Preconditioning and simplification of multiscale stochastic dynamics

Analysis and Reduction of Complex Networks Under Uncertainty

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Abstract

We outline the development of (a) preconditioning algorithms that enable sparse representation of uncertain dynamical systems, and (b) methods for the simplification of these system models.

The preconditioning approach is based on the definition of an appropriate multiscale stretching of the individual components of the dynamical system which, in particular, enables robust recovery of the unscaled transient dynamics. Efficient representations of the stochastic dynamics are then obtained through non-intrusive spectral projections of the stretched measures. Implementation of the present approach is illustrated through application to a chemical system with large uncertainties in the reaction rate constants. Computational experiments show that, despite the large stochastic variability of the stochastic solution, the resulting dynamics can be efficiently represented using sparse low-order expansions of the stochastic multiscale preconditioner and of the stretched variables.

Methods for simplifying uncertain dynamical models are also developed for systems defined as *networks* of interacting components. These methods introduce criteria for the deletion of nodes (state variables) and edges (dynamical processes) in order to create simpler models. In particular, we use computational singular perturbation to calculate probabilistic 'importance indices' for node-edge pairs and introduce a thresholding procedure based on conditional value-at-risk (CVaR) to eliminate model components that do not significantly influence the dynamics of user-targeted state variables. Several error metrics are used to evaluate simplified models for their ability to preserve probabilistic information about the dynamics of the full model. We further establish connections between probabilistic importance indices, global sensitivity analysis, and the variation (over parameter space) of locally-simplified deterministic models. As with the preconditioning approach above, the simplification methodology is demonstrated via application to detailed chemical kinetic systems with large uncertainties in the reaction rate parameters.