Meeting: 1001, Evanston, Illinois, SS 15A, Special Session on Mathematical Problems in Robotics

1001-92-213 **Michael A. Erdmann*** (me@cs.cmu.edu), Computer Science Department, Carnegie Mellon University, 5000 Forbes Avenue, Pittsburgh, PA 15213. *Protein Similarity from Isotopic Line Weavings.*

Proteins provide a rich domain in which to test theories of shape similarity. Sometimes the detection of common local structure is sufficient to infer global alignment of two proteins; at other times it provides false information. Proteins with very low sequence identity may share large substructures, or perhaps just a central core. There are even examples of proteins with nearly identical primary sequence in which alpha-helices have become beta-sheets.

The thesis of this talk is: Protein similarity detection leads naturally to algorithms operating at the metric, relational, and isotopic scales. Our work introduces a definition of similarity based on atomic motions that preserve local backbone topology without incurring significant distance errors. Similarity detection then seeks rigid body motions able to overlay pairs of substructures, each related by a substructure-preserving motion, without necessarily requiring global structure preservation. This definition is general enough to span a wide range of questions: One can ask for full rearrangement of one protein into another while preserving global topology, as in drug design; or one can ask for rearrangements of sets of smaller substructures, each of which preserves local but not global topology, as in protein evolution. (Received August 26, 2004)