Using DelPhi focusing module

Example demonstrating the use of the 'focusing' method to calculate electrostatic potential and electric field for a particular region with high precision (scale=4) with a reduced computational time. This is an alternative way to the previous example (example 3) where the potential and electric field were calculated in a single run at modest precision (scale=2). Improving the precision (scale=4) in a single run (as in example 3) would require much larger grid size resulting in large computational time. To overcome the large computational cost and at the same time to ensure the desired precision, here we present the 'focusing' method which require two runs. The first run would be low-resolution (scale=1) while the second would be fine-grain/high-resolution (scale=4) implementing the 'focusing' technique. For convenience, we keep the same test example inputs barnase and ASP39 of barstar in complex with barnase as earlier examples.

How to run:

Check that if you have all the input files: `barnase.pdb`, `amber.crg`, `amber.siz`, `param_phimap1.prm`, `param_phimap2_focus.txt`, `frc_in.pdb`

Run1 or Parent-run can be started using command given below after changing current directory to example directory:

```
$DELPHI_EXE param_phimap1.prm > focusing1.log
```

This will output phimap1.cube which is then read by the second parameter file (param_phimap2_focus.prm)

Run2 or Child-run can be started using command given below after changing current directory to example directory:

```
$DELPHI_EXE param_phimap2_focus.prm > focusing2.log
```

Output files: frc.out

*Note: `$DELPHI_EXE` is the full filename of the delphi executable

Details after the run:

The focusing method is usually used for large systems. Here for simplicity, we just use the focusing method in a regular sized system, which is a barnase and a residue from barstar. Using focusing method you need a parent run (Run 1) and a child run (Run 2). The parent run is used to calculate a big system in a relatively low resolution and then output the potential map. The child run will take the potential map from the parent run as input and obtain boundary conditions from it. Then the child run uses higher resolution to generate more accurate potentials and fields in a smaller region. This focusing is very useful when the entire system is very big but the region of interest is only a small part of the whole system.

In the parent run, we need to output a potential map using the lines below. In this example, the potential map is `phimap1.cube`, with a resolution of `scale=1.0`.

```
scale=1.0
out(phi,file="phimap1.cube",format=cube)
```

The child run reads the phimap1.cube and outputs `phimap2.cube`. The resolution of the child run is higher than in the parent run (`scale=4.0`) and the calculation box is smaller; the acenter option is used to indicate where is the center of the child box; the boundary condition is set as 3 to indicate the boundary values are calculated based on the input phimap1.cube; an frc option is used to calculate the potential and field on a residue from barstar.

```
scale=4.0
gsize=65
in(phi,file="phimap1.cube",format=cube)
acent(29.3265,39.6727,8.45517)
bndcon=3
in(frc,file="frc_in.pdb")
out(frc,file=frc.out)
site(a,p,f)
```

The results in frc.out are shown below:

ATOM DESCRIPTOR GRID PT. GRID FIELDS: (Ex, Ey, Ez)

N	ASP	39	4.1756	0.6405	-0.3778	-0.3490
CA	ASP	39	4.8222	0.4604	-0.5575	-0.2597
C	ASP	39	4.2671	0.4711	-0.7224	-0.1193
O	ASP	39	4.8549	0.5076	-0.7876	-0.0760
CB	ASP	39	4.9746	0.3860	-0.4938	-0.1966
CG	ASP	39	6.1325	0.6179	-0.8084	-0.8741
OD1	ASP	39	7.6227	0.2540	-0.7568	-1.7999
OD2	ASP	39	5.6482	1.6908	-1.3951	-0.6391
H	ASP	39	4.1805	0.8720	-0.2338	-0.2283
HA	ASP	39	5.5355	0.3913	-0.6681	-0.3523
HB3	ASP	39	4.3396	0.5483	-0.5301	0.0870
HB2	ASP	39	5.1324	0.0829	-0.2063	-0.0216

total energy = -3.39614 kt