Final Report: Analysis and Reduction of Complex Networks Under Uncertainty

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1 Project Overview

The project was a collaborative effort among MIT, Sandia National Laboratories (local PI Dr. Habib Najm), the University of Southern California (local PI Prof. Roger Ghanem), and The Johns Hopkins University (local PI Prof. Omar Knio, now at Duke University). Our focus was the analysis and reduction of large-scale dynamical systems emerging from networks of interacting components. Such networks underlie myriad natural and engineered systems. Examples important to DOE include chemical models of energy conversion processes, and elements of national infrastructure—e.g., electric power grids. Time scales in chemical systems span orders of magnitude, while infrastructure networks feature both local and long-distance connectivity, with associated clusters of time scales. These systems also blend continuous and discrete behavior; examples include saturation phenomena in surface chemistry and catalysis, and switching in electrical networks. Reducing size and stiffness is essential to tractable and predictive simulation of these systems. Computational singular perturbation (CSP) has been effectively used to identify and decouple dynamics at disparate time scales in chemical systems, allowing reduction of model complexity and stiffness. In realistic settings, however, model reduction must contend with uncertainties, which are often greatest in large-scale systems most in need of reduction. Uncertainty is not limited to parameters; one must also address structural uncertainties—e.g., whether a link is present in a network—and the impact of random perturbations, e.g., fluctuating loads or sources.

Research under this project developed new methods for the analysis and reduction of complex multiscale networks under uncertainty, by combining computational singular perturbation (CSP) with probabilistic uncertainty quantification. CSP yields asymptotic approximations of reduced-dimensionality "slow manifolds" on which a multiscale dynamical system evolves. Introducing uncertainty in this context raised fundamentally new issues, e.g., how is the topology of slow manifolds transformed by parametric uncertainty? How to construct dynamical models on these uncertain manifolds? To address these questions, we used stochastic spectral polynomial chaos (PC) methods to reformulate uncertain network models and analyzed them using CSP in probabilistic terms. Finding uncertain manifolds involved the solution of stochastic eigenvalue problems, facilitated by projection onto PC bases. These problems motivated us to explore the spectral properties stochastic Galerkin systems. We also introduced novel methods for rank-reduction in stochastic eigensystems—transformations of a uncertain dynamical system that lead to lower storage and solution complexity. These technical accomplishments are detailed below. This report focuses on the MIT portion of the joint project.

2 Technical Accomplishments

2.1 Simplification of chemical kinetic systems under uncertainty

Simulation of chemical systems with detailed kinetics can be computationally intensive. While homogeneous systems containing hundreds of species and thousands of elementary reactions can be integrated in reasonable times, a direct approach is not practical when numerous calculations are required, e.g., in the numerical simulation of reacting flow or in problems of optimization or sampling. Here, model reduction techniques are required for computational tractability. Simplified or reduced kinetic models can also provide insight into chemical systems by revealing key pathways and interactions. Many existing methods for reduction in a deterministic setting take advantage of timescale separation in chemical kinetic systems, where different timescales result from a range of slow and fast reactions. However, the relevant reaction rate parameters are typically uncertain and the impact of this uncertainty on model reduction had not previously been investigated.

We have used the method of computational singular perturbation (CSP) to calculate probabilistic 'importance indices' for species-reaction pairs on both fast and slow timescales. By modifying an existing deterministic algorithm, distributions of these indices are used to generate new reduced models that take account of rate parameter uncertainty. We replace the deterministic threshold used in the original algorithm with a new threshold based on the CVaR (conditional value-at-risk). First, a 95% confidence level for each importance index is found; the CVaR is then the expected value of an importance index given that it has exceeded the confidence level. This quantity provides a measure of risk and reduces the impact of both sampling errors and the subjective choice of threshold values.

Different error criteria are used to examine these new reduced models for their ability to either (1) yield predictions within probabilistic bounds determined by the full model, or (2) preserve entire output probability distributions of the full model. Objective (1) allows for greater model reduction by taking advantage of uncertainty to allow larger errors compared to the deterministic case. Objective (2) gives greater confidence in the quality of the reduced model over a wider range of parameters. These objectives do not always conflict; sometimes both objectives can be partially satisfied.

We compared our results with both existing deterministic algorithms and with an exhaustive search for the best reduced model of given size in a methane-air reaction mechanism at nominal rate parameters. Although the deterministic simplification algorithm performs well, it has not previously been compared to optimal results from an exhaustive search. We find that there is an opportunity for considerable improvement to the algorithm in terms of both error in ignition delay at nominal rate parameters and smallest achievable mechanism size. The modified algorithm succeeds in allowing smaller mechanism sizes, but does not give lower error with nominal rate parameters at sizes that can already be achieved. However, it significantly improves reproduction of the output distribution when sampling from a distribution of rate parameters.

2.1.1 Numerical examples

CSP versus optimal simplified models We first present results obtained in an entirely deterministic context. Skeletal mechanisms generated using the CSP simplification algorithm of Valorani et al. are compared to "optimal" simplified mechanisms of a given size, found through an exhaustive search of all possible simplified mechanisms. Exhaustive search has combinatorial complexity and is obviously not practical as a simplification algorithm, but the goal of this comparison is to assess how far the results of a fast *heuristic* simplification algorithm lie from the best possible skeletal model. This assessment has additional relevance below, where we consider two new error criteria

