Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Mimicking the folding pathway to improve homology-free protein structure prediction KARL FREED, JOE DEBARTOLO, ANDRES COLUBRI, University of Chicago, ABHISHEK JHA, MIT, JAMES FITZGERALD, Stanford University, TOBIN SOSNICK, University of Chicago — Since demonstrating that a protein's sequence encodes its structure, the prediction of structure from sequence remains an outstanding problem that impacts numerous scientific disciplines including many genome projects. By iteratively fixing secondary structure assignments of residues during Monte Carlo simulations of folding, our coarse grained model without information concerning homology or explicit side chains outperforms current homology-based secondary structure prediction methods for many proteins. The computationally rapid algorithm using only single residue (phi, psi) dihedral angle moves also generates tertiary structures of comparable accuracy to existing all-atom methods for many small proteins, particularly ones with low homology. Hence, given appropriate search strategies and scoring functions, reduced representations can be used for accurately predicting secondary structure as well as providing three-dimensional structures, thereby increasing the size of proteins approachable by homology-free methods and the accuracy of template methods whose accuracy depends on the quality of the input secondary structure. Inclusion of information from evolutionarily related sequences enhances the statistics and the accuracy of the predictions.

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Date submitted: 01 Dec 2009 Electronic form version 1.4