Segment-based molecular surface remeshing by pattern analysis

In this project we worked on molecular surface remeshing. We have achieved three main goals. First, we investigated the recent challenges in generic surface remeshing via a systematic literature review. We have carried out a comprehensive analysis of 104 articles from the state-of-the-art. The paper is under its revised version with IEEE trans. On Vis. Comp. Graph.

Second, we have presented one paper in the International Conference On Medical Imaging and Computer Aided Diagnosis, held in Oxford UK in January 20 and 21, 2020.

Third, we also have simple yet novel algorithm for angle improvement and valence optimization. The paper is accepted for publication with Computer Graphics International (CGI 2020); and it is also recommended for publication in The Visual Computer Journal (SCI Springer). For valence optimization we remove the bad valence vertices with its neighbor triangle making regular holes in the mesh. The holes are filled in a careful manner to improve their valences as well as angle quality. We also use a segmentation-based surface remeshing which segments the mesh into random segments and then each segment is independently remeshed. In addition, a point insertion scheme is applied to minimize the ratio of obtuse triangles. Experimental results show that our method not only improves the maximal and minimal angles to an angle bound of [30 120] degree but also improves the vertices' regularity, reduces the ratio of obtuse triangles, preserves the area and volume and always succeed with downstream applications.

Surface Remeshing Mesh Generation Molecular surface Computer Graphics Quality Improvement

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Currently, we have reached a significant minimization of the obtuse triangles from the molecular surface meshes. In addition, for valence optimization, our method gives more than 99% of the regular vertices i.e. vertices with valence equal to 5, 6 or 7. The main challenge with molecular meshes is the complexity of the models in size and shape. We have proposed a divide-and-conquer approach that segments the input mesh into segments and each segment is then independently remeshed. Similarly, second challenge was the defective input, which was handled with centroidal Voronoi tessellation initialization and local edge based operation. The results have been improved significantly. However, we are still working to further improve it to eliminate all obtuse triangles. We are also working for parallel processing and GPU implementations.

We are still working on the project for further improvements. Our current goal is the elimination of all obtuse triangles. Then, we will try parallel processing and GPU implementations for efficiency enhancement. Finally, we will focus on end-user tools developments so that our algorithms are deployed to the end-users.

For FY2020, we will need additional resources including GPU system to be used for efficiency enhancement. One conference is accepted so the travel expenses for its presentation in Switzerland is also planned in FY2020.

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Valence optimization for molecular surface remeshing

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