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Automated Parallel and Body-Fitted Mesh Generation in Finite Element Simulation of Macromolecular Systems

Yan Xie[1], Tiantian Liu[1], Bin Tu[2], Benzhuo Lu[1,*] and Linbo Zhang[1,*]

[1] *State Key Laboratory of Scientific and Engineering Computing, Institute of Computational Mathematics and Scientific/Engineering Computing, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing 100190, China.*
[2] *National Center for NanoScience and Technology, Chinese Academy of Sciences, Beijing 100190, China.*

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Abstract. Mesh generation is a bottleneck for finite element simulations of biomolecules. A robust and efficient approach, based on the immersed boundary method proposed in [8], has been developed and implemented to generate large-scale mesh body-fitted to molecular shape for general parallel finite element simulations. The molecular Gaussian surface is adopted to represent the molecular surface, and is finally approximated by piecewise planes via the tool `phgSurfaceCut` in PHG [43], which is improved and can reliably handle complicated molecular surfaces, through mesh refinement steps. A coarse background mesh is imported first and then is distributed into each process using a mesh partitioning algorithm such as space filling curve [5] or METIS [22]. A bisection method is used for the mesh refinements according to the molecular PDB or PQR file which describes the biomolecular region. After mesh refinements, the mesh is optionally repartitioned and redistributed for load balancing. For finite element simulations, the modification of region mark and boundary types is done in parallel. Our parallel mesh generation method has been successfully applied to a sphere cavity model, a DNA fragment, a gramicidin A channel and a huge Dengue virus system. The results of numerical experiments show good parallel efficiency. Computations of electrostatic potential and solvation energy also validate the method. Moreover, the meshing process and adaptive finite element computation can be integrated as one PHG project to avoid the mesh importing and exporting costs, and improve the convenience of application as well.

AMS subject classifications: 65N50, 65Y05, 92C40, 65N30

Key words: Parallel mesh generation, body-fitted, PHG, biomolecules, finite element simulation.

*Corresponding author. *Email addresses:* `xieyan@lsec.cc.ac.cn` (Y. Xie), `liutt@lsec.cc.ac.cn` (T. Liu), `tubin@lsec.cc.ac.cn` (B. Tu), `bzlu@lsec.cc.ac.cn` (B. Lu), `zlb@lsec.cc.ac.cn` (L. Zhang)

1 Introduction

Continuum model uses a continuum description of the discrete particles (e.g., water molecules, ions, or protein molecule), which has been widely used in molecular simulations as an effective way to reduce the computational cost. The Poisson-Boltzmann equation (PBE) represents a typical continuum model describing the electrostatic interactions and ionic density distributions of a solvated molecular system at equilibrium state. The most commonly and practically used numerical methods to solve the PBE include finite difference (FD) method [2, 33], finite element method (FEM) [20, 29, 35, 37, 39], and boundary element method (BEM) [4, 25, 27, 42].

So far, mesh generation is still a bottleneck for usage of FEM/BEM due to the highly irregular shape of biomolecular systems. For biomolecular simulations, this task is further complicated by the identification of the irregular molecular surface and an appropriate description of this surface for resolving the molecular structures in sufficient details. For boundary element method a molecular surface mesh suffices; while for finite element method or its coupling with boundary element methods, a volume mesh in the solvent region and/or the solute region is also needed [28]. Triangular and tetrahedral meshing are most widely used forms of unstructured mesh generation [32]. There have been a number of free programs developed to generate surface triangular meshes for biomolecules. However, few free software can be used to generate tetrahedral meshes for biomolecules directly. A frequently-used package, Tetgen [36], is able to generate tetrahedral meshes based on the surface triangular meshes. A common strategy to obtain the tetrahedral meshes for biomolecules is generating the surface triangular meshes first and then obtaining the tetrahedral volume meshes based on the surface meshes.

We have built a tool chain to generate high-quality meshes for practical protein systems by combining a few mesh generation tools which are based on Delaunay meshing. The tool chain has essentially these components: surface meshing, quality improving, volume mesh generation, and membrane-protein mesh construction is necessary. First, a triangulation of the Gaussian surface is generated using our recently developed program TMSmesh [6], which is a robust tool for meshing molecular Gaussian surfaces and has been shown to be capable of handling molecules consisting of more than one million atoms. In the second step, the program ISO2Mesh [17] is first used to simplify the surface mesh by reducing the number of faces or adding some nodes while preserving its manifoldness, volume, and boundary shape. If self-intersecting faces exist, then the program TransforMesh [41], which can robustly handle topology changes and remove self-intersections, is used to find and remove self-intersecting faces. Finally, in the third step, a tetrahedral volume mesh is generated using the program TetGen, which consists of four-node tetrahedral elements and is ready for 3D finite element simulations. More details can be found in [7]. With this tool chain we have successfully generated meshes for many protein systems and performed finite element simulations on them [37, 40].

Today's parallel computers enable us to solve a problem with a mesh containing tens of millions of vertices. However, CPU time and memory limitations still make it a chal-