PROBABILISTIC COARSE-GRAINING: FROM MOLECULAR DYNAMICS TO STOCHASTIC PDES

*M. Schöberl, C. Grigo, N. Zabaras, P.S. Koutsourelakis**

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Summary

The present paper is concerned with two problems in physical modeling for which dimensionality reduction is of paramount importance: a) coarse-graining (CG) of atomistic ensembles, and b) the construction of reduced-order (RO) models for the solution of PDEs with high-dimensional stochastic inputs. We demonstrate that both problems can be cast in a similar formulation and propose a generative probabilistic model in which the latent variables provide the coarse-grained or reduced-order description of the original system. A central component is the definition of a tunable coarse-to-fine probabilistic map (rather than fine-to-coarse maps that are generally employed) which relates the latent variables with the outputs/responses of the reference model. This implicitly defines the coarse-grained/reduced description and provides a vehicle for making predictions of the fine-scale/full-order observables. As a result, the identification of the coarse-grained/reduced description is simultaneously performed with the discovery of the CG/RO model. The probabilistic formulation accounts for a significant source of uncertainty that is often neglected in such tasks i.e. the information loss that unavoidably takes place in the coarse-graining process.

Additional details

Molecular dynamics simulations [1] are nowadays commonplace in physics, chemistry and engineering and represent one of the most reliable tools in the analysis of complex processes and the design of new materials [6]. Direct simulations are hampered by the gigantic number of degrees of freedom, complex, potentially long-range and high-order interactions, and as a result, are limited to small spatio-temporal scales with current and foreseeable computational resources. One approach towards making complex simulations practicable over extended time/space scales is coarse-graining (CG) [13]. Coarse-graining methods attempt to summarize the atomistic detail in the fine-grained (FG) description in fewer degrees of freedom which in turn lead to shorter simulation times, with potentially larger time-steps and enable the analysis of systems that occupy larger spatial domains. Generally the construction of coarse-grained description is based on physical insight and localized lumping of several atoms into larger pseudo-molecules.

Another popular set of models encountered in continuum thermodynamics involve PDEs. Many problems of significant engineering interest, such as as flow in porous media or the mechanical properties of composite materials, exhibit random, fine-scale heterogeneity which needs to be resolved giving rise to very large systems of algebraic equations upon discretization. Pertinent solution strategies, at best (e.g. multigrid methods) scale linearly with the dimension of the unknown state vector. Despite the ongoing improvements in computer hardware, repeated solutions of such problems, as is required in the context of uncertainty quantification (UQ), poses insurmountable difficulties. It is obvious that viable strategies for these problems, as well as a host of other deterministic problems where repeated evaluations are needed such as inverse, control/design problems etc, should focus on constructing solvers that exhibit *sublinear* complexity with respect to the dimension of the original problem [10]. In the context of UQ a popular and general such strategy involves the use of surrogate models or emulators which attempt to learn the input-output map implied by the full-order (FO) model. Such models, e.g. Gaussian Processes [2], polynomial chaos expansions [4], (deep) neural nets [3] and many more, are trained on a finite set of full-order model runs. Nevertheless, their performance is seriously impeded by the curse of dimensionality, i.e. they usually become inaccurate for input dimensions larger than a few tens or hundreds, or equivalently, the number of FO model runs required to achieve an acceptable level of accuracy grows exponentially fast with the input dimension.

The present work is motivated by the following, common questions:

- What are good coarse-grained variables (how many,

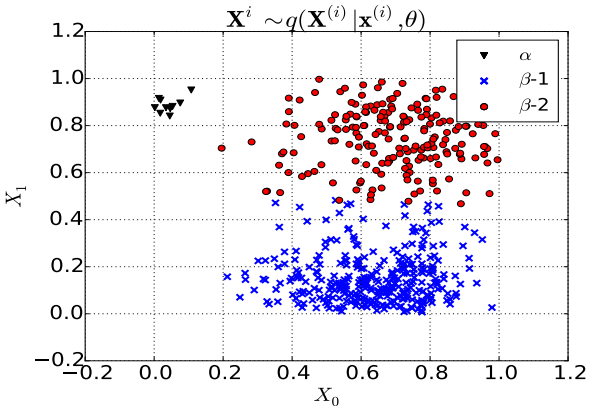

Figure 1: Visualization in two-dimensional (latent) CG-variable space of three alanine dipeptide conformations.

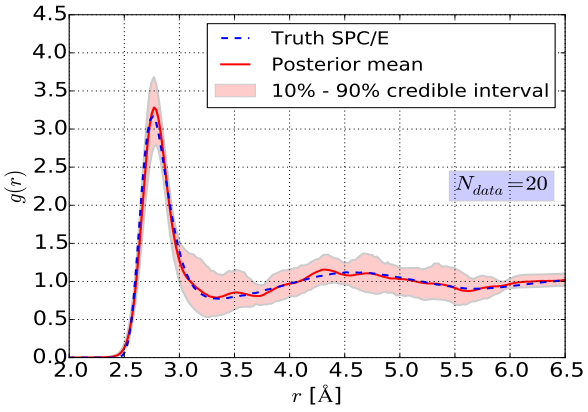

Figure 2: Prediction of Radial Distribution Function $g(r)$ using proposed CG model of SPC/E water trained with 20 FG realizations (posterior mean and quantiles) [11].

how are they related to the FG/FO description)?

- Given such a set, what is the right model for them?
- Given a good such model, how much can one predict about the evolution of the reference FG/FO system (reconstruction)?
- How much information is lost during the coarse-graining/reduction process and how does this affect predictions produced by the reduced model?
- Given finite simulation data at the fine-scale, how (un)certain can one be in their predictions?

To address these questions, we propose data-driven, generative probabilistic graphical models that are simultaneously capable of identifying a set of dimension-reduced variables as well as a CG/RO model (Figure 1). They also obviate the definition of restriction and lifting operators in the context of multiscale problems [8]. We demonstrate how such models can be trained using Stochastic Variational Inference techniques [5] in combination with Stochastic Optimization tools [7]. Even in the context of scarce FG/FO data, they can accurately identify CG/RO descriptions and produce predictive *probabilistic* estimates for any observables of the fine-grained (FG) or full-order (FO) models (Figure 2).

A critical question that is simultaneously addressed with the dimensionality reduction, is the construction of appropriate CG/RO models. The structural form of these models as well as the types of relations they imply, provide critical insight into the salient physical mechanisms that control emergent behavior. In the context of atomistic simulations, such models control the type and order of interactions between CG variables. In the case of stochastic PDEs, these relate to the microstructural features of the underlying random medium that are predictive of the FO response [12]. We follow two alternative strategies. In the first, we employ a rich set of feature functions in combination with sparsity-enforcing priors [9]. As a result we are capable bypassing a combinatorially large search through all possible candidate models. The second method employs a greedy, adaptive strategy by which feature functions/filters are learned and sequentially added in the construction of the CG/RO model.

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