Quantification and prediction of uncertainty in coarse-grained models of molecular simulations

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The work presented here is motivated by the need for compact representations of many-body stochastic molecular simulations, for use in engineering tasks such as process design and feedback control. Applications from polymer reaction and thin film deposition will be used to motivate the problem and demonstrate the methods. The major topic of this talk is the quantification and prediction of uncertainty in reduced order models of molecular simulations. While coarse-graining provides a method for computational reduction, this introduces error into the reduced order model. An approach based on spatial statistics will be presented, as a means to understand and predict model error so that these reduced order models can be used with confidence for design and control.