Calculating electrostatic component of solvation energy with Gaussian smooth dielectric function
(Not applicable to Delphi's MPI version)

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

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

Details:

Without the Gaussian option, DelPhi treats the biomolecule-water system as a two-dielectric system: a low dielectric constant within the molecule and a high dielectric constant in the water. When using the Gaussian method, DelPhi treats the biomolecule-water system as an inhomogeneous system, which is physically more reasonable. To use the Gaussian option, three flags are needed in the parameter file:

```
gaussian=1
srfcut=20
sigma=0.9
```

GAUSSIAN: gaussian=1 indicates that the Gaussian smooth dielectric method is selected. gaussian=0 is for the traditional homogenous method. Default value of gaussian is 0.
SIGMA: Sigma is the value of the variance of Gaussian distribution:

For example: sigma=2.0.

SRFCUT: When calculating the solvation energy using Gaussian smooth method, a cutoff of dielectric value is needed to determine the border between protein and water phases.
SRFCUT is used to specify this cutoff.
For example: srfcut=20.0.
Be aware that the solvation energy calculated using Gaussian model can NOT be combined with the Coulombic energy calculated in homogeneous model.

GAUSSIAN, SIGMA and SRFCUT are options for Gaussian smooth method, more detailed information can be found in the paper below:
L. Li, C. Li, Z. Zhang, E. Alexov, ,ÄúOn the Dielectric Constant of Proteins: Smooth Dielectric Function for Macromolecular Modeling and its Implementation in DelPhi,Äù, J. Chem, Theory Comput. 2013 Apr 9; 9(4): 2126-2136.

The result calculated by DelPhi is shown below:

```
 Energy> Total grid energy                          :     32580.86 kT
 Energy> Corrected reaction field energy            :     -3583.05 kT
```