Electrostatic component of binding energy using traditional 2-dielectric approach

The electrostatic component of binding energy can be obtained by two methods, Method-1 uses difference in grid energies, and Method-2 uses energy partitioning. In this process, three DelPhi runs are required as follows; the first run will be on the complex, second on the barnase and the third on the barstar molecules. One should keep the molecules at the same positions in all runs (this is mandatory for Method 1 calculations, since it uses grid energy differences and artificial grid energy terms must be canceled out). The files used in this example are present in Example_3.1.6/ and Example_3.1.6/2-dielectric/ directories, change current working directory to Example_3.1.6/2-dielectric/. Now we can do the DelPhi run using following command.

```
$DELPHI_EXE param_barnase-barstar_2-diel.prm \
                      > param_barnase-barstar_2-diel.log
$DELPHI_EXE param_barnase_2-diel.prm > param_barnase_2-diel.log
$DELPHI_EXE param_barstar_2-diel.prm > param_barstar_2-diel.log
```

The energy details for each of three runs is written in barnase-barstar_2-diel.dat, barnase_2-diel.dat and barstar_2-diel.dat files respectively. The relevant contents of the three .dat files are as below.

The content of barnase-barstar_2-diel.dat

```
Total grid energy                 : 132916.29 kT
Corrected reaction field energy   : -1737.31 kT
Total coulombic energy            : -44990.50 kT
Total required energy (everything
 calculated but grid)             : -46727.80 kT
```

The content of barnase_2-diel.dat

```
Total grid energy                 : 73515.44 kT
Corrected reaction field energy   : -1020.38 kT
Total coulombic energy            : -25009.84 kT
Total required energy (everything
 calculated but grid)             : -26030.23 kT
```

The content of barstar_2-diel.dat

```
Total grid energy                 : 59388.54 kT
Corrected reaction field energy   : -1265.7 kT
Total coulombic energy            : -19433.73 kT
```

```
Total required energy (everything
calculated but grid)                : -20699.43 kT
```

Now the electrostatic component of binding energy using Method-1 can be obtained from total grid energies of barnase-barstar complex, barnase and barstar as follows:

$\Delta G(bind) = G_{grid}(cpx) - G_{grid}(barnase) - G_{grid}(barstar)$

$\Delta G(bind) = 132916.29 - (73515.44 + 59388.54)kT = 12.31kT$

The electrostatic component of binding energy using Method-2 can be obtained from partitioned energies as follows

$$\Delta G(bind) = G_{coulombic} + G_{reaction\ field} + G_{ions} \quad (1)$$

$$= G_{ARET}(complex) - G_{ARET}(barnase) - G_{ARET}(barstar)$$

$$= -46727.80 - (-26030.23 + -20699.43)kT$$

$$= 1.86kT$$

where ARET = all required energy terms

Setting the grid position, scale and number same in monomer runs as the complex run, required by Method-1

First of all the we are required to run DelPhi with a given `scale` (say: `scale=2.5`) and `perfil` (say: `perfil=70`) as in provided barnase-barstar_2-diel.prm. On completion of this run the we need to obtain the `gsize` and grid center coordinates from the log file as below:

```
    gsize=`grep 'Grid size' param_barnase-barstar_2-diel.log | awk -F":" '{print $2}' | awk '{print $1}'`
    center=`grep 'Grid box is centered (A)' param_barnase-barstar_2-diel.log | awk -F":" '{print $2}' | awk '{printf "%f,%f,%f", $1, $2, $3;}'`
```

The two commands given below will print the appropriate `gsize` and `acenter` parameters to be included in file for monomers.

```
echo "gsize=$gsize";
echo "acenter=($center)";
```

The very same `gsize` value and grid center coordinates (use `acenter(x,y,z)` to set this parameter value, where (`x,y,z`) is the coordinates of grid center in DelPhi run for complex) should be used for the DelPhi runs of monomers (barnase and barstar). Here, make sure that perfil is not provided or commented in the DelPhi input parameter file for monomers.

Setting parameters for DelPhi run for Method-2

In all the runs (complex and monomers i.e. barnase-barstar, barnase and barstar) use same `scale` and `perfil`, but not `gsize` and `acenter`. Doing this will keep the grid resolution and percentage of grid filled by molecule(s) same but not the position and `gsize`.

Note that the calculated electrostatic component of binding energy via Method-1 and Method-2 is different. This is due to the fact that Method-1 does not fully cancel so termed “artificial grid energy” arising from real charges partitioning onto the grid. Thus we recommend using Method-2, the energy partitioning method in case of energy calculations with zero salt.