User Guide (Binary Version 0.4, October 14, 2013)

Treecode-Accelerated Boundary Integral (TABI) Poisson-Boltzmann solver

1. Introduction

This guide gives direction to use the binary Treecode-Accelerated Boundary Integral (TABI) Poisson-Boltzmann solver [1]. The code uses a well-posed boundary integral formulation of the Poisson-Boltzmann equation [2] to ensure rapid convergence of the GMRES iteration [3]. In addition, a fast treecode algorithm for the screened Coulomb potential [4] is applied to speed up the matrix-vector product in each GMRES iteration. The boundary integral formulation requires a triangular mesh to represent the molecular surface, which is generated by MSMS [5].

This material is based upon work supported by the National Science Foundation under NSF Grant DMS-0915057. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the National Science Foundation.

2. System Requirements

Users can download the binary file for their running systems. Currently, the binary files for Linux, Mac and Windows are available. One needs to download the following files suitable for their systems.

(1) tabipb.exe

(2) msms (saved as "msms.exe" for windows and "msms" for Linux and Mac)

(3) usrdata.in

(4) test_proteins (a folder with test proteins in forms of APBS's .pqr file, users can go to the web portal "http://pdb2pqr.nbcr.net" to generate the .pqr file for interested biomolecules)

Alternatively, one can put msms elsewhere and included it in system path (type "msms" to test). Users can download and install MSMS from "http://mgltools.scripps.edu/packages/MSMS/".

3. Input

The input parameters are set in the file "usrdata.in". The following is a sample file with explanations.

```
fname 1ajj              #PDB ID for testing proteins
den 1                   #MSMS density (vertices per angstrom^2)
epsp 1                  #dielectric constant for protein
epsw 80                 #dielectric constant for solvent
bulk_strength 0.15      #ionic concentration (M)
order 3                 #treecode multipole expansion order
maxparnode 500          #maximum particles per leaf for the tree
mac 0.8                 #multipole acceptance criterion
```

Type "./tabipb.exe" to run TABI solver. Make sure "usrdata.in" is in the same directory as tabipb.exe, and your target proteins in the format of APBS's .pqr files are stored in the subdirectory called "test_proteins".

4. Output

1) The TABI code produces an output file called surface_potential.dat containing (1) number of nodes, number of triangles, (2) node index, vertices, normal vectors, surface potentials [kcal/mol/ e_c], surface potential normal derivatives [kcal/mol/e_c/Å], (3) connectivity data for MSMS surface triangulation. The format is given below.

```
--------------------------------------------------
num_node num_triangle
node_index x y z norm_x norm_y norm_z phi norm_phi
...
node_index1 node_index2 node_index3
...
--------------------------------------------------
```

2) The TABI code also prints the free energy of solvation on the screen together with some other information such as CPU time and the GMRES residuals at each step.

5. Reference

[1] W.H. Geng and R. Krasny, A *treecode-accelerated boundary integral Poisson-Boltzmann solver for electrostatics of solvated biomolecules*, J. Comput. Phys., 247, 62-78 (2013).

[2] A. Juffer, E. Botta, B. van Keulen, A. van der Ploeg and H. Berendsen, *The electric potential of a macromolecule in a solvent: a fundamental approach*, J. Comput. Phys., 97, 144-171 (1991).

[3] Y. Saad and M.H. Schultz, GMRES: *A generalized minimal residual algorithm for solving non-symmetric linear systems*, SIAM J. Sci. Stat. Comput., 7, 856-859 (1986).

[4] P.J. Li, R. Krasny and H. Johnston, *A Cartesian treecode for screened Coulomb particle interactions*, J. Comput. Phys., 228, 3858-3868 (2009).

[5] M.F. Sanner, A.J. Olson and J.C. Spehner, *Reduced surface: An efficient way to compute molecular surfaces*, Biopolymers, 38, 305-320 (1996).

[6] N.A. Baker, D. Sept, S. Joseph, M.J. Holst, J.A. McCammon, *Electrostatics of nanosystems: application to microtubules and the ribosome*. Proc. Natl. Acad. Sci. USA, 98, 10037-10041 (2001).

6. Acknowledgment

NSF Grant DMS-0915057