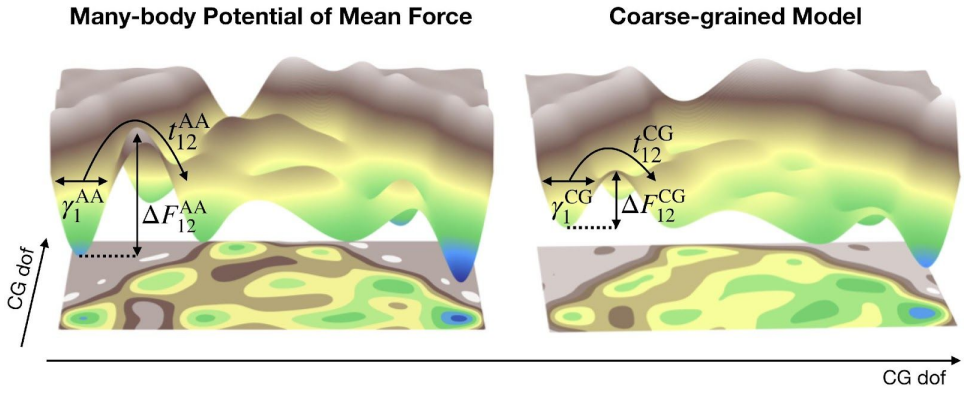
Systematic Coarse-graining

While atomically-detailed molecular simulations have emerged as powerful computational tools for studying specific soft matter systems, lower-resolution models are required to reach experimentally-relevant length and time scales. These coarse-grained (CG) models are not only more efficient, but also provide insight into the essential driving forces for particular phenomena. We develop methodologies for constructing accurate and transferable models, both from the ``bottom up''---targeting features of an underlying reference model---and from the ``top down''---reproducing particular experimental observables.



The removal of degrees of freedom from the system modifies the relationship between the relative time scales of distinct dynamical processes through both a loss of friction and a “smoothing” of the free-energy landscape (see Figure, Rudzinski, J.F. Computation 7(3), 42 (2019)). While these effects typically result in faster dynamics, decreasing the computational expense of the model, they also obscure the connection to the true dynamics of the system. The lack of consistent dynamics is a serious limitation for CG models, which not only prevents quantitatively accurate predictions of dynamical observables but can also lead to qualitatively incorrect descriptions of the characteristic dynamical processes. We have been developing methods that attempt to construct CG models with consistent dynamical properties.