abstract

Workshop on Topology: Identifying Order in Complex Systems
Topic:

Speaker:

Affiliation:

Date:

Time/Room:

The rapid improvements in computational power have enabled researchers to produce large amounts of molecular simulation data. Hence there is a pressing need to be able to analyze such data to enhance our understanding of molecular dynamics. However, given their massive size and typically high-dimensionality, it is hard to directly traverse and explore these data. In this talk, I will describe our recent work toward building a visualization platform to facilitate interactive exploration of the high-dimensional molecular simulation data. Our tools are based on a topological concept called the contour tree. Specifically, a set of molecular simulation data can be considered as a sample of the so-called protein energy landscape. Using the contour tree idea, we construct a two-dimensional terrain as a metaphor for the high-dimensional protein energy landscape. This two-dimensional terrain preserves certain topological information of the high dimensional landscape, and provides an intuitive environment where users can now easily inspect the high-dimensional data set. I will explain the mathematical ideas behind our tool, the construction of the terrain and the current utilities of our software in the talk.

This is joint work with W. Harvey, I-H. Park, C. Li, O. Rubel, V. Pascucci, and P.-T. Bremer