Binding of a peptide to a membrane: An application of non-liner PBE

This example will show how to use the focusing technique to improve the resolution.

Ensure that you have the following files in the directory:

binding.sh
charmm22.crg
pcpgps_aminos.siz
lys5.pdb
r4.pdb
lys5_r4.pdb

Run the script called "binding.sh".

Then with your command shell pointed to the directory of Example_3.1.9, execute command given below:
$ bash binding.sh

The script will execute 12 delphi runs - each set of 4 runs will calculate the energy of 5-lys, membrane itself and the complex. Focusing will be applied to improve the resolution. Nonlinear Poisson-Boltzmann equation will be solved. The distance between peptide and membrane is 4A, so the surface effects are not important.

Wait for DelPhi to complete the calculations which may take ~15-20 minutes (for serial Delphi).

The final focusing files are: lys5_r4_2.log (the complex)
$ grep 'Total non linear grid energy' lys5_r4_2.log
total nonlinear grid energy: 285679.17 kT

lys5_2.log (only the peptide):
$ grep 'Total non linear grid energy' lys5_2.log
total nonlinear grid energy: 2587.42 kT

r4_2.log (only the membrane):
$ grep 'Total non linear grid energy' r4_2.log
total nonlinear grid energy: 283099.28 kT

Thus, the binding energy is: 285679.17 -2587.42 -283099.28 = -7.53 kT

NOTE: You might have to change the relaxation parameter (relpar) if you see that the runs do not converge.