CHL Lab

Rosalind J. Xu 18’ June 2018

**Making a New Fragment for SolEFP**

If you have a novel moiety in your simulation, you need to make a new fragment to represent that moiety. If that moiety is for an amino acid side chain, you need to incorporate it to gmx.tc as well.

There are two types of scenarios: 1. You need to make a new fragment for a non-probe residue; 2. You need to make a new fragment for a probe residue. 2 requires slightly more steps than one. Bartek’s tutorial covers both 1 and 2, as well as how to add a new amino acid entry in gmx.tc. His tutorial can be found here: <https://github.com/globulion/slv/blob/master/doc/tutor/III.SolEFP.Parameters.md>

Ask Bartek for permission to access. You can also ask Casey to ask Bartek to give you permission.

The following steps cover how to deal with scenario 1 on Fock:

**1.** Generation of FCHK file in Gaussian: Use g03 utility on Fock. Ask Joe Cammisa to add you to the g03 user group. Create [molecule]-gauss-fchk.i from template.

Run commands:

tcsh

source /opt/gaussian/g03/bsd/g03.login

g03 [molecule]-gauss-fchk.i [molecule]-gauss-fchk.log (obtain [molecule].chk)

formchk [molecule].chk [molecule].fchk

**2.** Generation of CAMM file. Put [molecule].fchk in working directory.

slv\_gen-camm SCF 6-311++G\*\*

**3.** Generation of EFP file in GAMESS:

Install gamess in home directory. See <https://www.webmo.net/support/gamess_linux.html>

(When configuring: use ifort instead of gfortran; use mkl math library; choose sockets; opt out of LIBCCHEM)

Edit $SCR, $USERSCR, and $GMSPATH in rungms; set $EXTBAS in gms-files.csh to $GMSPATH/extbas/slvbas;

upload extbas folder containing slvbas file to $GMSPATH.

Add export PATH=$PATH:$HOME/programs/gamess to ~/.bashrc file.

Create [molecule]-gms-efp.inp from template. (Do not change the symmetry group options!)

Run commands:

rungms [molecule]-gms-efp 00 4 >& [molecule]-gms-efp.log &

Copy [molecule]-gms-efp.dat and [molecule]-gms-efp.efp from /tmp to working directory.

**4.** Generation of FRG files:

slv\_efp-frg [molecule].fchk [molecule].camm None [molecule].efp [molecule].frg 6-311++G\*\*

**5.** Add [molecule] fragment folder containing [molecule].frg, [molecule].efp and [molecule].xyz files to $SLV\_DATA/frg (echo $SLV\_DATA/frg to find out where this folder is). Add ‘[molecule]’ to slvpar.params in site-packages/solvshift in python2.7.

**6.** Follow Bartek’s tutorial for the syntax of gmx.tc, and how to add a new entry to it: <https://github.com/globulion/slv/blob/master/doc/tutor/III.SolEFP.Parameters.md>

If you need a QM visualization software for the atomic indexes, I recommend IQmol: <http://iqmol.org/downloads.html>