MATLAB version of the APBS

Abstract

This is the first version. This solver uses the biconjugate gradient stabilized method and the inexact LU decomposition to numerically solve the linearized PB equation on the finest (target) 3D-grid. This version requires the shifted dielectric and the ion accessibility coefficient (kappa function) maps as generated by the APBS code as well as the corresponding pqr file generated by the pdb2pqr code. It uses standard three-linear splines (spl0) to spread the charge density along the nearest grid points if needed. The resulting electrostatic potential and charge maps are saved in dx format. For visualization purpose, this code also generates two files (.fig and .tiff) corresponding to the graphical representation of the electrostatic potential surface.

Description

This code is based on Michel Holst's thesis and Nathan Baker's APBS approach. The box-method is used to discretize the following (linearized) PB equation

$$-\nabla. \left(\epsilon\left(\mathbf{r}\right)\nabla u\left(\mathbf{r}\right)\right) + \bar{\kappa}\left(\mathbf{r}\right)u\left(\mathbf{r}\right) = magic\sum_{i=1}^{N} z_i\delta\left(\mathbf{r} - \mathbf{r}_i\right) \tag{1}$$

where $u\left(\mathbf{r}\right) = e_c\Phi\left(\mathbf{r}\right)/K_BT$ and $magic = 4\pi e_c^2/K_BT$. For a diagonal dielectric tensor, the resulting discretized linear PB equations at the nodes $u_{ijk} = u\left(x_i, y_j, z_k\right)$ for $1 \le i \le N_x$, $1 \le j \le N_y$ and $1 \le k \le N_z$ reads

$$\left[\epsilon_{i-1/2,j,k}^x\frac{\left(h_{j-1}+h_j\right)\left(h_{k-1}+h_k\right)}{4h_{i-1}} + \epsilon_{i+1/2,j,k}^x\frac{\left(h_{j-1}+h_j\right)\left(h_{k-1}+h_k\right)}{4h_i}+\right.$$

$$\epsilon_{i,j-1/2,k}^y\frac{\left(h_{i-1}+h_i\right)\left(h_{k-1}+h_k\right)}{4h_{j-1}} + \epsilon_{i,j+1/2,k}^y\frac{\left(h_{i-1}+h_i\right)\left(h_{k-1}+h_k\right)}{4h_j}+$$

$$\epsilon_{i,j,k-1/2}^k\frac{\left(h_{i-1}+h_i\right)\left(h_{j-1}+h_j\right)}{4h_{k-1}} + \epsilon_{i,j,k+1/2}^k\frac{\left(h_{i-1}+h_i\right)\left(h_{j-1}+h_j\right)}{4h_k}+$$

$$\left.\kappa_{ijk}\frac{\left(h_{i-1}+h_i\right)\left(h_{j-1}+h_j\right)\left(h_{k-1}+h_k\right)}{8}\right]u_{ijk}+$$

$$\left[-\epsilon_{i-1/2,j,k}^x\frac{\left(h_{j-1}+h_j\right)\left(h_{k-1}+h_k\right)}{4h_{i-1}}\right]u_{i-1jk} + \left[-\epsilon_{i+1/2,j,k}^x\frac{\left(h_{j-1}+h_j\right)\left(h_{k-1}+h_k\right)}{4h_i}\right]u_{i+1jk}+$$

$$\left[-\epsilon_{i,j-1/2,k}^y\frac{\left(h_{i-1}+h_i\right)\left(h_{k-1}+h_k\right)}{4h_{j-1}}\right]u_{ij-1k} + \left[-\epsilon_{i,j+1/2,k}^y\frac{\left(h_{i-1}+h_i\right)\left(h_{k-1}+h_k\right)}{4h_j}\right]u_{ij+1k}+$$

$$\left[-\epsilon_{i,j,k-1/2}^k\frac{\left(h_{i-1}+h_i\right)\left(h_{j-1}+h_j\right)}{4h_{k-1}}\right]u_{ijk-1} + \left[-\epsilon_{i,j,k+1/2}^k\frac{\left(h_{i-1}+h_i\right)\left(h_{j-1}+h_j\right)}{4h_k}\right]u_{ijk+1} =$$

$$magic\frac{\left(h_{i-1}+h_i\right)\left(h_{j-1}+h_j\right)\left(h_{k-1}+h_k\right)}{8}f_{ijk} \tag{2}$$

in which

$$h_i = x_{i+1} - x_i,\ h_j = y_{j+1} - y_j\ h_k = z_{k+1} - z_k$$

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The delta functions appearing in the right hand side of the starting equations are approximated with linear B-splines (spl0) which spread the point like charge along the nearest neighborhood. The resulting f_{ijk} represent the smearing of the point charges along the grid points.

