Calculating the total electrostatic energy of a protein (at Zero salt concentration)

How to run:

Check that you have all the input files: `1brs.pdb`, `amber.crg`, `amber.siz`, `param_protein.prm.` To run it, type following command and press enter:

```
$DELPHI_EXE param_protein.prm > protein.log
```

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

Details of the run: This example is used to calculate total electrostatic energy of a protein (at Zero salt concentration) and the electrostatic potential map. For other molecules such as DNA, RNA, etc, the method is similar. 1brs.pdb is the file containing atomic coordinates of the protein 'barnase'. amber.crg and amber.siz files contain the charge and size information, respectively.

After the run, in log file you will see the result shown as below:

```
 Energy> Total grid energy                          :     32580.86 kT
 Energy> Corrected reaction field energy            :     -3583.05 kT
```

The "Corrected reaction field energy" is the electrostatic component of solvation energy;

"Coulambic energy" is the coulombic interaction energy between charged atoms in homogeneous medium with an internal dielectric constant of indi. In this particular instance, indi is set as 2.0 “All required energy terms but grid energy” is the sum of the above two energy terms and represents the total electrostatic energy of the protein.

The electrostatic potential map output file (`phimap.cube`) may be used to various visualization purposes by graphical interfaces such as Chimera, VMD, Pymol etc. Similarly, modeling the same protein with Gaussian-based smooth dielectric function can be done by invoking DelPhi and appropriate parameter file as:

```
$DELPHI_EXE param_protein_gauss.prm > protein_gauss.log
```

After the run is completed, one finds the output information in the log file:

```
Energy> Corrected reaction field energy : -3583.05 kT
```