Electrostatic component of solvation energy of two charges embedded in spherical dielectric cavity (particle mesh representation):

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 spherical particle mesh with a maximum radius of 9 Ö and two charges of +10 eu embedded in the particle mesh.

The corresponding analytical expressions are provided in the references above. One can simplify the analytical expressions, at a particular positioning of the charges .
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

This example illustrates how to use ProNOI (Smith, Nicholas, et al. "Protein Nano-Object Integrator (ProNOI) for generating atomic style objects for molecular modeling." BMC structural biology 12.1 (2012): 31. http://compbio.clemson.edu/downloadDir/ProNO_Integrator.zip) to generate a spherical cavity and to place two charges inside. The PDB-like file is then input to DelPhi to calculate electrostatic energy. The electrostatic energy can be calculated via analytical function (Li, Lin, et al. "DelPhi: a comprehensive suite for DelPhi software and associated resources." BMC biophysics 5.1 (2012): 9.) and results compared.

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_pronoi.prm > proNOI.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 atoms represent the spherical cavity. The N and CA atoms are the two charges, as shown below:

```
ATOM   3569  SPH                0.504   0.873  -8.943
ATOM   3570  SPH               -0.504   0.873  -8.943
ATOM   3571  SPH               -1.008   0.000  -8.943
ATOM   3572  SPH               -0.504  -0.873  -8.943
ATOM   3573  SPH                0.504  -0.873  -8.943
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     :     -5230.22 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               :     -8040.20 kT
 Energy> Coulombic energy                              :      2809.98 kT
```

Note that the calculated energy (-5230.22 kT) is very close to the analytical solution (-5083.19 kT).
In this case, the analytical and calculated energies differ slightly more than the 'large sphere' example.
This is due to the fact that the dielectric cavity (represented here) is not a perfect sphere, especially the molucular surface is not a precise spherical surface. One can improve the presentation to make it more spherical by increasing the probe radius (from prbrad=1.4 to say prbrad=10.0) to smooth the protrusions and crevices among the atoms.