For more details, including used unit system, please refer to the Michel Holst's thesis and the APBS user guide online. To visualize more clearly the problem, let's explicitly write the first equations for a cubic grid of 5x5x5 containing general coefficients

$$a_{222}u_{222} + a_{122}u_{122} + a_{322}u_{322} + a_{212}u_{212} + a_{232}u_{232} + a_{221}u_{221} + a_{223}u_{223} = f_{222}$$

$$a_{322}u_{322} + a_{222}u_{222} + a_{422}u_{422} + a_{312}u_{312} + a_{332}u_{332} + a_{321}u_{321} + a_{323}u_{323} = f_{322}$$

$$a_{422}u_{422} + a_{122}u_{122} + a_{322}u_{322} + a_{212}u_{212} + a_{232}u_{232} + a_{221}u_{221} + a_{223}u_{223} = f_{422}$$

$$a_{232}u_{232} + a_{132}u_{132} + a_{332}u_{332} + a_{222}u_{222} + a_{242}u_{242} + a_{231}u_{231} + a_{233}u_{233} = f_{232}$$

$$\ldots$$

in which the nodes are arranged using the natural ordering

$$U = [u_{111}, u_{211}, .., u_{N_x11}, u_{121}, .., u_{221}, u_{321}, .., u_{N_x21}..., u_{N_xN_yN_z}]^T$$

Note that the prescribed values of nodes u_{1jk}, $u_{N_x,j,k}$, $u_{i,1,k}$, $u_{i,N_y,k}$, u_{ij1} and u_{ijN_z} along the faces of the box coming from the Dirichlet boundary conditions will have their corresponding elements removed in such a way that only equations for the interior nodes remain. In other words, we will only consider the following set of unknown nodes

$$U = [u_{222}, u_{322}, .., u_{N_x-1,22}, u_{232}, .., u_{332}, u_{432}, .., u_{N_x-2,32}..., u_{N_x-1,N_y-1,N_z-1}]^T$$

in such a way that the previous equations become

$$a_{222}u_{222} + a_{322}u_{322} + a_{232}u_{232} + a_{223}u_{223} = f_{222} - a_{122}u_{122} - a_{212}u_{212} - a_{221}u_{221} \equiv b_{222}$$

$$a_{322}u_{322} + a_{222}u_{222} + a_{422}u_{422} + a_{332}u_{332} + a_{323}u_{323} = f_{322} - a_{312}u_{312} - a_{321}u_{321} \equiv b_{322}$$

$$a_{422}u_{422} + a_{322}u_{322} + a_{232}u_{232} + a_{223}u_{223} = f_{422} - a_{122}u_{122} - a_{212}u_{212} - a_{221}u_{221} \equiv b_{422}$$

$$a_{232}u_{232} + a_{332}u_{332} + a_{222}u_{222} + a_{242}u_{242} + a_{233}u_{233} = f_{232} - a_{132}u_{132} - a_{231}u_{231} \equiv b_{232}$$

in which the boundary $u's$ are conveniently brought to the right-hand-side of the equations. The resulting left-hand side equations can be written in compact form in term of matrix vector product as follows

$$Au = b$$

in which

$$u\,(p) = u_{ijk}, \qquad b\,(p) = b_{ijk}, \qquad p = (k-2)(N_x - 2)(N_y - 2) + (j-2)(N_x - 2) + i - 1$$

$$i = 2, .., N_x - 2, \quad j = 2, .., N_y - 2, \quad k = 2, .., N_z - 2$$

and A is a (seven banded block tri-diagonal form) $(N_x - 2)(N_y - 2)(N_z - 2)$ by $(N_x - 2)(N_y - 2)(N_z - 2)$ squared symmetric positive definite matrix containing the following nonzero elements (see figure 1):

