Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Frustration in protein elastic network models[1] TIMOTHY LEZON, IVET BAHAR, Department of Computational Biology, University of Pittsburgh — Elastic network models (ENMs) are widely used for studying the equilibrium dynamics of proteins. The most common approach in ENM analysis is to adopt a uniform force constant or a non-specific distance dependent function to represent the force constant strength. Here we discuss the influence of sequence and structure in determining the effective force constants between residues in ENMs. Using a novel method based on entropy maximization, we optimize the force constants such that they exactly reporduce a subset of experimentally determined pair covariances for a set of proteins. We analyze the optimized force constants in terms of amino acid types, distances, contact order and secondary structure, and we demonstrate that including frustrated interactions in the ENM is essential for accurately reproducing the global modes in the middle of the frequency spectrum.

[1]This research was funded by NIH grant 5R01 GM086238-02.

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Date submitted: 18 Nov 2009 Electronic form version 1.4