Uncertainty Quantification in Molecular Dynamics Simulations: Forward and Inverse Problem

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Abstract
Molecular dynamics (MD) is widely employed in both industrial and academic environments, playing a key role in the study of a variety of systems, ranging from liquids to solids, as well as biomolecules, such as proteins and nucleic acids (DNA, RNA). MD simulations provide a suitable and convenient method to explore the dynamical properties of a system at the atomic level which, in general, are difficult and expensive to investigate experimentally. The main weakness of MD, however, is that the reliability of its predictions strongly depends on the accuracy with which the potential function used to compute the forces can model the atomic interactions occurring in the real system of interest. Consequently, defining the potential is the most delicate stage of an MD simulation. Typically, MD potentials are formulated in terms of two-body or many-body contributions, long range and short-range terms, each requiring a suitable functional form. For many systems, literature shows that MD potentials are characterized by broad uncertainties, thus making them a key source of uncertainty.

This talk discusses the application of uncertainty quantification (UQ) methods to MD simulations. Two fundamental, distinct sources of uncertainty are investigated in this work, namely parametric uncertainty and intrinsic noise. Intrinsic noise is inherently present in the MD setting, due to fluctuations originating from thermal effects. Parametric uncertainty, on the contrary, is introduced in the form of uncertain potential parameters, geometry, and/or boundary conditions. The UQ problem is presented in both its main components, namely the forward propagation, which aims at characterizing how uncertainty in model parameters affects selected observables, and the inverse problem, which involves the estimation of target model parameters based on a set of observations. The talk highlights the challenges arising when parametric uncertainty and intrinsic noise combine to yield non-deterministic, noisy MD predictions of target macroscale observables. Polynomial Chaos (PC) expansions and Bayesian inference provide us the tools to develop a framework enabling us to isolate the impact of parametric uncertainty on the MD predictions and, at the same time, properly quantify the effect of the intrinsic noise. Systematic applications to a set of problems of various complexity leads to the observation that an uncertain PC representation built via Bayesian regression is the most suitable model for the representation of uncertain MD predictions of target observables in the presence of intrinsic noise and parametric uncertainty.

Biography
Francesco Rizzi received his Bachelor Degree in Environmental Engineering in 2007, and M.Sci. in Computational Physics in 2009, both from the University of Udine, Italy. He then moved to Johns Hopkins University, where he obtained a M.Sci. and Ph.D. in Mechanical Eng. in 2012. He is currently a postdoc at Sandia California. Prior to joining Sandia, he worked as a postdoc in the Dept. of Mechanical and Materials Science at Duke University. Main research interests include resilience, uncertainty quantification, fluid mechanics, high-performance computing and molecular dynamics.