User Guide (version 0.2, July 13, 2013)

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

1. Introduction

This package contains the code written in Fortran 90/95 for the Treecode-Accelerated Boundary Integral Poisson-Boltzmann (TABIPB) 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].

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 on their systems. 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 TABIPB executable file. Optionally, 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 TABIPB 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 TBIPB 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 protein coordinates (.xyzr) and partial charges (.pqr); obtained by running script convpdb.pl from package MMTSB feig.bch.msu.edu/mmtsb/convpdb.pl) together with CHARMM; these files are input to MSMS; we also provide the _apbs.pqr files for running APBS [6].
   An alternative way is to use the APBS defined pqr file to generate the .xyzr and .pqr file, a script written in f90 is available upon request.
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 main.f90 (e.g. dielectric constants (eps0 and eps1), ionic bulk strength (M), parameters related to GMRES solver, and treecode parameters). In the readin.f90 file, the user can set the PATH, provide PDB ID and MSMS density (number of vertices per $Å^2$, e.g. 1). After running the Makefile, an executable file "TABIPB.out" will appear. Type "./TABIPB.out" to run TABIPB solver.

5. Output

1) The TABIPB 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 TABIPB 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