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TITLE

Meshing challenges in constructing implicit solvation models of biomolecular structures

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Finite element simulations have become an important tool in the analysis of biomolecular functional models, such as electrophoresis, electrostatics and diffusion influenced reaction rate constants. For efficient and accurate finite element solutions, adaptive and quality meshes are a necessary first step. The primary difficulty remains in generating satisfactory surface or volumetric meshes for complicated macromolecules or protein structures. In this talk, I will discuss the challenges in constructing quality meshes for implicit solvation models of biomolecular structures. We have developed a comprehensive scheme for this problem. Starting from atomic resolution data in the Protein Data Bank (PDB), a smooth volumetric electron density map is constructed from atomic data using weighted Gaussian isotropic kernel functions and a two-level clustering technique. This enables the selection of a smooth implicit solvation surface approximation to the Lee-Richards molecular surface. Next, a modified dual contouring method is used to extract triangular/quadrilateral meshes for the surface, and tetrahedral/ hexahedral meshes for the volume inside or outside the molecule within a bounding sphere/box of influence. Then, geometric flow techniques are used to improve the surface and volume mesh quality. In addition, the constructed piecewise-linear meshes can be used as control meshes to construct high-order elements such as T-Spline surfaces. Several examples are presented, including generated meshes for biomolecules that have been successfully used in finite element simulations involving solvation energetics and binding rate constants.

Biography

Jessica Zhang is an Assistant Professor in Mechanical Engineering at Carnegie Mellon University with a courtesy appointment in Biomedical Engineering. She received her Ph.D. in Computational Engineering and Sciences in 2005 from the University of Texas at Austin. Her research interests include computational geometry, mesh generation, computer graphics, visualization, finite element method, isogeometric analysis and their application in computational biomedicine and engineering. She co-authored over 60 publications in international journals and conference proceedings. She is the recipient of the Office of Naval Research Young Investigator Award and the George Tallman Ladd Research Award.