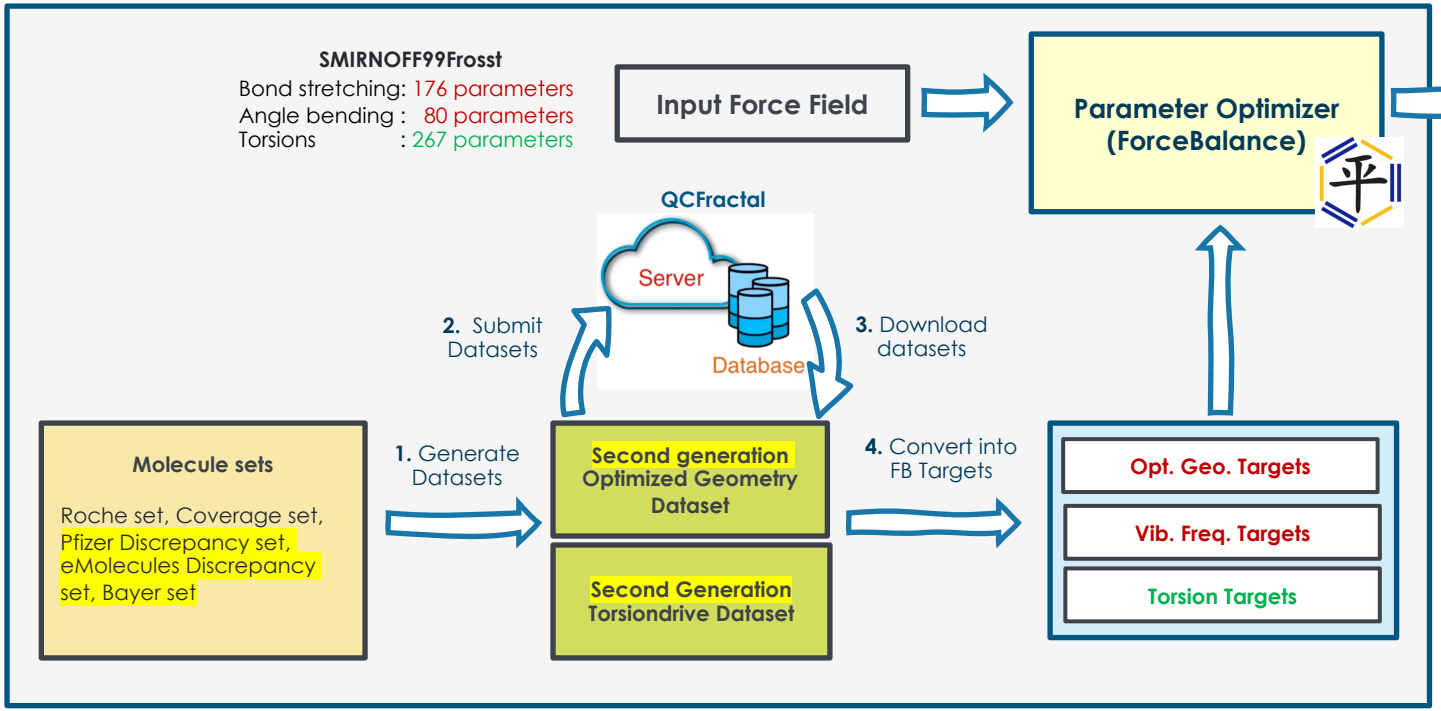
b14	[#6:1]-[#8:2]
b14a	[#6X3:1]-[#8X1-1:2]

(3) Addition of b36a: Double bond between N^+ and N^-

b36	[#7:1]=[#7:2]
b36a	[#7+1:1]=[#7-1:2]



Toward v1.2.0 “Parsley” with a new design of dataset



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Preliminary fitting

Preliminary fitting (v1.2.0-pre)	V1.2.0
2,974 optimized geometries	4745 optimized geometries
278 vibrational frequencies	1189 vibrational frequencies
581 1-D torsions	710 1-D torsions

- Input force field: same initial force field used in v1.1.0 fitting;
- The objective function decreased from **1.028e+4** to **3.127e+3** in **28** steps.

