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Model the Solvent-Excluded Surface of 3D Protein Molecular Structures Using Geometric PDE-Based Level-Set Method

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Abstract. This paper presents an approach to model the solvent-excluded surface (SES) of 3D protein molecular structures using the geometric PDE-based level-set method. The level-set method embeds the shape of 3D molecular objects as an isosurface or level set corresponding to some isovalue of a scattered dense scalar field, which is saved as a discretely-sampled, rectilinear grid, i.e., a volumetric grid. Our level-set model is described as a class of tri-cubic tensor product B-spline implicit surface with control point values that are the signed distance function. The geometric PDE is evolved in the discrete volume. The geometric PDE we use is the mean curvature specified flow, which coincides with the definition of the SES and is geometrically intrinsic. The technique of speeding up is achieved by use of the narrow band strategy incorporated with a good initial approximate construction for the SES. We get a very desirable approximate surface for the SES.

AMS subject classifications: 65D07, 65D10, 65D17, 65D18

Key words: Solvent-excluded surface, implicit surface, mean curvature specified flow, level-set method.

1 Introduction

The research of proteins brings the surprising information that the geometric shape of proteins is very important in their function. Proteins are considered as 3D objects with the

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envelope of surface. Most proteins function through interactions with each other at their molecular surfaces (interfaces). Hence, a proper description of the protein molecular surfaces is essential to the understanding of the life process. Moreover, it also has important implications for the calculations in protein folding, stability, docking and structure-based drug design. The geometric details of the molecular surfaces, called active sites, such as pockets, protrudes and cavities etc., can open up a patch of studying the life function from the viewpoint of the molecular structures. Therefore, the molecular modeling requires special concerns in defining and representing the molecular surfaces of proteins on which interactions occur. There are three common definitions of the molecular surfaces: the Van Der Waals (vdW) surface, the solvent-accessible surface (SAS) and the solvent-excluded surface (SES). The SES is preferred over the SAS as a more suitable description of the topology and details on the surface of proteins, as well as the significant implications in protein recognition, energetics, and stability calculations.

There have been a number of techniques in molecular structure modeling. Unstructured mesh based on the Voronoi-Delaunay framework and the advancing front technique was presented in [30]. Molecular skin model, an explicit triangular description with shape and topology adaptation, was introduced in [18,19]. A spline parametric approximation method using solvent probe molecules with variable radius was proposed in [8,9]. A compressed volumetric representation of biomolecular structures was given in [10]. A novel concept of minimal molecular surfaces is presented in [2]. A level-set method [12] based on the solvation free energy functional in the variational implicit solvent model is used to numerically capture arbitrarily shaped solute-solvent interfaces for biomolecular models in the aqueous environment. A level-set front-propagation method to identify the molecular surface and detect the interior cavities within protein structure by a unified and efficient work is adopted in [11]. Based on the Gaussian density map method [4,15,16], molecular surfaces are approximated as an isocontour of implicit solvation models. Recently a mesh generation combining a modified dual contour method with implicit solvation model in the form of the Gaussian density map is implemented in [42], which extracts triangular and interior/exterior tetrahedral meshes of molecular structures. Generating a high-quality and adaptive unstructured mesh for molecular structures is very important and challenging because of their applications in so many areas.

Since the level-set method was invented by Osher and Sethian [28,29,36], it has been successfully applied to a broad range of problems, such as interface evolution, fluids, materials, combustion, image processing and computer vision, etc.. The level-set method provides a powerful strategy for deforming surfaces, which can easily handle complicated topologies and topologies changing (split apart or merge together), as well as noisy or highly non-uniform data sets. It treats a 3D surface as the level-set of a 3D scalar function, that is, embeds the deformable surfaces as the level surface of a volume, and an evolution equation on the volume governs the behavior of the level surfaces that lie within it. It has a lot of advantages in their applications in 3D graphics. For surface morphing [21, 23, 32], the level-set method can be applied to a wide range of shapes