Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2018-0098

Vol. **25**, No. 4, pp. 1235-1258
April 2019

COMPUTATIONAL SOFTWARE

DASHMM Accelerated Adaptive Fast Multipole Poisson-Boltzmann Solver on Distributed Memory Architecture

Bo Zhang[1,*], Jackson DeBuhr[1], Drake Niedzielski[2], Silvio Mayolo[3], Benzhuo Lu[4] and Thomas Sterling[1]

[1] *Center for Research in Extreme Scale Technologies, School of Informatics Computing, and Engineering, Indiana University, Bloomington, IN, 47404, USA.*
[2] *Department of Physics, Rensselaer Polytechnic Institute, Troy, NY, 12180, USA.*
[3] *Department of Computer Science, Tennessee Technological University, Cookeville, TN, 38505, USA.*
[4] *State Key Laboratory of Scientific/Engineering Computing, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing, 100190, China.*

Received 9 April 2018; Accepted (in revised version) 25 September 2018

Abstract. We present DAFMPB (DASHMM-accelerated Adaptive Fast Multipole Poisson-Boltzmann solver) for rapid evaluation of the electrostatic potentials and forces, and total solvation-free energy in biomolecular systems modeled by the linearized Poisson-Boltzmann (LPB) equation. DAFMPB first reformulates the LPB into a boundary integral equation and then discretizes it using the node-patch scheme [33]. It solves the resulting linear system using GMRES, where it adopts the DASHMM library [14] to accelerate the matrix-vector multiplication in each iteration. DASHMM is built on top of a global address space allowing the user of DAFMPB to operate on both shared and distributed memory computers with modification of their code. This paper is a brief summary of the program, including the algorithm, implementation, installation and usage.

AMS subject classifications: 45B05, 31C20, 92C05, 68N19

Key words: Poisson-Boltzmann equation, boundary element method, DASHMM, distributed computing.

*Corresponding author. *Email addresses:* zhang416@indiana.edu (B. Zhang), debuhj@gmail.com (J. DeBuhr), niedzd97@gmail.com (D. Niedzielski), sdmayolo42@students.tntech.edu (S. Mayolo), bzlu@lsec.cc.ac.cn (B. Z. Lu), tron@indiana.edu (T. Sterling)

Program Summary

Program title: DAFMPB

Nature of problem: Numerical solution of the linearized Poisson-Boltzmann equation that describes electrostatic interactions of molecular systems in ionic solutions.

Software license: GNU General Public License, version 3

CiCP scientific software URL:

Distribution format: .gz

Programming language(s): C++

Computer platform: x86_64

Operating system: Linux

Compilers: GCC 4.8.4 or newer. icc (tested with 15.0.1)

RAM:

External routines/libraries: HPX-5 version 4.1.0, DASHMM version 1.2.0

Running time:

Restrictions:

Supplementary material and references: `https://github.com/zhang416/dafmpb`

Additional comments:

1 Introduction

The Poisson-Boltzmann (PB) continuum electrostatic model has been adopted in many simulation tools for theoretical studies of electrostatic interactions between biomolecules such as proteins and DNA in aqueous solutions. Various numerical techniques have been developed to solve the PB equations and help elucidate the electrostatic role in many biological processes, such as enzymatic catalysis, molecular recognition and bioregulation. Packages such as DelPhi [27, 28], MEAD [7], UHBD [3, 36], PBEQ [21], ZAP [19], and MIBPB [10] are based on finite-difference methods. Packages such as the Adaptive Poisson-Boltzmann Solver (APBS) [2] are based on finite volume/multigrid methods. In a circumstance where the linearized PB is applicable, the partial differential equations can be reformulated into a set of surface integral equations (IEs) by using Green's theorem and potential theory [8, 12, 16, 17, 22, 26, 32, 33, 35, 44, 49, 51]. The unknowns in the IEs are located on the molecular surface, and the resulting discretized linear system can be solved very efficiently and accurately with certain fast algorithms, such as the fast multipole method (FMM) [8, 32, 51], pre-corrected FFT [26], or tree codes [17]. This strategy has been implemented in the Adaptive Fast Multipole Poisson-Boltzmann (AFMPB) solver [31, 51], the predecessor of DAFMPB, and many other recent works [12, 16, 44], where [12, 16] also utilized GPU acceleration.