Topological Ball Decomposition of Growing Macromolecules for Fast Visualization by Flow Complexes

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Abstract. Understanding molecular surfaces is essential for computations of chemical and physical properties for protein-protein interactions, especially when the surfaces are defined by the varying isosurfaces of different electron density levels of molecules. Edelsbrunner proposed a new paradigm called the skin surface. We propose to represent such smooth deformable surface by a quadratic complex which is formed by vertices, quadratic curves and patches (triangular and rectangular). The main aim of this paper is to visualize the surface of a macromolecule for real time applications as well as allowing the model to grow for purposes such as changing different radii of the solvents or electron density levels. The approach is to first construct a flow complex consisting of finite and infinite simplices with every simplex intersecting with the skin surface in either an empty set or, in a topological disk for different degrees of growth of the surface model. The construction is efficient and produces a triangulation which is watertight and with no self-intersection. The flow complex provides a frame work that is also general enough for other molecular surface models such as unions of balls, as well as general geometric modelling such as CAD/CAM designs.

Models	Figure no.	# Atoms	DSTA	RDSTA	SFCA	SFC
1j5f	1(a)	357	785s	141s	41s	1.2s
adna	1(b)	490	492s	95s	15s	0.8s
133D	1(c)	292	632s	61s	13s	0.7s
101b	1(d)	556	554s	132s	23s	0.9s
1AIE	1(e)	335	682s	153s	37s	1.0s
1D63	N/A	573	N/A	192s	25s	1.7s
114D	1(f)	488	612s	151s	17s	1.4s
161D	N/A	406	561s	145s	22s	0.9s
1XD7	1(g)	883	N/A	412s	72s	3.1s

Table 1: Comparison with existing algorithms. By taking the average time to compute growing models at 10 different α values, the time for flow complex construction can be ignored. (The label "N/A" indicates a molecule is too large to be computed by that algorithm.)

Implementation and Results. Table 1 lists the experimental results of the examples in Figure 1, along with a comparison with various algorithms to generate the skin surfaces. The table reflects the different results of our skin flow complex algorithm (SFCA), the dynamic skin triangulation algorithm (DSTA) [1] and the restricted Delaunay skin meshing algorithm (RDSMA) [2]. A Pentium 4 2.4GHZ PC with 512MB RAM is used in this test and we construct the skin surfaces of each example in 10 different α values and take the average construction time. Since our goal is to generate growing skin surfaces for real time applications, time is the main criterion in this comparison. By taking the average time to compute growing models at 10 different α values, the time for the flow complex construction shown in the last column of Table 1 becomes insignificant. By comparing the average time for computing a growing molecular model, we observe that our flow complex approach is much faster and outruns the other two algorithms with obviously higher efficiency, especially for the purpose to visualize growing models.

References

[1] H. Cheng. Algorithms for Smooth and Deformable Surfaces in 3D. *Ph.D. Thesis, Computer Science Dept., UIUC., URL: http://www.comp.nus.edu.sg/~hcheng/PhD.pdf*, 2002.

[2] H.-L. Cheng and X.-W. Shi. Quality Mesh Generation for Molecular Skin Surfaces Using Restricted Union of Balls. *Proc. IEEE Visualization*, pages 399–405, 2005.

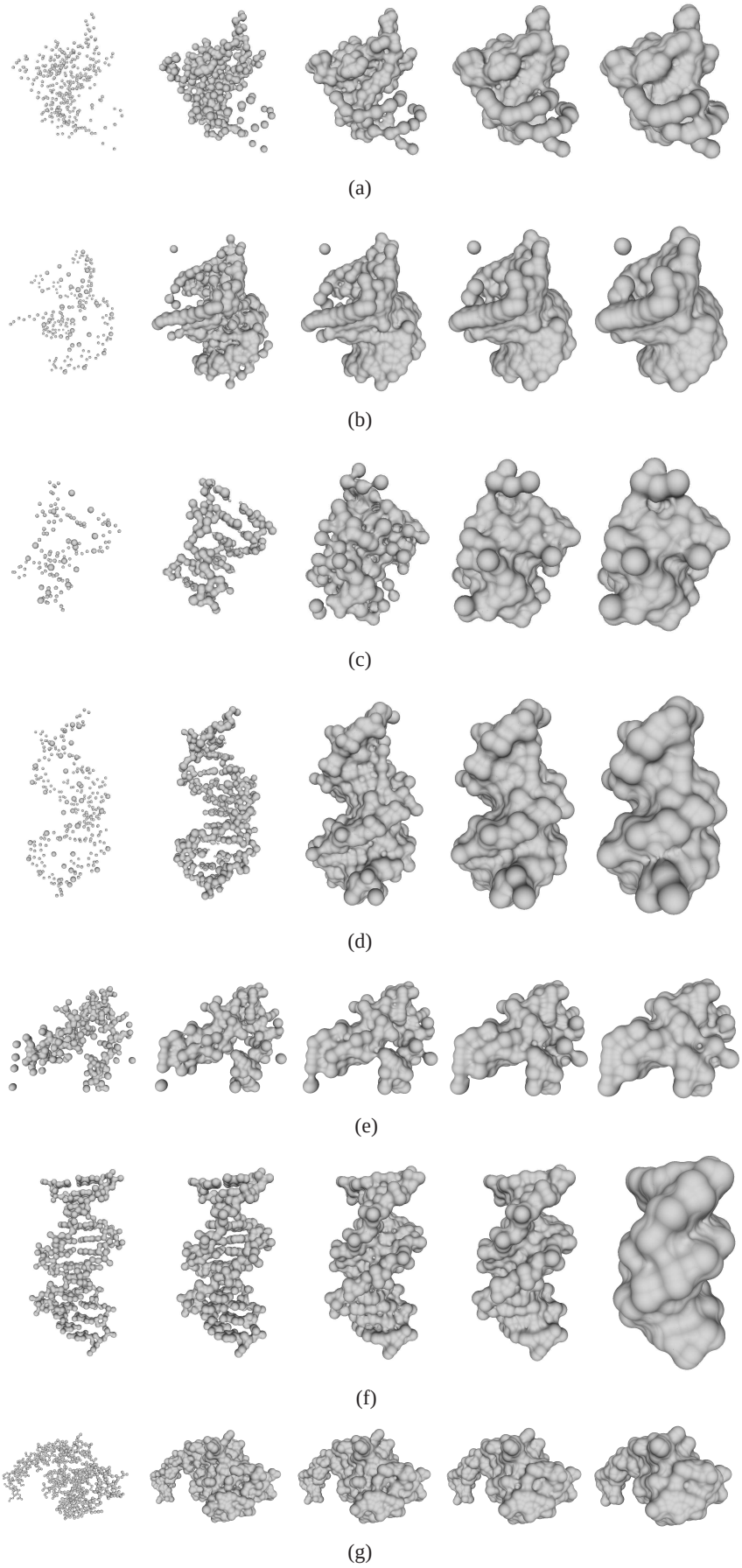

Figure 1: Figure (a) shows the growing skin models of a DNA molecule with PDB ID: 1J5F. Figure (b) shows the growing skin models of "Gramicidin A" molecule. Figure (c) shows the growing skin models of the crystal structured N4-Methylcytosine Guanosin Base-Pairs in a synthetic hexanucleotide. Figure(d) shows the growing skin models of a DNA molecule with PDB ID: 101b.Figures (e-g) show the growing skin models of DNA molecules with PDB IDs: 1AIE, 114D, 1XD7.