Special Colloquium

UCR

Mathematics

Department

DR. HUAN LEI

PACIFIC NORTHWEST NATIONAL LABORATORY

"DATA-DRIVEN APPROACHES TO QUANTIFY QUASI-EQUILIBRIUM AND NON-EQUILIBRIUM DYNAMICS FOR MULTIPHYSICS BIOSYSTEMS"

One of the grand challenges of modeling multiphysics biosystems roots in the multifaceted amorphous nature of these systems. Traditional computational approaches developed on isolated scales, or coupled between phenomenological descriptions with ad hoc scale separation show limitations due to lack of universal field variables of such systems. We propose a data-driven method to quantify quasi-equilibrium and non-equilibrium properties for complex physical systems with high dimensional stochastic space based on generalize polynomial chaos (gPC) expansion and Mori-Zwanzig projection method. To alleviate the high -dimensionality, we propose a numerical method to enhance the sparsity by defining a set of collective variables within active subspace, which enable us to accurately quantify the quasi-equilibrium properties with respect to the amorphous states where traditional approaches such as sparse grid method shows limitation therein. Moreover, non-equilibrium properties further depends on the non-local memory term arising from the high-dimensional unresolved states. We propose a data-driven method based on appropriate parameterization to compute the memory kernel of the generalized Langevin Equation (GLE). The approximated kernel formulation satisfies the second fluctuation-dissipation conditions with consistent invariant measure. The proposed method enables us to characterize transition properties such as reaction rate where mean field approximation shows limitation.

Wednesday, February 15th, 2017

Room 284, the 2nd Floor of the Surge Building

Tea Time @ 3:40 p.m.

Talk Begins @ 4:10 p.m.

Ends @ 5:00 p.m.

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