MATLAB example: The two Born-ions model

Abstract

Let's consider the two-ions complex model at room temperature (T=298.15 C). Inside the radius (r=1A) the low dielectric coefficient representing the (solute) molecule is set equal to $\epsilon^x = \epsilon^y = \epsilon^z = 2.0$. The positive ion (with valence equal to $z = +1$) is located at the position $(1, 1, 1)$ in amstrongs and the negative ion (with valence equal to $z = -1$) is located at the position $(-1, -1, -1)$. Both ions are immersed in a solvent medium of dielectric coefficient that mimic water, e.g., with $\epsilon^x = \epsilon^y = \epsilon^z = 78.54$ (solvated state). The bulk ionic strength is set equal to zero. To solve the PB equation we will use a cubic grid of 65 points and a box length of 12 A centered at the origin of the reference system $(0, 0, 0)$. We will use the linear B-spline to obtain the fractional charge at the node points.

Part I

Using the MATLAB PB SOLVER

Input files as generated by the APBS and pdb2pqr codes

The "twoions.pqr" file corresponding to the model described above reads

ATOM 1 I1 ION 1 1.000 1.000 1.000 1.000 1.000

ATOM 2 I2 ION 1 -1.000 -1.000 -1.000 -1.000 1.000

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

read

mol pqr twoions.pqr # Two-ion complex

end

elec name comp_solv # Solvated complex

mg-manual

dime 65 65 65 # Grid dimensions

nlev 4 # Multigrid levels

glen 12 12 12 # Grid lengths

gcent mol 1 # Grid center

mol 1

lpbe # Linearized PB

bcfl mdh # Full multipole boundary condition

ion 1 0.000 2.0 # Zero ionic strength

ion -1 0.000 2.0 # Zero ionic strength

pdie 2.0 # Solute dielectric

sdie 78.54 # Solvent dielectric

chgm spl2 # Cubic spline charge discretization

srfm mol # Molecular surface

srad 1.4 # Solvent probe radius

swin 0.3 # Surface spline window

sdens 10.0 # Sphere density

temp 298.15 # Temperature

write pot dx twoions-pot

write charge dx twoions-charge

write dielx dx twoions-dielx

write diely dx twoions-diely

write dielz dx twoions-dielz

write kappa dx twoions-kappa

calcenergy total # Total energy

calcforce no # No forces

end

quit

For example, if you saved both files 'twoions.pqr" and 'twoions.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 twoions.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 twoions-dielx.dx, twoions-diely.dx, twoions-dielz.dx, and the ion accessibility map twoions-kappa.dx. We also obtain the charge density twoions-charge.dx and the electrostatic potential twoions-pot.dx maps which will be used later for testing purpose.

MATLAB input file

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

65 65 65

12 12 12

298.15

0.0 78.54

twoions-dielx.dx

twoions-diely.dx

twoions-dielz.dx

twoions-kappa.dx

twoions.pqr

twoions_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 line contains the bulk properties (ionic strenght $I_s = \sum c_i z_i^2$ and the solvent dielectric coeffcient for the solvated states or the molecular dielectric coefficient for the reference state); 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 (working) folder (for instances 'Matlab_PB_solver') where all the Matlab files of our code are saved. In the folder "twoions_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 twoions.inm, twoions-ion.pqr, twoions-dielx.dx, twoions-diely.dx, twoions-dielz.dx, and twoions-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 "twoions.inm" such that we have to set the name of the inputfile as follows

  inputfile='twoions.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 'twoions_model' in the directory 'C:/Users/me/Documents/Matlab_PB_solver/' containing the following files

  twoions_model_MATLAB_charge_density.dx
  twoions_model_MATLAB_potential_solution.dx
  twoions_model_MATLAB_potential_solution.jpg
  twoions_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.

Part II

Testing our code

Before using our Matlab code

Before running the "comparison.m" file in the Matlab console you must create a folder (for instances "Potential") 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 in that folder the APBS and MATLAB electrostatic potential solutions. In our example they are APBS-twoions-pot.dx and twoions_model_MATLAB_potential_solution.dx.

Next, you must edit three lines in the "comparison.m" file to know:

- The line number 19 contains the path to the folder "Potential". In our example you have to set the path as follows

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

- The line number 27 contains the number of grid points in the format $[N_x N_y N_z]$. In our example we have to set

  dime= [65 65 65];

- The line number 29 contains the length of the boxside in the format $[L_x L_y L_z]$ in anstromgs. In our example we have to set

  glen= [12 12 12];

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

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

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 'COMPARATIVE_ANALYSIS' in the directory 'C:/Users/me/Documents/Matlab_PB_solver/' containing the following files

Absolute Error between MATLAB and APBS solutions.dx

Absolute_error.fig

Absolute_error.tiff

APBS-twoions-pot_and_twoions_model_MATLAB_potential_solution.fig

APBS-twoions-pot_and_twoions_model_MATLAB_potential_solution.tiff