- The main diagonal elements

$$d_0(p) = \left[\epsilon^x_{i-1/2,j,k} \frac{(h_{j-1} + h_j)\,(h_{k-1} + h_k)}{4h_{i-1}} + \epsilon^x_{i+1/2,j,k} \frac{(h_{j-1} + h_j)\,(h_{k-1} + h_k)}{4h_i} + \right.$$

$$\epsilon^y_{i,j-1/2,k} \frac{(h_{i-1} + h_i)\,(h_{k-1} + h_k)}{4h_{j-1}} + \epsilon^y_{i,j+1/2,k} \frac{(h_{i-1} + h_i)\,(h_{k-1} + h_k)}{4h_j} +$$

$$\epsilon^k_{i,j,k-1/2} \frac{(h_{i-1} + h_i)\,(h_{j-1} + h_j)}{4h_{k-1}} + \epsilon^k_{i,j,k+1/2} \frac{(h_{i-1} + h_i)\,(h_{j-1} + h_j)}{4h_k} +$$

$$\left. \kappa_{ijk} \frac{(h_{i-1} + h_i)\,(h_{j-1} + h_j)\,(h_{k-1} + h_k)}{8} \right] \tag{3}$$

- The Next upper band diagonal, which is shifted in one column to the left from the first column, contains the following elements
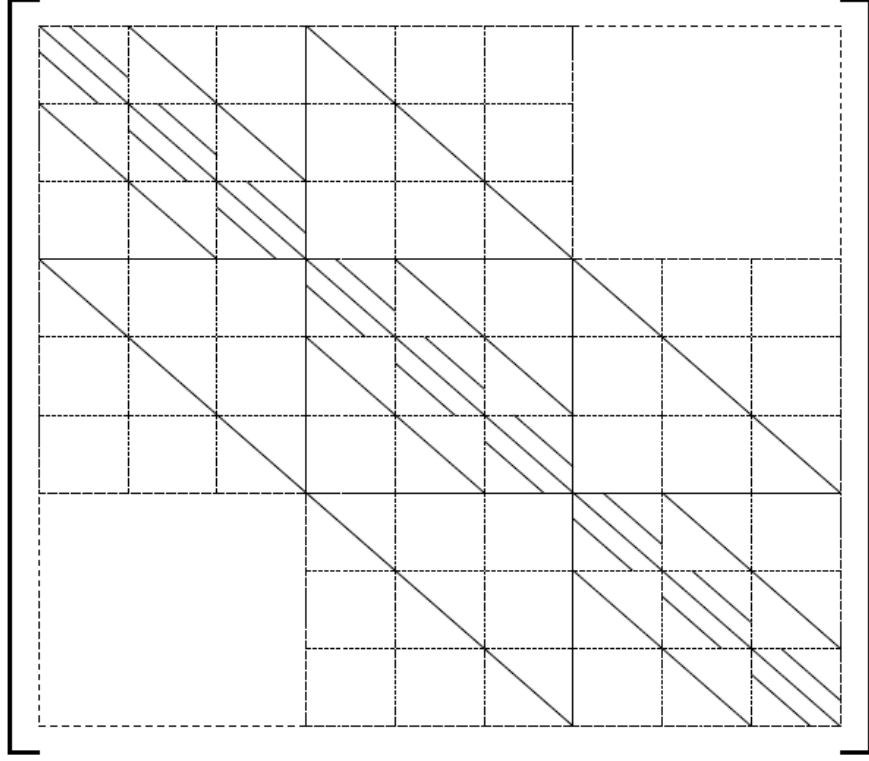
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Figure 1: A Matrix representation

$$\left[d_1(p) = -\epsilon_{i+1/2,j,k}^x \frac{(h_{j-1} + h_j)\,(h_{k-1} + h_k)}{4h_i} \right] \tag{4}$$

- The second upper band diagonal which is shifted $N_x - 2$ columns from the first column

$$d_2(p) = \left[-\epsilon_{i,j+1/2,k}^y \frac{(h_{i-1} + h_i)\,(h_{k-1} + h_k)}{4h_j} \right] \tag{5}$$

