CIBM SEMINAR SERIES

Computation and **I**nformatics in **B**iology and **M**edicine
Training Program

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Multiscale Surface Techniques: Labeling and Matching the Protein Surface

Abstract:

Protein interactions form the basis for a number of biological processes. Understanding these interactions, and how they arise, is therefore critical to a complete understanding of biology. Our work tackles this challenge on two fronts: by providing better visualizations to help scientists better understand complex proteins, and by providing tools to help identify potential matches for known binding sites.

We begin with the solvent-excluded surface, a mesh that describes the boundary of interaction of the protein with its environment. While the solvent-excluded surface on its own is a valuable tool for understanding protein interaction, its complexity can pose challenges for both visualization as well as analysis. In this talk, we show how by thinking of the surface at multiple scales, we can provide novel solutions to problems in both domains.

In the first half of this talk, we will describe how we can apply high-quality labels to a surface by utilizing a set of simplified proxy surfaces, called "Text Scaffolds". These labels remain close to the region they describe, but are designed for maximum legibility, even on highly complex surfaces, such as those of a protein.

In the second half, we will describe a new multi-scale surface descriptor which can compactly describe regions of the surface of a molecule. We show how simple variants of mesh operations can be used to compute the descriptors without resorting to expensive parameterizations, and additionally provide a statistical approximation at reduced computational cost. We show how these descriptors apply to a number of uses in visualization, analysis, and matching of surfaces, particularly to tasks in protein surface analysis. We describe preliminary results from the use of these descriptors, along with other physio-chemical properties, to find novel binding site matches.

Tuesday, September 15th, 2009

4:00 pm
Biotechnology Center Auditorium
425 Henry Mall