**On how to edit mcce source code**

1. Copy the source code to your local directory from /home/mcce/mcce3.0/
2. Edit files in there
3. To compile, go to lib and type

make clean

make

1. Go back to the mcce main directory and type

Make

1. If you ever edit mcce.h the header file, make sure you edit in all mcce.h

In the main dir

In lib

In tools/zopp

In tools/merge

In tools/fitit

In tools/add\_sas

**How the opp files are created:**

In mcce2.5.1 and mcce3.0, opp files are saved as one binary file called energies.opp, so if you want to see what’s inside it, you must call zopp –x energies.

Let’s say you want to edit each file in opp files, here is the flow of how these files are created.

In energies.c:

1. Inside conf\_energies method, four columns are created (line ~890)
   * 1. counter
     2. prot.res[i].conf[j].uniqID
     3. pairwise\_ele[counter] : this comes from DelPhi straight from run01.frc or run02.frc
     4. vdwt : from vdw\_conf method in vdw\_conf.c

these columns are save inside a file called rot.res[kr].conf[kc].uniqID.opp, if you want to see this file, set the following to flags in run.prm f (DELPHI\_CLEAN) and ./ (PBE\_FOLDER)

1. Inside conf\_rxn method, 6 columns are added to (line ~ 2045)
   * 1. prot.res[i].conf[j].iConf
     2. prot.res[i].conf[j].uniqID
     3. prot.res[i].conf[j].tmp\_pw\_ele \* k\_single\_multi : pairwise\_ele[counter]\* k\_single\_multi
     4. prot.res[i].conf[j].tmp\_pw\_vdw : this comes from conf\_energies method
     5. prot.res[i].conf[j].tmp\_pw\_ele : this comes from the pairwise\_ele[counter]
     6. prot.res[i].pw\_bound : this comes from DelPhi (run01.frc)

**note: mcce2.5.1 doesn’t have the last column**

these columns are save inside a file called rot.res[kr].conf[kc].uniqID.opp, if you want to see this file, set the following to flags in run.prm f (DELPHI\_CLEAN) and ./ (PBE\_FOLDER)

In make\_matrices.c

The opp files created from energies.c are read in here and saved into the final opp **FILE**. You can find the place at which the information is read and save under the following comment // read from energies.c and save into ematrix

Then, there are saved inside energies.opp. If you want to view them, you use zopp –x anyname, which is in return invoke extract\_matrix method in make\_matrices.c. The number of columns in extract\_matrix must match the number of columns in zopp program. In zopp program (opp.c), also edit the code Inside of main method of opp.c

**Note**: make sure you recompile the zopp code. The zopp code needs mcce.a, make sure you delete the old one and move the new one from mcce3.0/lib to zopp dir and then recompile by typing make