Dynamic Maintenance and Visualization of Molecular Surfaces (Extended Abstract)

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The high combinatorial complexity of macromolecules makes it challenging to compute and update their structures and properties in real time. Several different approaches have been developed to achieve this efficiency for molecular surface computations [7]. Other work on surface representations features the use of metaballs, molecular surfaces and blobby models [9]. In this paper we extend this work by describing algorithms that dynamically update and render exact smooth trimmed NURBS (non-uniform rational B-splines) representations for moving or growing the molecular surfaces. Trimmed NURBS are an industry-wide CAD/CAGD standard and fast becoming optimized for graphics rendering software (OpenGL)/hardware [6, 8].

In [1] we present an exact trimmed NURBS boundary representation of the Lee-Richards solvent contact molecular surface [3]. We show in this paper how this trimmed NURBS representation can be efficiently maintained to animate both the solvent accessible surface and the Lee-Richards solvent contact surface of a molecule.

In our approach we combine the use of efficient data structures [4] that have already been shown useful for molecular modeling [5] with the use of standard graphics libraries. The basic idea is to dynamically maintain the primary structures and exactly compute and update representations (tensor product rational B-splines, trimmed NURBS) of the molecular surface which are directly displayed by optimized trimmed NURBS rendering functions of OpenGL. In particular we focus on the special case of dynamic, continuous modification of the solvent radius.

We analyze the complexity of two main classes of updates that yield families of molecular surfaces obtained for different solvent radii: (1) updates that keep the Power Diagram fixed (quadratic growing of the radius of the solvent ball); (2) updates that modify the Power Diagram (linear growing of the radius of the solvent ball). Full details can be found in [2].

In both cases efficiency is achieved through the introduction of a novel geometric construction. In case (1) we use a constructive approach to duality that generalizes the standard "lifting" scheme [4], proving that the Power Diagram of a molecule (3D union of balls) constitutes a compact representation of the collection of all the Power Diagrams of the trimming circles of all the patches in the molecular surface. In particular the cell of the 3D Power Diagram relative to a ball B is the dual of the 2D Power Diagram of the trimming circles of B. As a first approximation (with the bonus of being simpler and more efficient) we consider the molecular surfaces obtained by disproportionally increasing the solvent radius so that the associated Power Diagram remains unchanged. We show how we can keep track of the topological changes that occur in the trimming curves of the patches that form the molecular surface so that its boundary representation can be updated efficiently. Furthermore, we compute and dynamically update an exact boundary representation of the molecular surface so that the same dynamic data-structure is also suitable for molecular modeling operations such as those supporting synthetic drug design.

In previous work on dynamic triangulations the focus has been mostly on the simpler Delaunay/Voronoi structures. Little has been done on the more general case of dynamic Regular Triangulation/Power Diagrams and for dimensions greater than two. Moreover, the kinds of dynamic operations developed are usually insertion/deletion of a single point. Such local operations become inefficient when we need to perform even a simple but global modification. Here we adopt an approach for global modifications where after a preprocessing each patch in the molecular surface is treated independently. By the "dividi et impera" paradigm we achieve the efficiency solving several small problems in place of a single large one.

In the case (2) setting, where the 3D Power Diagram is subject to flips, we use the same construction as in [5] based on the definition of a 4D complex of convex polytopes $\mathcal{C}$ whose "horizontal" slices are all the possible 3D Power Diagrams of the growing balls for any growth factor r. Hence we apply a simple hyperplane sweep algorithm to optimally maintain the dynamic Power Diagram of the linearly growing balls. Thus in this case we exactly compute the offset of the union of balls (so that its topology can be precisely determined), even when it requires a change in the nearest neighbor relations among the atoms corresponding to flips in the associated Regular Triangulation. More in general, for a set of balls in d-dimensional space this requires the construction of a complex of convex polytopes in $(d+1)$-dimensional space whose "horizontal" slices are all the possible Power Diagrams.

In this complex setting we still efficiently update the boundary representation of the dynamic molecular surface. In particular using a well chosen coordinate system we simplify the computation of the trimming curves. For example, the trimming circle for two spheres of radii r_1 and r_2 whose centers are the distance l apart for the solvent radius r is the circle of center $(a_1(r)/a_2(r), 0)$ and radius $[a_1(r)^2 + a_2(r)^2]^{1/2}/a_1(r)$, where $a_1(r) = r_1 + r$ and $a_2(r) = [l^2 + r_1^2 - r_2^2 + 2r(r_1 - r_2)]/(2l)$. In general, we explicitly compute the coordinates of all the control points and weights of the trimming curves in the 2-D parameter space as functions of the solvent radius r.

