

A Brief Overview of The Force Field Toolkit (ffTK)

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Available Methods for Obtaining Parameters

Analogy (Re-use of parameters from similar structures)

ParamChem <https://www.paramchem.org/>

SwissParam <http://swissparam.ch/>

Zoete *et al.*; *J. Comp. Chem.* 32(11) **2011**, pp.2359-2368

MATCH <http://brooks.chem.lsa.umich.edu/software>

Yesselman *et al.*; *J. Comp. Chem.* 33(2) **2012**, pp.189-202

Development

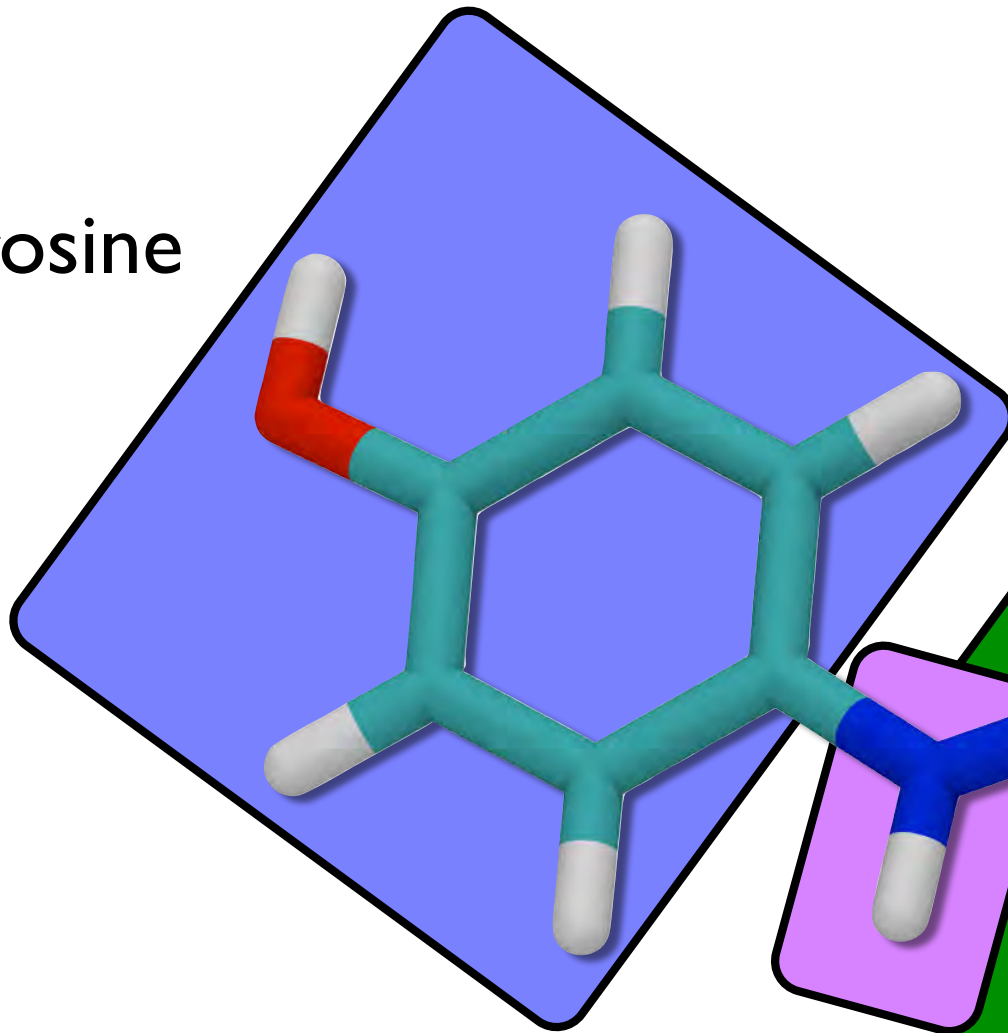
ParaTool <http://www.ks.uiuc.edu/Research/vmd/plugins/paratool/>

