MATLAB Solver example: The Born-ion model

Abstract

Let's consider the born-ion model at room temperature (T=298.15 C). Inside the born radius (r=3A) the low dielectric coefficient representing the molecule is set equal to $\epsilon^x = \epsilon^y = \epsilon^z = 1.0$. This ion is located at the origin of the reference system and it is immersed in a solvent medium of dielectric coefficient that mimic water, e.g., with $\epsilon^x = \epsilon^y = \epsilon^z = 78.54$. The bulk ionic strength is set equal to zero. The born ion charge valence is set equal to $z = +1$. To solve the PB equation we will use a cubic grid of 65 points and a box length of 12 A centered at the ion position. We will use the linear B-spline to obtain the fractional charge at the node points.

Input files as generated by the APBS and pdb2pqr codes

The "born-ion.pqr" file corresponding to the model described above reads

```
ATOM 1 I ION 1 0.000 0.000 0.000 1.00 3.00
```

As an example, the "born.in" input file used by the APBS reads

```
# READ IN MOLECULES
read
mol pqr born-ion.pqr
end
# COMPUTE POTENTIAL FOR SOLVATED STATE
elec name solvated
mg-auto
dime 65 65 65
cglen 50 50 50
fglen 12 12 12
fgcent mol 1
cgcent mol 1
mol 1
lpbe
bcfl mdh
pdie 1.0
sdie 78.54
chgm spl0
srfm spl2
srad 1.4
swin 0.3
sdens 10.0
temp 298.15
calcenergy total
calcforce no
write pot dx born-pot
```

write charge dx born-charge
write dielx dx born-dielx
write diely dx born-diely
write dielz dx born-dielz
write kappa dx born-kappa
end
quit

For example, if you saved both files 'born-ion.pqr" and 'born.in' in the directory 'C:/Users/me/Documents/APBS_PB_solver/', you may type in your command prompt window

C:/Users/me/Documents/Matlab_PB_solver>apbs born.in

In this way we obtain the input files in dx format required by the MATLAB version of the APBS to solve the PB equation. Specifically, we obtain the shifted dielectric coefficients maps born-dielx.dx, born-diely.dx, born-dielz.dx, and the ion accessibility map born-kappa.dx. We also obtain the charge density born-charge.dx and the electrostatic potential born-pot.dx maps which will be used later for testing purpose.

MATLAB input file

Now we are ready to write the input file "born.inm" as follows

65 65 65
12 12 12
298.15
born-dielx.dx
born-diely.dx
born-dielz.dx
born-kappa.dx
born-ion.pqr
born_ion_model

The first line corresponds to the number of grid of points $[N_x N_y N_z]$; the second line corresponds to the length in Anstrong of the boxsides $[L_x L_y L_z]$; the next line corresponds to the temperature in Celsius degree; next is the name of the dx file containing the shifted dielectric coefficients along the x direction; next is for the one corresponding to the y-direction and next the one in the z-direction. The seventh line corresponds to the name of the ion accessibility coefficient map. The next one corresponds to the name of the pqr file generated by the pdb2pqr code and the last line corresponds to the name of the folder that will be created into the current folder (for instances 'Matlab_PB_solver') where all the Matlab files of our code are saved. In the folder "born_ion_model" you will find all the files generated by our Matlab code, namely electrostatic potential and the charge maps in dx format, and the electrostatic potential surface $u_{ij(N_z+1)/2}$ in both jpg and fig format.

Before using our Matlab code

Before running the "main.m" file in the Matlab console you must create a folder (for instances "Matlab_Input_Files") in the same directory (For instances 'C:/Users/me/Documents/Matlab_PB_solver/') in which all the Matlab files of our code are saved. Then you must save the input files born-ion.inm, born-ion.pqr, born-dielx.dx, born-diely.dx, born-dielz.dx, and born-kappa.dx in the folder "Matlab_Input_Files".

Next, you must edit two lines in the "main.m" file to know:

- The line number 57 contains the path to the folder "Matlab_Input_Files". In our example you have to set the path as follows

  MYPATH='C:/Users/me/Documents/Matlab_PB_solver/Matlab_Input_Files';

- The line number 65 contains the name of the inm input file. In our example we termed it as "born-ion.inm" such that we have to set the name of the inputfile as follows

  inputfile='born-ion.inm';

Now we are ready to run the main.m file. In the command window of Matlab you may type

>>run C:/Users/me/Documents/Matlab_PB_solver/main

You are done. On the same command window you will see information about the different steps that our code performs to get the required solution.

Matlab output files

In this example you will find a created folder named 'born_ion_model' in the directory 'C:/Users/me/Documents/Matlab_PB_solver/' containing the following files

born_ion_model_MATLAB_charge_density.dx
born_ion_model_MATLAB_potential_solution.dx
born_ion_model_MATLAB_potential_solution.jpg
born_ion_model_MATLAB_potential_solution.fig

Accuracy and efficiency of our Matlab code

You may change same parameters of our code in order to make it faster and more efficient. In particular, the default accuracy is set equal to 10^-9. You may change it by editing the main.m file and change the variable 'accuracy' for the required precision. You may also change the tolerance in the inexact LU decompostion. The default value for the variable 'tolerance' is set equal to 0.25.