962-92-6 **Bonnie Berger*** (bab@theory.lcs.mit.edu), Lab for Computer Science, NE43-330, Massachusetts Institute of Technology, 545 Tech Square, Cambridge, MA 02139. *Mathematical challenges in protein motif recognition.*

One of the most important and challenging problems in computational biology is that of predicting the three-dimensional structure or shape of a protein from its amino acid sequence. As a first step to tackling this problem, many researchers have focused on the structural motif recognition problem: given a known super-secondary structural motif, or fold family, determine whether this motif occurs in a given amino acid sequence.

In this talk, I will present algorithms that use probabilistic techniques to improve existing methods for recognizing protein structural motifs. We have implemented these algorithms and have tested them on 2-stranded and 3-stranded coiled coils, and recently have adapted them to the less local beta-helical motif.

I will also talk about some of the biological implications of our work. In particular, our programs have been useful in identifying coiled-coil-like motifs in the envelope proteins of many viruses, such as the influenza virus, Moloney murine leukemia virus, HIV, SIV, and visna virus, whose structures have since been solved. This in turn has led to antiviral drug discovery by the Kim lab. Our programs also predict many bacterial proteins of unknown structure that play a role in human infectious disease to be beta helices; these proteins include virulence factors, adhesins, and toxins in pathogenesis, as well as surface proteins from Chlamydia and the intestinal bacterium *Helicobacter pylori.*

(Portions of this work are joint with Peter S. Kim, Ethan Wolf, Mona Singh, David Wilson, Andrea Cochran, Jonathan King, Lenore Cowen, and Phil Bradley.) (Received May 01, 2000)