

Dmitry A. Kondrashov, Ph.D.CIBM Postdoctoral Fellow
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University of Wisconsin-Madison***Optimization and Evaluation of Simple
Models of Protein Motion
Using X-Ray Crystal Data******Abstract:***

Fluctuations of proteins near their native conformations play important roles in function. Simple coarse-grained models, such as the Gaussian Network Model, have been shown to capture some of the features of equilibrium protein dynamics. We extend this model to include more than one interaction parameter between residues, by using B factors from over 100 ultra-high resolution X-ray crystal structures to optimize the interaction parameters. Adding a single parameter to the model results in substantial improvement of the prediction. We also analyze simple models that include directions of motion and validate their predictions against anisotropic B-factors. We find that two models, Anisotropic Network Model and Block Normal Modes, show substantial agreement with experiments. Applications of the methods to prediction of functionally relevant protein motion will be illustrated.

**Tuesday, November 29th
4:00 p.m.**Auditorium (Room 1111)
Genetics/ Biotechnology Center
425 Henry Mall