Reliable Extreme-Scale Stochastic Dynamics Simulation based on Generalized Interval Probability – II. Multiscale Quantification

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1. Introduction

This paper addresses a different set of problems from the ones discussed in a separate paper, entitled "Reliable Extreme-Scale Stochastic Dynamics Simulation based on Generalized Interval Probability – I. Uncertainty Dynamics", where the basics of generalized interval probability and stochastic dynamics simulation under both aleatory and epistemic uncertainties are introduced.

In modeling and simulation of multiscale complex systems, information collected by either physical or computational experiments is likely to have different forms and qualities, because of the constraints in instrument limitation, time, and cost associated with the experiments. Measurement and simulation results from different scales and physical domains need to be integrated consistently to make robust decisions under aleatory and epistemic uncertainties.

2. Cross-scale cross-domain information assimilation and model validation

We recently developed a generalized hidden Markov model (GHMM) to capture dependency relationships of uncertain variables at multiple scales or in different physical domains. The spatial and scale correlations among hidden and observable variables are represented by generalized interval probability. These scales may also be constituted by domains (e.g., time, different loosely coupled model environments, and physical domains).

The information with both uncertainty components can be assimilated based on a *generalized interval Bayes' rule* (GIBR), which is computationally much more efficient than those combination and update rules proposed in other forms of imprecise probability. The GHMM has been applied in multiscale materials-product design [1], where nanoscale properties are inferred from mesoscale and macroscale experimental measurements. It has also been applied in the validation of molecular dynamics (MD) simulation of nuclear materials irradiation [2], where the MD models are validated from macroscopic experiments with the consideration of measurement errors. Similar to the Bayesian approach, the validation of simulation models under both epistemic and aleatory uncertainties at multiple scales can be performed based on GIBR.

One example is shown in Fig.1, where interval cumulative distribution functions (c.d.f.'s) of point defect generation from MD simulations can be constructed with the incorporation of model and parameter errors. They are then updated from the macroscopic measurements of electrical resistivity change rates based on GIBR. The comparison between prior and posterior interval probabilities provides the necessary information for validation. Interval probability provides the extra information of how significant the epistemic component of uncertainty is in the model validation. With this extra information, a different decision, such as the need to collect more data or reduce measurement errors, can be made, instead of just whether the model is validated or not.

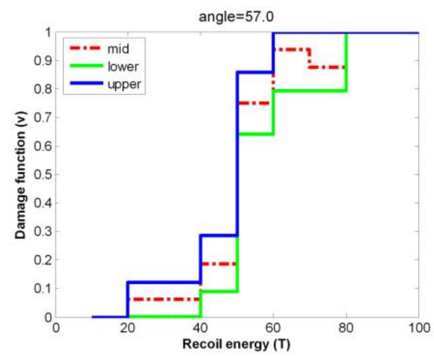

Fig.1: Interval c.d.f. of Frenkel pair generation from MD simulations at different recoil energy levels

3. Reliable kinetic Monte Carlo simulation

Kinetic Monte Carlo (KMC) simulation has been widely used in predicting chemical reaction, material degradation, crack propagation, protein folding, and many others as the alternative to solving the chemical master equation. Unknown, imprecise, or non-stationary propensity function in KMC is a common issue to affect its accuracy and reliability of prediction. A reliable kinetic Monte Carlo (R-KMC) simulation approach [3] that incorporates epistemic uncertainty with interval-valued parameters in stochastic simulation has been developed.

The simulation mechanism is rigorously based on the theoretical model of interval master equation. A multi-event random set sampling algorithm was developed to simulate based on interval-valued propensities. The simulated system is evolving simultaneously with the best- and worst-case scenarios based on the mathematically verifiable algorithm. It is shown that R-KMC converges to the classical KMC when interval-valued propensities shrink to real values. The feasibility and efficiency of the R-KMC mechanism in simulating chemical reactions have been demonstrated.

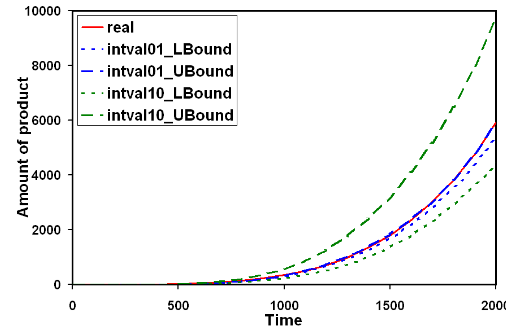

Fig.2: interval-valued average time in R-KMC gives best-case and worst-case estimations of species

As shown in Fig.2, the evolution of the number of species in reactions is captured with the consideration of epistemic uncertainty. Interval bounded results are given without the need of multiple simulation runs for sensitivity analysis, which saves time and energy in extreme-scale computation.

4. Sample-free global sensitivity analysis

Different from the traditional variance-based statistical sensitivity analysis, where data from either physical experiments or Monte Carlo sampling are required, we developed a sample-free global sensitivity analysis approach [4] so that the sensitivity of model parameters and inputs can be assessed without the assumption of probability distributions and samplings.

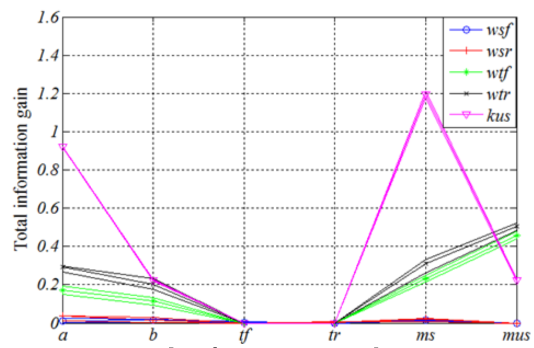

Fig.3: An example of sensitivity rankings among six inputs w.r.t. five outputs with sensitivity zones

Based on generalized interval, several metrics of indeterminacy and information gain are defined so that the uncertainty effect of input on the output in a functional relationship $\boldsymbol{f}(\boldsymbol{x})=\boldsymbol{y}$ can be assessed without the information of statistical variances or local gradients. The sensitivity levels of inputs can be ranked based on the least information of lower and upper bounds only. Fig.3 shows an example of sensitivity rankings among six inputs with respect to five outputs in an engineering design problem. The rankings are based on sensitivity zones and improve the robustness. The new sample-free global sensitivity analysis approach provides a computationally efficient approach to analyze complex systems with the minimum level of functional evaluations.

References

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