GAAMP <http://gaamp.lcrc.anl.gov/para-fit.html>

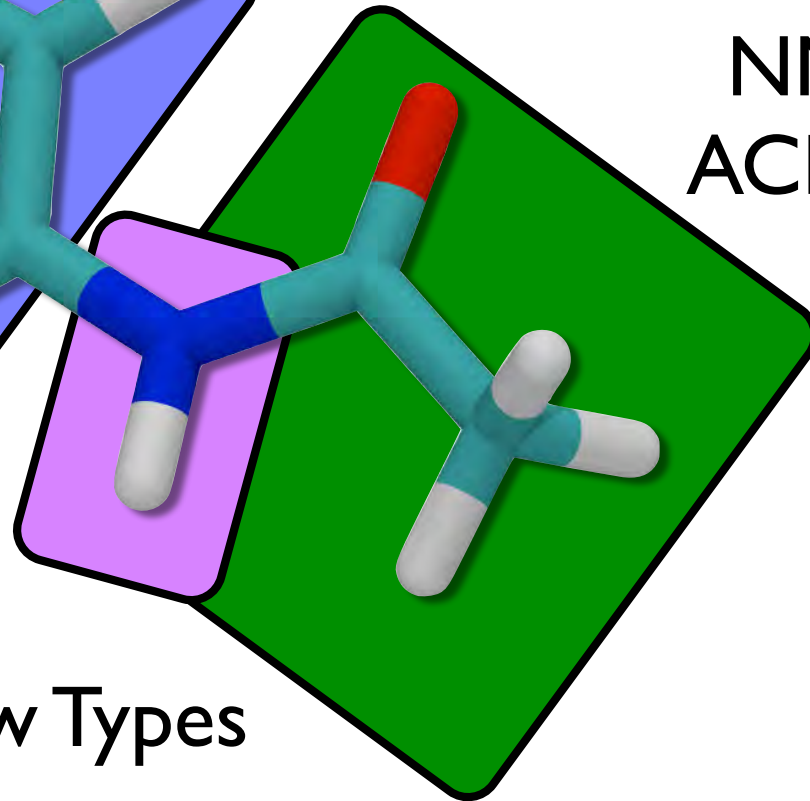
ffTK <http://www.ks.uiuc.edu/Research/vmd/plugins/fftk/>

