Klein Bottle Discovered in Molecular Conformation Data

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Sandia and the University of New Mexico recently applied methods from dimension reduction and computational topology to the analysis of molecular conformation data. The data described the conformation of a simple cyclo-octane ring and was initially selected to provide a test bed for the algorithms. This "simple" dataset was discovered to have a surprisingly rich mathematical structure.

The dataset consisted of ~1M points in 72 dimensions, with each point corresponding to a molecular conformation of cyclo-octane (see Figure 1). This dataset was previously thought to have a manifold structure, locally equivalent to a smooth surface. However, we discovered that it in fact had an algebraic structure, smooth almost everywhere, but with singularities in the form of self-intersections. By understanding these self-intersections, we were able to split the algebraic structure into two manifold components (see Figure 2). We used methods from computational topology to identify the components. The first was a sphere, and the second (much to our surprise) was a Klein bottle.

A Klein bottle is a surface with only one side. It is a mathematical object that exists in four dimensions -- any three dimension visualization will have certain artificial singularities (as can be seen in Figure 2). We are currently investigating the physical meaning of this Klein bottle in terms of the molecular conformations.

This is joint work with Shawn Martin (1415), W. Michael Brown (1412), Evangelos Coutsias (UNM), and Jean-Paul Watson (1412).

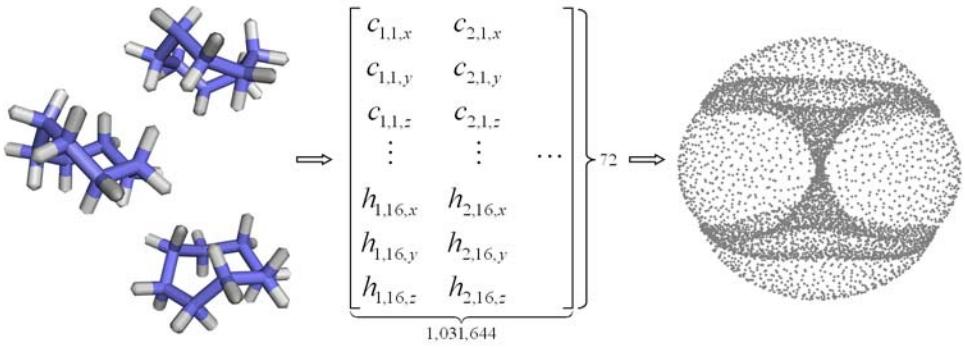

Figure 1. Conformation Space of Cyclo-Octane. The set of conformations of cyclo-octane can be represented as a surface in a high dimensional space. On the left, we show various conformations of cyclo-octane. In the center, these conformations are represented by the 3D coordinates of their atoms. On the right, a dimension reduction algorithm is used to obtain a lower dimensional visualization of the data.

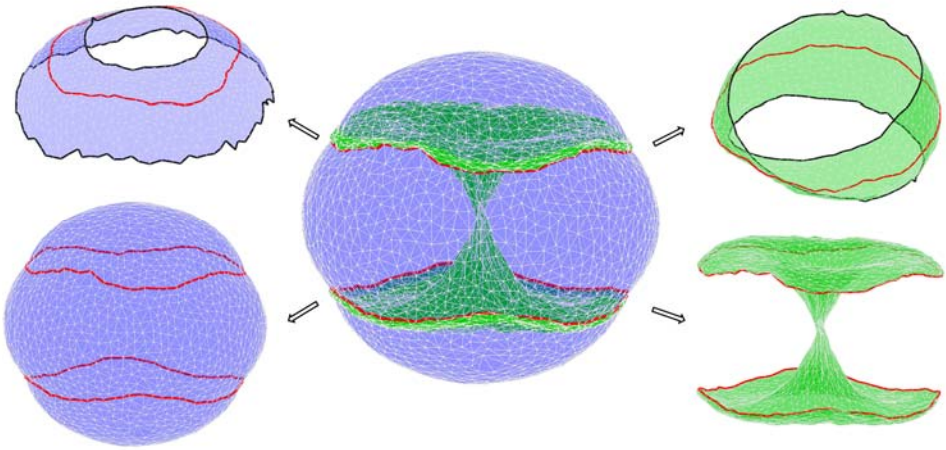

Figure 2. Decomposing Cyclo-Octane. The cyclo-octane conformation space has an interesting decomposition. The local geometry of a self-intersection consists of a cylinder (top left) and a Mobius strip (top right), while the self-intersection is a ring traversing the middle of each object (shown in red). Globally, cyclo-octane conformations can be separated into a sphere (bottom left) and a Klein bottle (bottom right).

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