

Abstract Submitted  
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**Investigating the impact of representation upon coarse-grained models**<sup>1</sup> THOMAS FOLEY<sup>2</sup>, Pennsylvania State University, M SCOTT SHELL<sup>3</sup>, University of California, Santa Barbara, WILLIAM NOID<sup>4</sup>, Pennsylvania State University — The first step in building a coarse-grained (CG) model is choosing a representation or ‘mapping’ of the original system at a reduced resolution. In practice, the mapping is often chosen on the basis of ‘physical intuition.’ Consequently this crucial step would greatly benefit from the development of systematic and principled methodologies. Accordingly, we have studied the relationship between the mapping and the resulting CG model. As a starting point, we have analytically derived, as a function of the CG mapping, the exact many-body potential of mean force (PMF) for the simple Gaussian Network Model (GNM) of protein fluctuations. We use this as a simple model for investigating the effect of the CG mapping upon the information loss and quality of the CG model. Moreover, by considering the GNM’s for different proteins, we investigate the significance of high resolution structural features for the quality of the CG model.

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<sup>2</sup>Department of Physics and Chemistry

<sup>3</sup>Department of Chemical Engineering

<sup>4</sup>Department of Chemistry

Thomas Foley  
Pennsylvania State University

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