Abstract Submitted
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**The impact of resolution upon the complexity, information, thermodynamics, and transferability of coarse-grained models**[1] THOMAS FOLEY, Pennsylvania State University, M. SCOTT SHELL, University of California, Santa Barbara, WILLIAM NOID, Pennsylvania State University, NOID/SHELL TEAM — By eliminating atomic degrees of freedom, coarse-grained (CG) models allow highly efficient simulations of complex phenomena. However, as a consequence of changing the model resolution, the coarse-graining procedure alters the apparent thermodynamic properties and model transferability. The present work analyzes the effects of model resolution upon the exact many-body potential of mean force (PMF), $W$, and, in particular, its entropic component, $S_W$. We demonstrate that $S_W$ quantifies the loss of information from the atomistic model and impacts the complexity, thermodynamics, and transferability of the CG model. In order to investigate these formal results, we analytically calculate the exact PMF for the popular Gaussian Network Model of proteins and quantify both the energy-entropy balance as well as the entropic contribution to intramolecular interactions as a function of resolution. Interestingly, seven diverse proteins demonstrate strikingly similar shifts in energy-entropy balance with decreasing model resolution. We expect that these results may provide general insight into both the thermodynamic properties and transferability of coarse-grained models for soft materials.

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Thomas Foley
Pennsylvania State University

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