

Molecular surface meshing and applications in numerical simulation

Benzhuo Lu, Chinese Academy of Sciences

Efficient and Qualified Mesh Generation for Gaussian Molecular Surface Using Adaptive Partition and Piecewise Polynomial Approximation, Recent developments for mathematical modeling and numerical simulation of biomolecular systems raise new demands for qualified, stable, and efficient surface meshing, especially in implicit-solvent modeling. We developed a ray-casting and surface-tracing method for manifold triangular meshing for large Gaussian molecular surfaces. A new algorithm is recently developed to greatly improve the meshing efficiency and qualities. In the first step, a new adaptive partition and estimation algorithm is proposed to locate the cubes in which the surface are approximated by piece-wise trilinear surface with controllable precision. Then, the piecewise trilinear surface is divided into single valued pieces by tracing along the fold curves, which ensures that the generated surface meshes are manifolds. The mesh quality can be further improved using post-processing techniques. An alternative way is to combine the molecular surface mesh identification and volume mesh generation together during mesh refinement procedure when using FEM. Numerical test results show that TMSmesh 2.0 is capable of handling arbitrary sizes of molecules and achieves ten to hundreds of times speedup over the previous algorithm. In all of our extensively tested molecules, the resulted surface meshes are all manifolds and can be used in boundary element method (BEM) and finite element method (FEM) simulations.