

Center for Biocomplexity Colloquium

John Chodera

**California Institute for Quantitative Biosciences (QB3)
University of California, Berkeley**

“How do Biomolecules move?”

Tuesday, April 6, 2010

4:00pm

117 Hayes-Healy Hall

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

Abstract: Biological macromolecules, like proteins and nucleic acids, are the elementary molecular machines in all living things. While an impressive variety of biophysical techniques are now available to probe how they move and interact, fundamental physical limitations mean that the information obtained from such experiments will always be indirect, requiring additional interpretation in order to understand the essential details of how molecular motions and interactions, and how these are perturbed in disease states.

I will illustrate how we are developing powerful new techniques based on discretization of the transfer operator and Markov chains that allow us to use atomistic molecular dynamics simulations -- typically only able to describe the behavior of single molecules over nanoseconds -- to understand the statistical behavior of many molecules over microseconds or longer. Using IBM Blue Gene, the Folding@Home worldwide distributed computing project, and the computational speed boost provided by graphics processing units (GPUs), we are able to probe fundamental biophysical processes such as protein folding and ligand binding, with the eventual goal of contributing to the rational design of new therapeutic agents.

Short Bio: John Chodera is a Distinguished Postdoctoral Fellow with the California Institute for Quantitative Biosciences (QB3) at the University of California, Berkeley. After receiving a B.S. in Biology from Caltech, he received his doctorate in Biophysics with Ken Dill at the University of California, Berkeley, and spent two years in the lab of Vijay Pande at Stanford (head of the Folding@Home project) as a postdoctoral researcher. His interests include the development of efficient algorithms and use of high-performance and distributed computing for the study of biomolecular systems, as well as the development of new algorithms for rational drug design and the emergence of resistance mutations.