In either case we prove and also demonstrate via our implementation that: (a) for small solvent radius changes the global topological structure of the molecular surface remains unaltered, requiring scaling and a dynamic maintenance of the arrangement of domain B-spline trimming curves, and (b) for large solvent radius changes the regions in which the eventual updates of the topological structure is required, is also localized. Both of the constructions are defined in general for the union of growing balls in any fixed dimension.

Figure 1 shows a sequence of solvent excluded surfaces obtained for increasing solvent radius. The full animation can be downloaded from: `http://king.ticam.utexas.edu/CCV/VisualEyes/visualization/molecular/Nutrasweet_ConnollySurface/gramicidin.mpg`.

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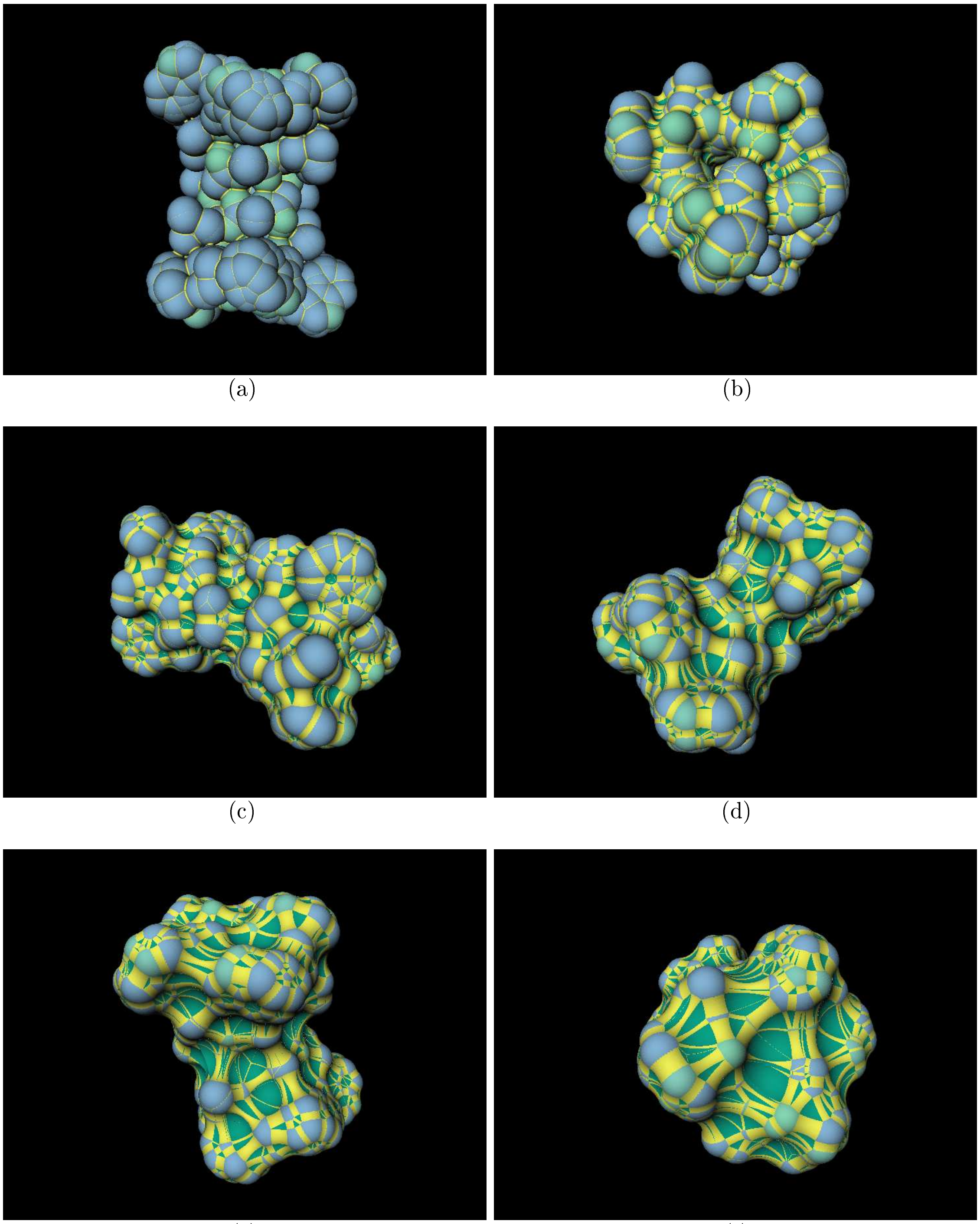

(a) (b) (c) (d) (e) (f)

Figure 1: The solvent excluded surface of the gramicidin molecule obtained with six different solvents of increasing radius.