Preliminary fitting

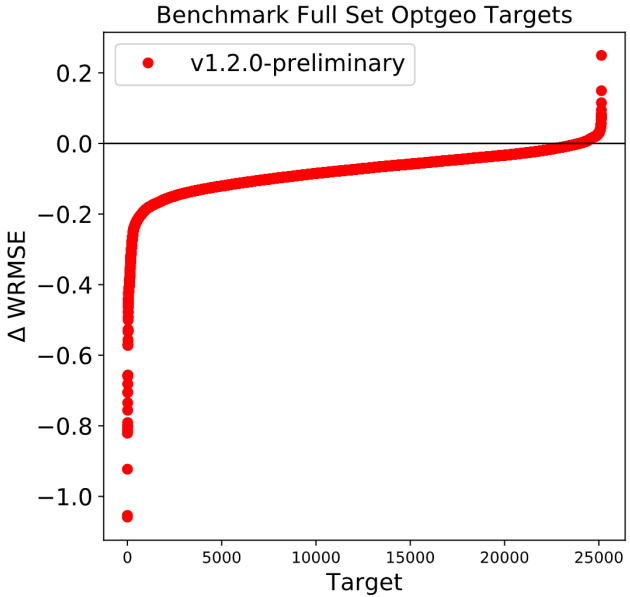
Benchmark Results

Two types of benchmarks were done: (1) QM vs MM optimized geometries and (2) the relative energies between conformers at QM optimized geometries.

The final objective function value(X2) from FB single point calculation gives a brief overview of the agreement between QM and MM. The lower X2 is, the better the force field reproduces QM structures and energetics.

	X2 for primary set	X2 for full set
Initial force field	1435	29,469
v1.0.0	948	20,672
v1.1.0	936	20,097
v1.2.0-preliminary	766	16,939

Reproducibility of QM optimized geometries

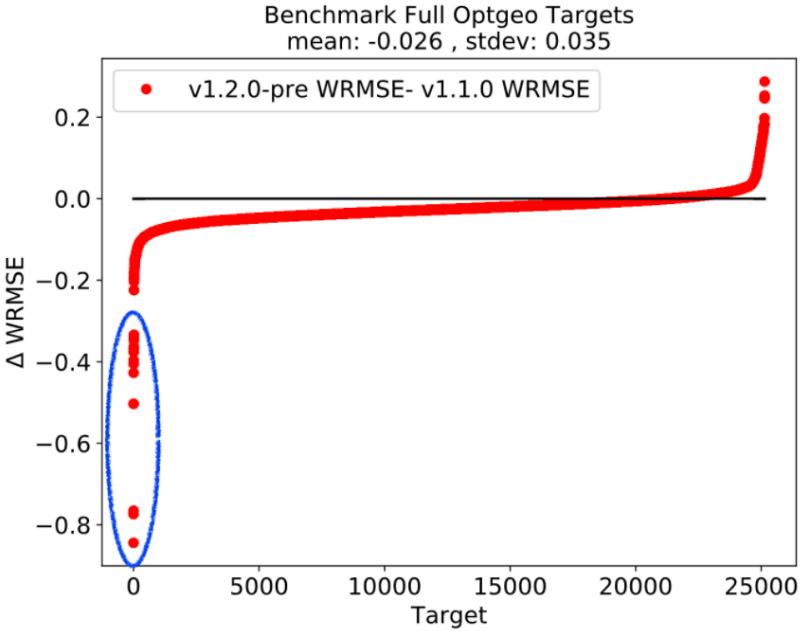


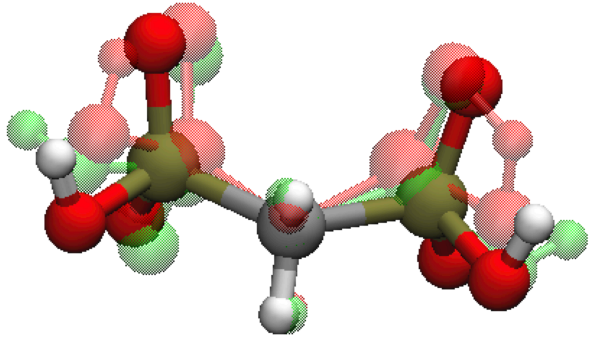
- y values in the plots(ΔWRMSE) are the difference in the WRMSE between different v1.2.0-pre and initial force field

$$\mathrm{WRMSE} = \sqrt{\sum_{i}^{N} \frac{\left(\frac{\text{QM internal coord.(i) - MM internal coord.(i)}}{\text{denom.}}\right)^2}{N}}$$

- Negative y value indicates better reproduction in v1.2.0-pre compared to initial force field.

