Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

AWSEM-MD: Coarse-grained Protein Structure Prediction Using Physical Potentials and Bioinformatically Based Local Structure Biasing ARAM DAVTYAN, University of Maryland at College Park, WEIHUA ZHENG, NICK SCHAFER, University of California at San Diego, CECILIA CLEMENTI, PETER WOLYNES, Rice University, GAREGIN PAPOIAN, University of Maryland at College Park, PAPOIAN GROUP TEAM, WOLYNES GROUP COLLABORATION — The Associative memory, Water mediated, Structure and Energy Model (AWSEM) is a coarse-grained protein model. When combined with a sequence alignment method, AWSEM can be used to perform de novo protein structure prediction. Herein we present structure prediction results for a particular choice of sequence alignment method based on short residue sequences called fragments. We demonstrate the model's structure prediction capabilities for three variants on a standard sequence alignment protocol, all of which assume that the structure of the target sequence is not known. We show that the inclusion of structures from homologous sequences in the fragment memory search improves structure prediction only marginally. However, when the fragment search is restricted to only homologous sequences, AWSEM can perform high-resolution structure prediction.

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Date submitted: 10 Nov 2011 Electronic form version 1.4