



## Bioinformatics Seminar

---

Speaker: Oliver Brock, UMASS Amherst

Title: Re-thinking Conformation Space Search for Protein Structure Prediction

Date: Monday, 14 November 2005

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:

The protein structure prediction problem remains one of the great challenges in molecular biology. It sometimes is referred to as the second half of the Human Genome Project, since knowledge of the structure of proteins encoded in the genome can lead to an understanding of cellular processes. Currently, there are two competing views on how the protein structure prediction problem may be solved. The NIH-funded Protein Structure Initiative (PSI) relies on structural genomics, a combination of experimental techniques and homology modeling. The alternative view attempts to predict the structure of proteins entirely based on computation. In this talk, I will argue that, despite the progress made in the PSI, computational methods are likely to play an important role in addressing the protein structure prediction problem. I will also present our recent work in efficient conformation space search. Due to the enormous size of conformation space, this search is currently believed to be the primary obstacle on the path towards accurate computational protein structure prediction. We exploit recent insights from machine learning and robot motion planning to render this search more effective. Our approach improves the Monte Carlo approach, which has been used for conformation space search almost exclusively for over 50 years.

---

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.

Massachusetts Institute  
of Technology  
77 Massachusetts Avenue  
Cambridge, MA 02139

*For General Questions, please contact [kvdickey@mit.edu](mailto:kvdickey@mit.edu)*