Solving non-linear Poisson-Boltzmann equation to calculate the electrostatic solvation and total electrostatic energies of a protein

How to run:
Check that you have all the input files: 1brs.pdb, amber.crg, amber.siz, param_nonlinear.prm

To run it, type:
<path>/delphi param_nonlinear.prm > nonlinear.log
Press enter key, you should get the results.
Output files: phimap.cube
*Note: <path> is the folder where you put delphi executable file

Details after the run:
This example is used to calculate the electrostatic component of solvation energy of a protein. The difference between this example and basic example 2 is: in example 2, we solve linear Poisson-Boltzmann equation, while here we solve non-linear Poisson-Boltzmann equation to demonstrate the non-linear effects which are important for highly charged systems. To invoke non-linear calculations, several extra lines are needed in the parameter file:
salt=0.15
nonit=800
relpar=1.0 #optional, but highly recommended, line for relaxation parameter

However in some cases the selection of relpar=1.0 might not result in convergence.
In such cases, the user is advised to try out different variables.

Where salt is the salt concentration in molars, nonit is the maximum number of steps in the calculation (note that you may want to increase this number if convergence is not achieved within 800 iterations). relpar - we recommend relpar to take values from 0.8 to 1.0. The resulting nonlinear.log is shown below:

```
 Energy> Total grid energy                              :     61484.49 kT
 Energy> Corrected reaction field energy                :     -1005.93 kT
 Energy> Coulombic energy                               :    -28450.24 kT
 Energy> rho*phi/2 term in solution                     :        -1.29 kT
 Energy> Osmotic pressure term                          :         1.11 kT
 Energy> Total non linear grid energy                   :     61484.67 kT
 Energy> All required energy terms but grid energy      :    -29456.00 kT
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Note: The electrostatic component of solvation energy is given by ,ÄúCorrected reaction field energy,Äù(rxn) term = -1005.93 kT. The total electrostatic energy in non-linear case includes electrostatic stress and osmotic pressure along with electrostatic component of solvation energy and Coulombic energy, as G(total) = G(Coulombic) + G(rxn)+ G(salt press) + G(rho*phi/2) = -28450.24 -1005.93 +1.11-1.29=-29456.35 (note this number -29456.35 is slightly different from the number reported as ,ÄúAll required energy terms but grid energy   :   -29456.00 kT,Äù, because of the numerical truncations of individual energy terms). Note that electrostatic stress term is denoted as ,Äúrho*phi/2 term,Äù in the output file. Note also that the difference of osmotic pressure and electrostatic stress is a measure of non-linearity ,Äì the more distinctive they are, the more pronounced the non-linear effects are.

Although we call this the total energy (G(total)) term, it doesn‚Äôt equal to the explicit ion contribution to the energy.