

# Center for Biocomplexity Colloquium

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***“Advanced Optimization and Sampling Strategies in  
Structural Biocomputing”***

Thursday November 6, 2008

4:00pm

184 Nieuwland Science Hall

*\*Tea at 3:30pm in 257 Hurley\**

Effective exploration of complex high dimensional energy surfaces is among the most severe limiting factors encountered in any in silico investigations performed on biological systems. The development of novel optimization algorithms capable of leading coarse-grained or atomistic simulation into the era of systems biology research will require the synergetic adaptation of many methods and concepts. Significant challenges must be met and success is not entirely at hand.

In this talk we overview the most relevant factors that significantly limit the scope of computational investigations in structure based biocomputing. Then we walk through some of our state of the art approaches that are designed to eliminate these limitations. In particular both essential dimensionality and optimization/sampling algorithms will be addressed and combined to lead towards novel simulation protocols. Finally we will briefly overview some of the past, present and future applications.