Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Generalized rules for the optimization of elastic network models
TIMOTHY LEZON, ERAN EYAL, IVET BAHAR, University of Pittsburgh —
Elastic network models (ENMs) are widely employed for approximating the coarse-grained equilibrium dynamics of proteins using only a few parameters. An area of current focus is improving the predictive accuracy of ENMs by fine-tuning their force constants to fit specific systems. Here we introduce a set of general rules for assigning ENM force constants to residue pairs. Using a novel method, we construct ENMs that optimally reproduce experimental residue covariances from NMR models of 68 proteins. We analyze the optimal interactions in terms of amino acid types, pair distances and local protein structures to identify key factors in determining the effective spring constants. When applied to several unrelated globular proteins, our method shows an improved correlation with experiment over a standard ENM. We discuss the physical interpretation of our findings as well as its implications in the fields of protein folding and dynamics.

Timothy Lezon
University of Pittsburgh

Date submitted: 20 Nov 2008 Electronic form version 1.4