

Abstract Submitted  
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**Uncertainty Quantification in MD Simulations: Forward Propagation and Parameter Inference**<sup>1</sup> FRANCESCO RIZZI, OMAR KNIO, Johns Hopkins University, HABIB NAJM, BERT DEBUSSCHERE, KHACHIK SARGSYAN, MAHER SALLOUM, HELGI ADALSTEINSSON, Sandia National Laboratories — This work focuses on quantifying uncertainty in molecular dynamics (MD) simulations accounting for both intrinsic noise and parametric uncertainty. We consider isothermal, isobaric MD simulations of TIP4P water at ambient conditions. Due to the thermal noise in the system, this yields non-deterministic, noisy predictions for the water observables. Selected macroscale observables are expressed in terms of polynomial chaos (PC) expansions using both a non-intrusive spectral projection (NISP) and Bayesian inference approach. We show that the effect of the thermal noise can be controlled, and that the two methods yield similar results. We illustrate the possibility of determining or refining a set of force-field parameters for water using a reformulated Bayesian approach based on PC expansions. We present a synthetic problem where presumed “true” values of the TIP4P model parameters are used to generate a collection of noisy data of selected water observables. Exploiting the PC representation, we show how the “true” force-field parameters can be accurately and efficiently recovered using low-order surrogate models.

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