Bio-Geometric Modeling

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Molecules have forever been modeled geometrically, either as stick-diagrams, emphasizing the covalent bonds between atoms, or as space-filling diagrams, representing the space they occupy. This talk aims at further developing the geometric view of the molecular world. It introduces the filtration of alpha complexes, which are combinatorial objects dual to the space filling diagrams obtained by continuously growing the atom balls. These combinatorial objects lead to fast and robust algorithms for visualization and analysis.

We demonstrate that each space filling diagram is connected the same way as its dual complex, meaning the two are homotopy equivalent. We can therefore express the connectivity of the space filling diagram by the homology groups of the dual complex. We also introduce persistent homology groups to capture the scale-dependence of a topological feature.

We show that the dual complex of a space filling diagram can be used to compute the volume and surface area without constructing the diagram. Similarly, it can be used to compute the weighted area derivative of the surface, which is believed to have a significant contribution to the force that drives the folding process simulated by molecular dynamics.