Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Systematic Coarse-Graining of Peptides to Understand their Effective Molecular Interactions LUCA LARINI, GREGORY A. VOTH, Center for Biophysical Modeling and Simulation and Department of Chemistry, University of Utah, Salt Lake City, UT, 84112, USA — The process of building reliable coarse-grained models is a major challenge for both theory and simulation. Force matching is a systematic method to produce quantitatively accurate coarse-grained potentials from atomistic simulation data. This method provides a sound theoretical background that can also be used to gain deeper insight into the system under examination. In this way, force matching can be employed as a tool for analysis. Application to a simple biological molecule will be described in order to gain a better understanding of the effective forces acting on the system.

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Date submitted: 02 Dec 2008 Electronic form version 1.4