User Guide (Version 0.4, October 14, 2013)

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

1. Introduction

This package contains the code written in Fortran 90/95 for the 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

1) Compiler: Intel Fortran compiler (ifort) or GNU Fortran (gfortran). A sample Makefile is provided in the package.

2) Molecular surface generation software: MSMS [5]. The users need to download and install MSMS (http://mgltools.scripps.edu/packages/MSMS/). For convenience the package includes an MSMS executable file suitable for Linux. The MSMS executable file should be put in the same directory as the TABI executable file. Alternatively, MSMS can be installed elsewhere and included in the system path.

3. Files in the package

1) dgmres_dep.f: GMRES solver file from netlib.
2) main.f90: main file of the TABI solver.
3) Makefile: file containing compiling information; type “make” to compile and link.
4) readin.f90: file for reading the output from MSMS (vertices and normal vectors of molecular surface triangulation).
5) surface_potential.dat: sample TABI solver output file containing (1) vertices, normal vectors, surface potential, normal derivative of surface potential, (2) connectivity data for MSMS triangulation.
6) test_proteins: sub-directory containing the files of protein coordinates and partial charges given in the Naming format of PDBID_apbs.pqr, which is supported by APBS. The supplied code will read these files and generate the .xyzr files as the input of MSMS, which generates vertex and face files of triangulation .
7) treecode3d_pb.f: treecode related subroutines for building tree and computing particle-particle and particle-cluster interactions.

8) var_modules.f90: file containing the *allocatable* variables distributed in the different modules.

4. 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
```

After running the Makefile, an executable file “tabipb.exe” will appear. 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”. Users can go to the web portal “http://pdb2pqr.nbcr.net” to generate the .pqr file for interested biomolecules

5. 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.

6. 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).

7. Acknowledgment

NSF Grant DMS-0915057