

Abstract: Issues in modeling and simulation of reduced-order models include model selection, calibration, validation, and error estimation, all in the presence of uncertainties in the data, prior information, and the model itself. These issues are addressed via the Occam-Plausibility ALgorithm (OPAL), which chooses, among a large set of models, the simplest valid model that may be used to predict chosen quantities of interest. An illustrative example application to coarse-grained models of atomistic polyethylene is given.