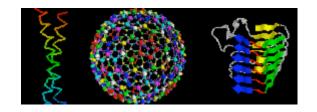
MIT
Department of Mathematics
& The Theory of
Computation Group
At CSAIL



Bioinformatics Seminar

Speaker: Amy Keating, Biology, MIT

Title: Computational Strategies for Predicting and Designing Protein Structure

and Interactions.

Date: Monday, 10 April 2006

Time & Location:

Refreshments: 11 am in the Theory of Computation Lab at MIT's Building 32,

Stata Center Room G-575

Talk: 11:30 am the Theory of Computation Lab at MIT's Building 32, Stata

Center, Room G-575

URL: http://www-math.mit.edu/compbiosem/

Abstract:

High-resolution, physics-based modeling is an important tool for predicting and designing protein structure. However, the extreme complexity of these problems, along with constraints introduced by computational search algorithms, necessitate the use of many approximations. This talk will address some of these, including the use of side-chain rotamers, the use of a fixed backbone, the use of pair-wise decomposable energy functions and issues related to how to model unfolded states. The nature of the problems will be illustrated, and possible solutions will be discussed. Examples will be drawn from the modeling of coiled-coil and Bcl-2 family proteins.

The seminar is co-hosted by Professor Peter Clote of Boston College's Biology and Computer Science Departments and MIT Professor of Applied Math Bonnie Berger. Professor Berger is also affiliated with CSAIL & HST.

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