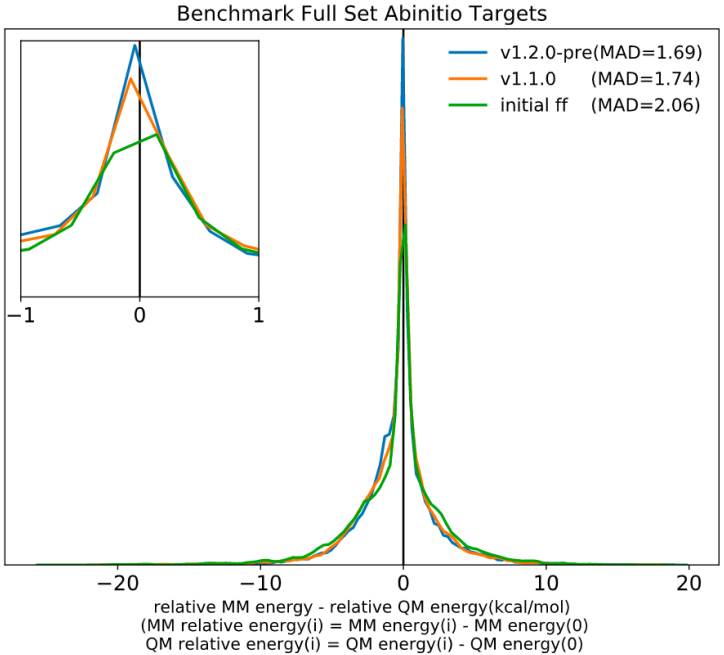
Reproducibility of QM optimized geometries

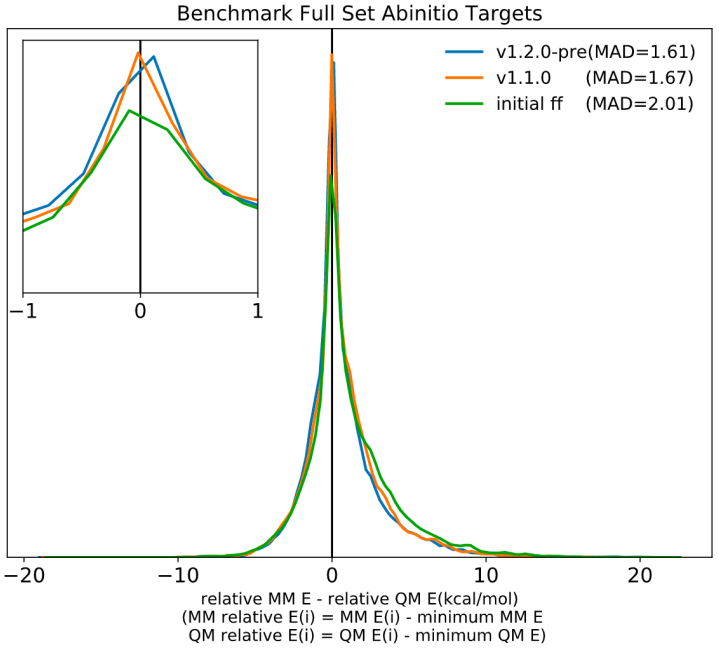




QM optimized geometry of [P@@](=O)(O)[O-])[P@](=O)(O)[O-].
(transparent red: MM optimized geometry with v1.1.0 force field,
transparent green: v1.2.0-pre force field)

Pre-liminary results





Thank you!

And please look forward to the next release of v1.2.0 Parsley!

Contributors:

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Christopher Bayly, David Mobley, Lee-Ping Wang