Binding of a peptide to a membrane

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
```

Open the bash script ./binding.sh in a text editor.
In line 3, locate "DELPHI_COMMAND" and replace its value "_DELPHI_COMMAND_" with the appropriate command to run delphi.

E.g. To run delphi's sequential version, replace "_DELPHI_COMMAND_" with "<absolute/path/of/Delphi/executable>"

Run the script called "binding.sh".
To run this script, you must make sure that the file is marked as executable.

Then with your command shell pointed to the directory of example5, type
$ ./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. Thus, we will apply the grid energy difference method to calculate the binding energy. Note that method 2 from the previous example can't be used, because part of the system is outside the final focusing box. Note also that 1/2 of the pairwise interaction energy will be lost to the charges outside the box. In this particular case, this results in a correction of a fraction of kT, so it can be neglected.

Wait for delphi to complete the calculations. The expected runtime is 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.