An Example: Acetaminophen

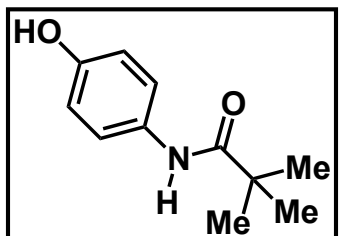
Tyrosine



NMA or
ACE-patch

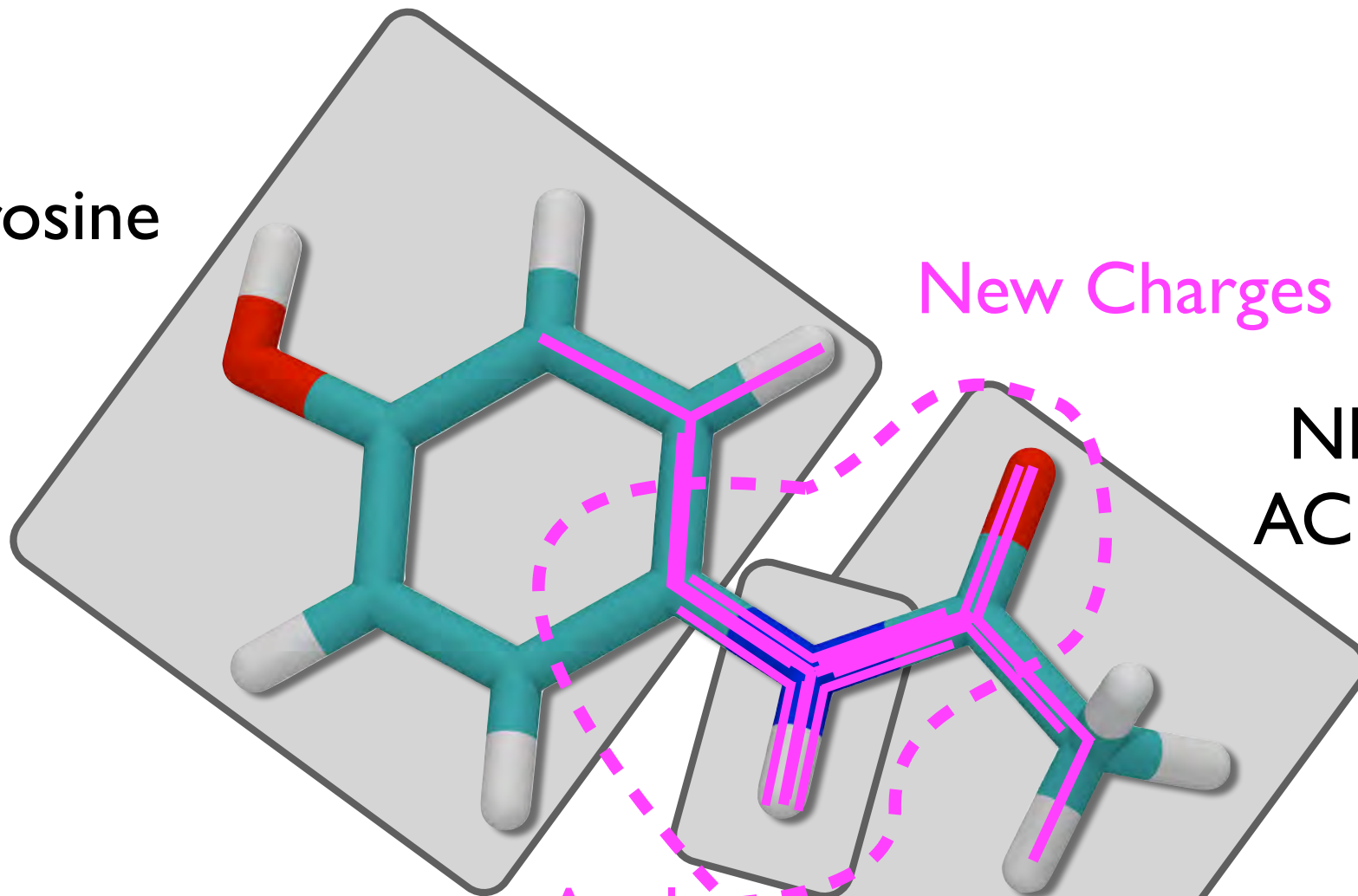


New Types



An Example: Acetaminophen

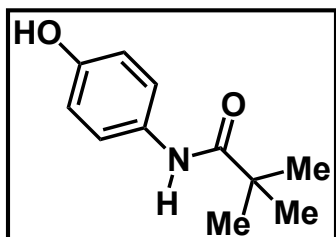
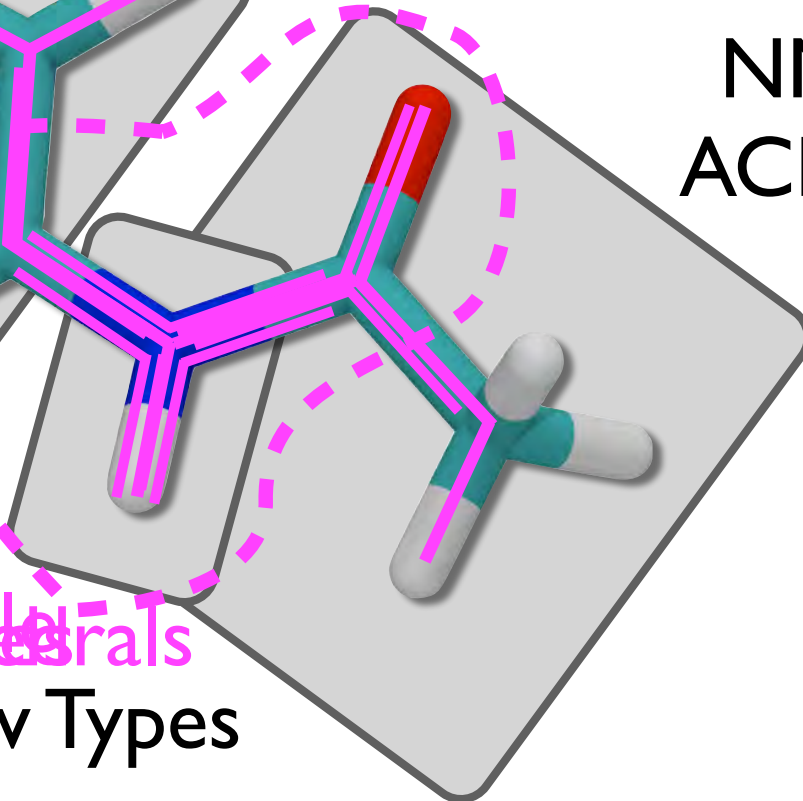
Tyrosine



