High-resolution Prediction and Refinement of Protein Structures

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***Short Abstract* — A precise understanding of cellular regulatory system hinges on an accurate prediction of protein structures. Although protein structures can be solved experimentally, *de novo* predictions by computers will be much cheaper. However, high-resolution predictions of protein structures have been challenging throughout the history. Recently, we have implemented multiple methods to achieve correct folds of proteins using AWSEM, a coarse-grained model feasible for personal computers. Based on our initial predictions, atomistic simulations were used to further refine the model prediction. Our results show a further improvement over existing methods and indicate a new avenue for the prediction of protein structures.**

***Keywords* — Structure Prediction, AWSEM, Refinement.**

A precise understanding of cellular regulatory system hinges on an accurate description of the functions of the participating proteins, which in turn, relies on an accurate prediction of protein structures. Although protein structures can be solved experimentally, an accurate *de novo* prediction of protein by computers will be much more feasible and cheaper. However, a high-resolution prediction of protein structures has been challenging throughout the history of protein folding studies [1]. Especially, to reach a high-resolution structure, expensive computational resources are needed [2, 3]. Recently, we have implemented multiple methods to achieve high-resolution structures of proteins using AWSEM (The associative memory, water mediated, structure and energy model) [4, 5, 6], a coarse-grained model that is computationally manageable for personal computers. Our initial predictions already reach sub-angstrom regime in the best cases. Based on our first-level predictions, atomistic simulations with multiple enhance-sampling techniques were used to further refine the model predictions. Our results show a further improvement over the existing methods, and indicate a new avenue for the prediction of protein structures.

Acknowledgements: This work was funded by NSF (Grant PHY-1427654).

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