

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Intermediate Resolution Models and Protein Folding and Allostery¹ ABHIJEET KAPOOR, Iowa State University, ALEX TRAVESSET, Iowa State University and Ames Lab — Intermediate Resolution Models (IRM)s model proteins with nearly all atom precision but consider solvent implicitly, and treat electrostatics as short-range interactions. In this talk, we describe a new IRM. We discuss its differences from other existing IRMs and test it again a set of 13 proteins. The model successfully folds 12 of them into its native state, starting from a random configuration. The stability of the native state versus other states with different topologies (arrangement of the secondary structure) is also discussed. Implications for general protein motion are also presented.

¹This work is supported by NSF, through grant DMR-0748475.

Alex Traveset
Iowa State University and Ames Lab

Date submitted: 18 Nov 2012

Electronic form version 1.4