New Charges

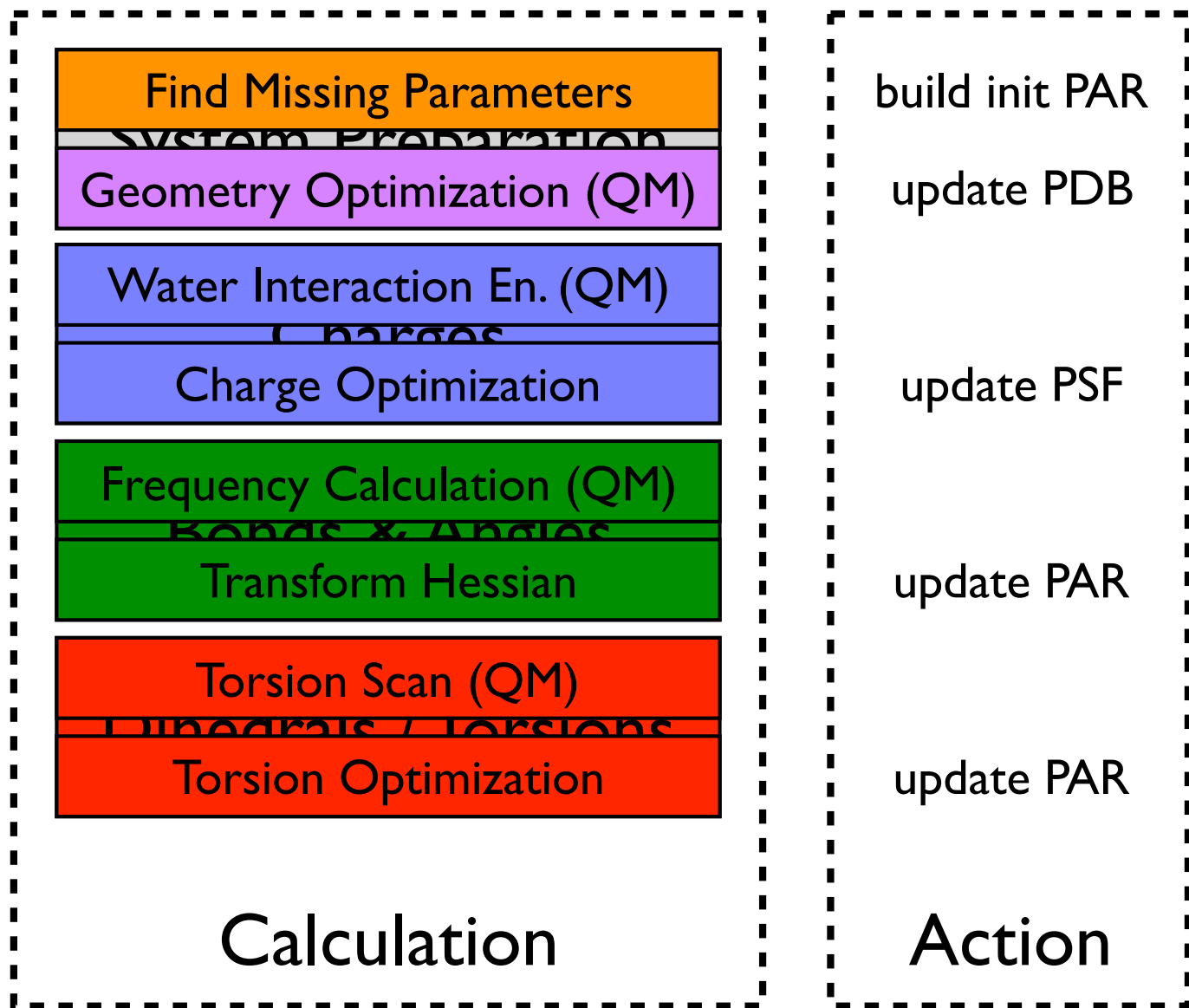
NMA or
ACE-patch

Bonds
Angles
New Types



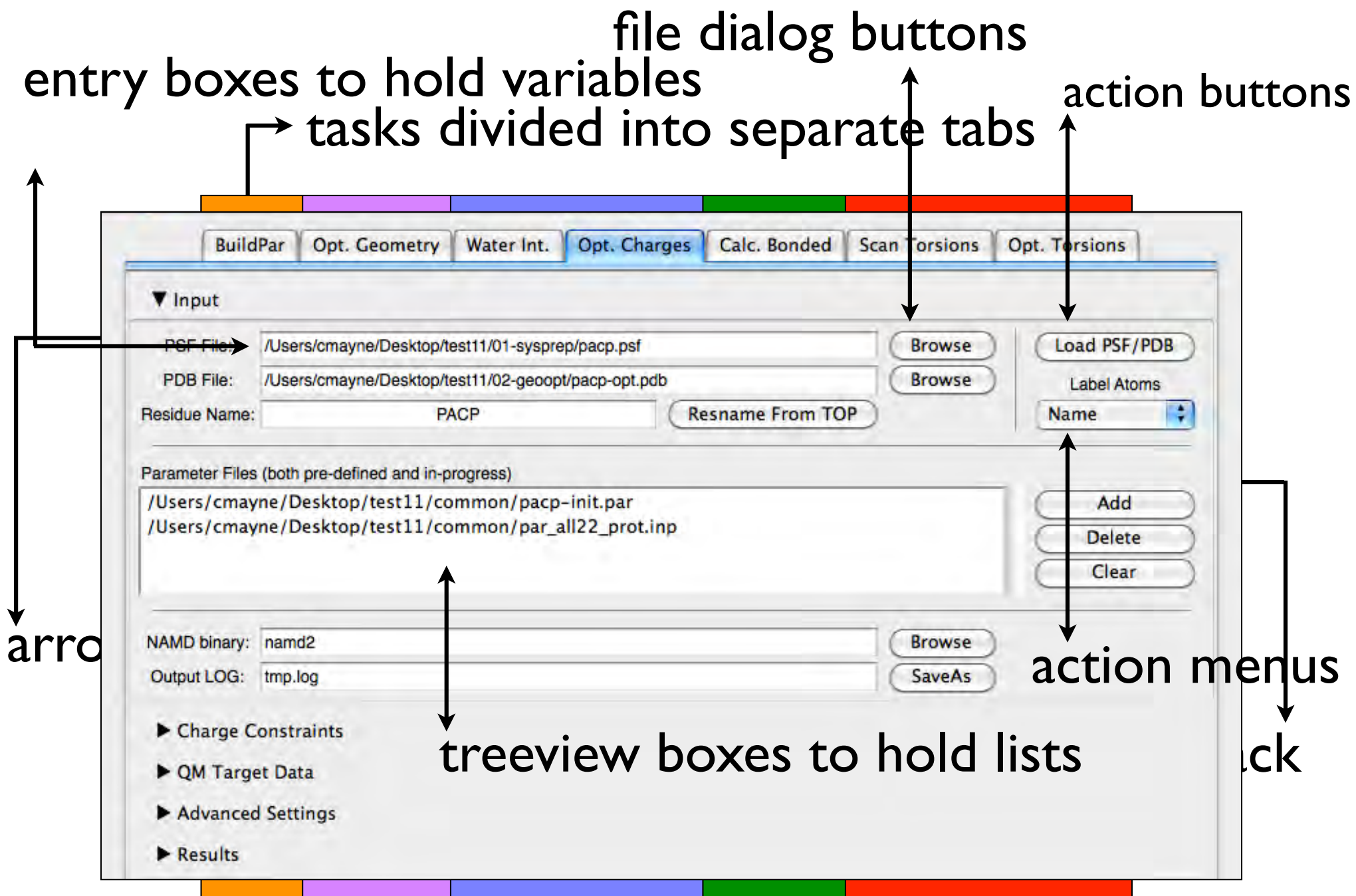
ffTK Facilitates the Parameterization Workflow

PSF/PDB



PAR File

ffTK Interface



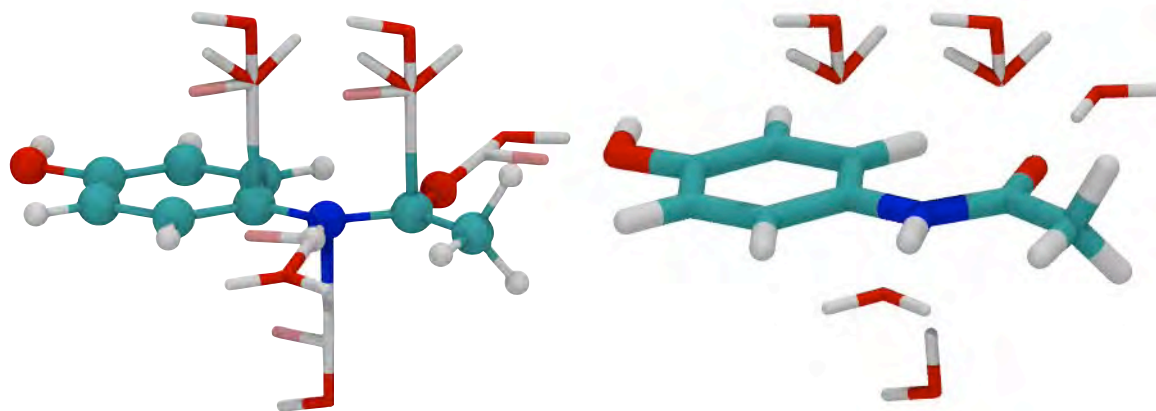
ffTK 1.0 is Available in VMD 1.9.1

Setup necessary QM calculations

Visualize calculation input/output

Multidimensional optimization
of developing parameters

Read/Write files (pdb, par, log, gau)



Full documentation online:
<http://www.ks.uiuc.edu/Research/vmd/plugins/fftk/>

Tutorial is available

