Computational Mathematics Seminar Series

Quantifying Quasi-equilibrium and Non-equilibrium Properties for Complex Multiphysics Systems

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Digital Media Center 1034
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Abstract:
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. For quasi-equilibrium properties, we demonstrate that sparse grid method suffers instability problem due to the high-dimensionality. Alternatively, we
propose a numerical method to enhance the sparsity by defining a set of collective variables within active subspace, yielding more accurate surrogate model recovered by compressive sensing method. Moreover, non-equilibrium properties further depends on the non-local memory term representing 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) by merely using trajectory data. The approximated kernel formulation satisfies the second fluctuation-dissipation conditions naturally with invariant measure. The proposed method enables us to characterize transition properties such as reaction rate where Markovian approximation shows limitation.

Speaker's Bio:
Huan Lei received his Ph.D. on Applied Mathematics from Brown University in 2012. He joined the Pacific Northwest National Laboratory (PNNL) as a postdoctoral associate. Currently, he is a research staff scientist in the Division of Advanced Computing, Mathematics \& Data at PNNL. His research work is mainly on developing mesoscale models and numerical methods applicable to multi-physical systems beyond equilibrium; in particular, non-equilibrium dynamic processes and intrinsic transition between the metastable states.

This lecture has a reception @ 03:00 pm

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