Example showing total electrostatic energy of two charges embedded in a dielectric cavity (Single Large-Sphere representation)

This example is used to compare the delphi output with the corresponding analytical solution.
See the following reference for more details:
1. Gilson, M. K.; Rashin, A.; Fine, R.; Honig, B. On the Calculation of Electrostatic Interactions in Proteins. J. Mol. Biol. 1985, 184 (3), 503,Äì516.
2. Li, Lin, et al. "DelPhi: a comprehensive suite for DelPhi software and associated resources." BMC biophysics 5.1 (2012): 9.

This example considers a large sphere with a radius of 10 Angstrom and two charges of +10 eu embedded in the sphere.
The corresponding analytical expressions are provided in the references above. At a particular positioning of the charges one can simplify the analytical expressions
and deliver the corresponding analytical total energy. In this particular case, the analytical total energy is -5083.19 kT.

You can visualize the geometry from the input pdb file: cavity1.pdb

How to run:
Check and make sure that you have all the input files: cavity1.pdb, my.crg, my.siz, param_large_sphere.prm

To run it, type:
<path>/delphi param_large_sphere.prm > largesphere.log
Press enter key, you should get the results.
*Note: <path> is the full path where the delphi executable is located.

In this example, we have created a system of spherical cavity, in which two charges are located. The cavity is centered at (0,0,0) with radius of 10 √Ö, the two charges are centered at (5,5,0) and (5,-5,0), respectively, and each of them has a +10e charge. In the cavity1.pdb file, the SPH atom represents the large sphere. The N and CA atoms are the two charges, as shown below:

```
ATOM   3573  SPH                0.000   0.000   0.000
ATOM   4384  N                  5.000   5.000   0.000
ATOM   4385  CA                 5.000  -5.000   0.000
```

The my.siz and my.crg files provide the size and charge information of each entity. The user can run DelPhi to obtain the total electrostatic energy.

```
 Energy> All required energy terms but grid energy     :     -5104.00 kT
```

Note that total electrostatic energy (All required energy terms but grid energy: -5104.00 kT) has the following components:

```
 Energy> Corrected reaction field energy               :     -7913.99 kT
 Energy> Coulombic energy                              :      2809.98 kT
```

Note that the calculated energy (-5104.0 kT) is very close to the analytical solution (-5083.19 kT).

Further improvement can be made by increasing the resolution (as shown in reference 2)