Generation of Amber polarizable force fields [ref]

Tutorial by:
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In R.E.D. Server Development/PyRED released in November 2014, the resp program version 3.1 is interfaced. This “iresp” version allows the derivation of non-polarizable and polarizable atomic charges for the Amber additive and non-additive force field models. iresp is available for download from the following web page: http://q4md-forcefieldtools.org/REDServer-Development/resp/.

The quantum mechanics (QM) Gaussian program is selected during the input submission procedure using the web interface: one has to register and use a private account:
See http://q4md-forcefieldtools.org/REDServer-Development/faq.php#3

Input molecules of PyRED are provided in the PDB file format:
See http://q4md-forcefieldtools.org/REDServer-Development/Documentation/readme.txt

1- Define specific keywords in the Project.config file:

See http://q4md-forcefieldtools.org/REDServer-Development/Documentation/Project.config
The user has to define the total charge and spin multiplicity of the molecules involved in force field generation if they are different from zero and one, respectively. She/he can also define bond(s), angle(s) and/or dihedral(s), which can be constrained during geometry optimization. Charge constraints can be requested during the charge fitting step to lead to molecular fragments as well, etc...

2- Define specific keywords in the System.config file:

See http://q4md-forcefieldtools.org/REDServer-Development/Documentation/System.config

- First, select the *charge model* as well as the *levels of theory* (i. e. the *methods* and the *basis sets*) used in geometry optimization and molecular electrostatic potential computation:

```
# RESP-A1 is the default; so this keyword is not really needed...
#  (just pick up a charge model involving two fitting steps: RESP-A1 or RESP-X1)
CHR_TYP        = RESP-A1
# MP2 in geometry optimization could be used, but it is far more expensive...
# These keywords are only implemented for the Gaussian program by now.
METHOD_OPTCALC = B3LYP
BASSET_OPTCALC = 6-311++G(d,p)
METHOD_MEPCALC = MP2
BASSET_MEPCALC = aug-cc-pVTZ
```


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- Then, select the last force field set available in PyRED:

```
# AMBERFF10 is the default; so this keyword is not really needed...
# To be used with the frcmod.user file (see below)
FFPARM = AMBERFF10
```

Finally, select the *model of polarization*:

```
# The default: non-polarizable RESP charges are derived
POLARIZ = NOPOLARIZT
# The Thole exponential model – Tinker like
POLARIZ = THOLEXPTNK
# The Thole linear model
POLARIZ = THOLLINEAR
```

One has also the opportunity to provide user defined polarizability values and user defined atom independent screening length values (values with four digits after the decimal point) using the following keywords: `C3-POL-ATOMTYPE`, `C2-POL-ATOMTYPE`, `C1-POL-ATOMTYPE`, `H-POL-ATOMTYPE`, `N-POL-ATOMTYPE`, `NO-POL-ATOMTYPE`, `O3-POL-ATOMTYPE`, `O2-POL-ATOMTYPE`, `F-POL-ATOMTYPE`, `CL-POL-ATOMTYPE`, `BR-POL-ATOMTYPE`, `I-POL-ATOMTYPE`, `S4-POL-ATOMTYPE`, `S-POL-ATOMTYPE`, `P-POL-ATOMTYPE`, and `SCREENLENGTH`.

Remarks:

- The polarizability values used during the charge fitting step are printed in the "mol3" file format. Thus, the user has access to the values used during the charge fitting step. They can also be read by the LEaP program if needed.
- Simultaneous use of polarizable charges and lone-pairs is not implemented yet.

3- Define specific force field parameters in the frcmod.user file (optional):

On the top of the force field set selected using the `FFPARM` keyword an additional ensemble of force field parameters can be provided by the user in the "frcmod.user" file. These additional force field parameters could consist in key dihedral force field and/or van der Waals parameters, that were specifically developed for the model of atomic charges derived in this tutorial.

An example of use of the "frcmod.user" file is available at:
See http://q4md-forcefieldtools.org/Tutorial/Tutorial-4.php#9.

4- Create an archive file to upload the different PyRED inputs

See http://q4md-forcefieldtools.org/REDServer-Development/popup/poparchive.php

```
tar -zcvf Archive.tgz Mol_red*.pdb Project.config System.config frcmod.user
```

[ref] P. Cieplak, J. W. Caldwell, P. A. Kollman, *J. Comput. Chem.* 2001, 22, 1048.
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