Abstract Submitted
for the 4CF15 Meeting of
The American Physical Society

Partial Unfolding and Refolding for Structure Refinement: A Unified Approach of Geometric Simulations and Molecular Dynamics[1] PAUL CAMPITELLI, AVISHEK KUMAR, BANU OZKAN, MICHAEL THORPE[2], Department of Physics and Center for Biological Physics, Arizona State University, OZKAN GROUP TEAM — The most successful protein structure prediction methods to date have been template-based modeling (TBM) or homology modeling, which predicts protein structure based on experimental structures. These high accuracy predictions sometimes retain structural errors due to incorrect templates or a lack of accurate templates in the case of low sequence similarity, making these structures inadequate in drug-design studies or molecular dynamics simulations. We have developed a new physics based approach to the protein refinement problem by mimicking the mechanism of chaperons that rehabilitate misfolded proteins. The template structure is unfolded by selectively (targeted) pulling on different portions of the protein using the geometric based technique FRODA, and then refolded using hierarchically restrained replica exchange molecular dynamics simulations (hr-REMD).

[1]Partial Unfolding and Refolding for Structure Refinement: A Unified Approach of Geometric Simulations and Molecular Dynamics
[2]Rudolf Peierls Center for Theoretical Physics, University of Oxford

Paul Campitelli
Department of Physics and Center for Biological Physics, Arizona State University

Date submitted: 09 Sep 2015 Electronic form version 1.4