Adaptive Validation and Error Estimation of Coarse-Grained Models of Atomic Systems

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Model validation in the presence of uncertainties in observational data, in parameters, and due to the generally subjective process of selecting the model itself, lies at the very foundations of the scientific method. Scientific knowledge is acquired through observations of physical events and through the development of scientific hypotheses on the causes of the events. The former requires the acquisition of relevant observational data and the latter are the consequences of inductive logic leading to mathematical and computational models, the validity of which must be tested against experiments or observations.

In this lecture, we consider issues of model selection and validation in connection with the coarse graining of atomic systems: the creation of models of atomistic systems by aggregating clusters of atoms into “beads” or “super atoms”, so as to dramatically reduce the number of degree of freedom and also to extend time scales in which physical quantities of interest can be observed. The overriding issues in developing coarse-grained (CG) models are how accurately they approximate key quantities of interest captured by the all-atom (AA) system; that is, is the CG model valid in some sense, and more fundamentally, how does one select the CG model itself to faithfully represent relevant properties of the AA model? We describe a general Bayesian framework for model selection and validation for coarse-grained molecular models. An adaptive algorithm is presented for model selection and validation in the presence of uncertainties. Examples are presented for representative polymeric structures. In addition, a posteriori error estimates are derived for errors created inherent in coarse-grain models.