

SELECTION, CALIBRATION, AND VALIDATION OF COARSE-GRAINED MODELS OF ATOMISTIC SYSTEMS IN THE PRESENCE OF UNCERTAINTIES

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The enormous size and complexity of atomistic MD models needed to capture important biological and manufacturing processes that occur on microscopic scales far exceeds the capacity of today's largest supercomputers or even those envisioned decades into the future. Thus, methods for reducing the number of degrees of freedom of atomistic models is viewed as a necessary approach to MD-studies. These aggregated lower-dimensional models that function on coarser spatial scales are called **coarse-grained** (CG) models.

In this study, we develop theories and methods for selection, calibration, and validation of coarse grained models of atomistic systems. As a starting point, a so-called all-atom (AA) model of a material body is defined. From there, we develop basic principles for developing CG based on Bayesian methods of statistical calibration, information theory, and methods of model selection that employ Bayesian notions of model plausibility.

While each step in the coarse-graining process can introduce significant uncertainties in the target predictions, these principles will provide a unified framework for assessing the predictability of CG models and for systematically addressing issues of model calibration, validation, and the quantification of uncertainty in quantities of interest. Applications to representative molecular models, including polymers used in nano-manufacturing processes, are presented.