- The third upper band diagonal which is shifted $(N_x - 2)(N_y - 2)$ columns from the first column

$$d_3(p) = \left[-\epsilon_{i,j,k+1/2}^k \frac{(h_{i-1} + h_i)\,(h_{j-1} + h_j)}{4h_k} \right] \tag{6}$$

The remaining elements of the upper triangular squared matrix A are set equal to zero. By symmetry we obtain the lower triagonal elements of the matrix A. Because the matrix A is sparse and large, we can implement efficient methods that optimally solve the linear system for U. Specifically, we use the biconjugate gradient stabilized method combined with the inexact LU decomposition of the matrix A. Having the numerical values for the nodes in the interior of the box, we finally add the previously removed prescribed values along the six faces to get the solution over the complete set of grid points.

Computational algorithm

1. We read the input file .inm to get the APBS input files (shifted dielectric coefficients, kappa function and pqr data file) as well as the number of grid points, the box Lengths, and temperature.

2. By using linear B-splines, we discretize the charge density to get f_{ijk} for $i = 1, .., N_x$, $j = 1, .., N_y$, $k = 1, .., N_z$. We also calculate the Dirichlet boundary condition along the six faces of the box $u_{1jk}, u_{N_x,j,k}, u_{i,1,k}, u_{i,N_y,k}, u_{ij1}$ and u_{ijN_z} using the temperature, the value of the bulk dielectric coefficient (usually water) and ionic strength.

3. By using the expressions (3), (4),(5), and (6), we evaluate the nonzero components of the matrix A, e.g., the diagonal elements $d_0(p), d_1(p), d_2(p)$, and $d_3(p)$, for $p = (k-2)(N_x-2)(N_y-2) + (j-2)(N_x-2) + i - 1$ and $i = 2, .., N_x - 1$, $j = 2, .., N_y - 1$, $k = 2, .., N_z - 1$. The values for the shifted dielectric coefficients and kappa function elements are obtained from the APBS input files. The values of the mesh size h_i, h_j and h_k are obtained from the number of grid points and the Length of the box. Next, we built the sparse upper triangular matrix A by filling with zeros the remaining elements of the matrix A. Next, we obtain the lower triangular elements of the matrix A by using the following symmetry property $A_{pq} = A_{qp}$ for $q = 1, .., (N_x - 2)(N_y - 2)(N_z - 2)$ and $p = q, .., (N_x - 2)(N_y - 2)(N_z - 2)$.

4. By using the values obtained for the discretized charge density f_{ijk} and the values of the Dirichlet boundary elements multiplied by the appropriate shifted dielectric coefficient values, we evaluate the elements of b_{ijk}. We use the natural ordering $p = (k-2)(N_x -$

$2)(N_y-2)+(j-2)(N_x-2)+i-1$ and $i = 2, .., N_x-1, \quad j = 2, .., N_y-1, \quad k = 2, .., N_z-1$ to construct the corresponding vector $b(p)$ (one index) from the data array structure (three indices) b_{ijk}.

5. We use the inexact LU decomposition of the matrix A. The default tolerance value is set equal to 0.25 which provides a fast evaluation of the matrices L and U.

6. The resulting L and U matrices, the matrix A and the vector b are used to approximately solve $Au = b$ for the vector u using the biconjugate gradient stabilized method. The default accuracy is set equal to 10^-9 and the maximum number of iteration equal to 800.

7. We use the natural ordering relationship to convert the resulting vector $u(p)$ to data array structure to get the numerical solution for u_{ijk} for $i = 2, .., N_x-1, \quad j = 2, .., N_y-1, \quad k = 2, .., N_z - 1$.

8. Finally we add the previously removed values of the nodes at the faces of the box to obtain the solution for the nodes u_{ijk} over the complete set of grid points, namely for $i = 1, .., N_x, \quad j = 1, .., N_y, \quad k = 1, .., N_z$.

9. The electrostatic potential u_{ijk} and the charge f_{ijk} maps are saved in dx format files.

10. The electrostatic potential surface $u_{ij(N_z+1)/2}$ is saved in tiff and fig format files for visualization purpose.