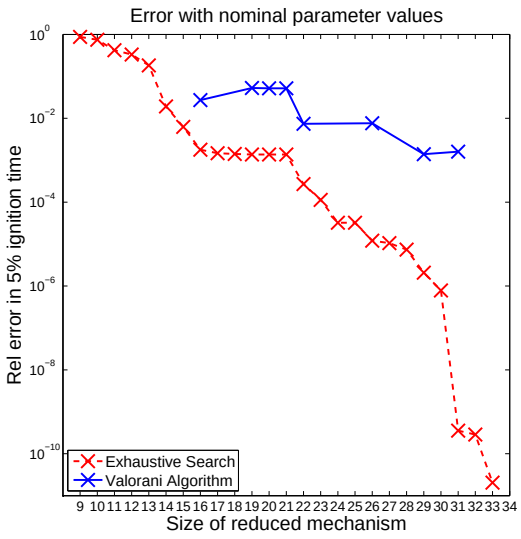

Figure 1: Relative error in ignition delay predictions, for mechanisms obtained via CSP simplification (blue) and optimal mechanisms obtained via exhaustive search (red).

that incorporate uncertainty, then introduce a *new* heuristic simplification algorithm designed to do a "good" job minimizing these errors.

Figure 1 shows relative error in ignition delay time as predicted by simplified mechanisms of differing sizes (where size corresponds to the number of retained species). The simplified mechanisms are found through CSP simplification or by exhaustive search, as described above. The "full" mechanism in this example is GRIMech 3.0 with C_3 and NO_x chemistry removed. (Removal of these species/reactions is simply a practical choice, intended to make exhaustive search more computationally feasible.) The ignition delay of a hydrogen-enriched methane-air mixture under constant-pressure and adiabatic conditions is calculated for three different initial temperatures and mixture compositions; the figure shows the *relative* error in this ignition delay, averaged over all three cases.

Both the optimal and CSP-produced simplified mechanisms show a trend of smaller errors with larger mechanism sizes. Error of the optimal mechanisms is strictly non-increasing with mechanism size, as expected. For intermediate sizes, the CSP-produced mechanisms yield errors that are within one order of magnitude of the optimal (minimal) error; this performance may be considered quite reasonable, given the vastly different computational costs of the two simplification schemes.

Figure 2 shows the species actually removed in the CSP-simplified model and in the optimal simplified model of any size. Species removed by CSP simplification form nested sets—i.e., if a species is removed in mechanism of size n, it necessarily will be removed in mechanisms of size $n-1$ or smaller, as the latter result from larger values of the importance index threshold parameter. Exhaustive search, on the other hand, has no such constraints; thus, the removed species in an optimal mechanism of a given size do not need to be nested.

It is also worth noting that these results do not fully evaluate the generality of the simplified mechanisms. While the exhaustive-search mechanisms are *optimal for the prescribed error criterion*, it is entirely possible that the CSP-simplified mechanisms might better predict ignition delays at alternate initial conditions, or better reproduce different functionals of the species trajectories. While the heuristic CSP simplification algorithm takes into account the dynamics and structure of the chemical mechanism, it does not optimize for any particular output error criterion.

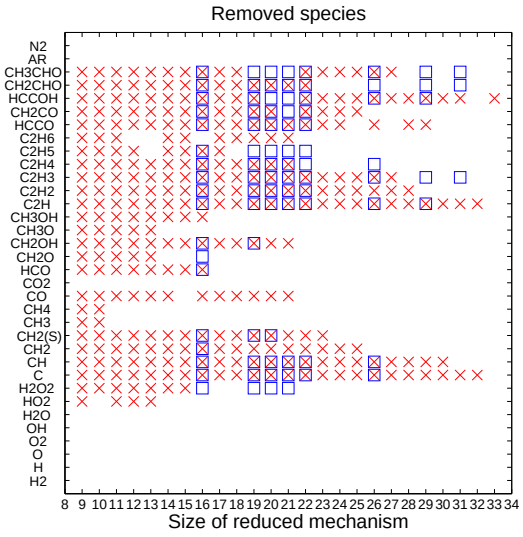

Figure 2: Species removed by CSP simplification (blue squares) and by exhaustive search for an optimal mechanism of given size (red '×'s).

New error criteria for reduction under uncertainty One of the key notions we explored in this research project is whether uncertainty provides opportunities for model reduction over a deterministic case. In other words, is it possible—and reasonable—to reduce a detailed mechanism that has uncertain parameters *further* than a detailed mechanism with precise/deterministic parameters?

We approached this question by devising output error criteria that will guide model reduction under uncertainty. A first criterion states that the difference between the simplified model prediction y_s and the detailed model prediction y_d of some output quantity of interest should be *normalized* by the standard deviation of the detailed model prediction. The criterion is thus

$$\text{err} = \frac{|y_s - y_d|}{\sigma_d}. \tag{1}$$

A more general criterion comes from the realization that, given a probabilistic description of uncertainty in the rate parameters, both the full-model and simplified-model outputs are random variables. Accordingly, one may choose among many established notions of "distance" between probability measures. Here, we employ the Kullback-Leibler (K-L) divergence. If y_s has probability density p_s and y_d has probability density p_d, the K-L divergence from p_d to p_s is

$$\begin{aligned} D_{KL}\left(p_d \| p_s\right) &= \int p_d(y) \log \frac{p_d(y)}{p_s(y)}\, dy \\ &= \mathbb{E}_{p_d}\left[\log \frac{p_d(y)}{p_s(y)}\right]. \end{aligned} \tag{2}$$

We note that the K-L divergence can reduce to (1) in the case of Gaussian output distributions with identical variance.

CSP simplification with risk-based thresholding We have modified the CSP simplification algorithm to account for parametric uncertainty in the detailed mechanism. CSP-based simplification relies on the evaluation of slow and fast CSP importance indices I^s_{km} and I^r_{km}, which quantify

the importance of reaction k to the slow or fast evolution of species m. Uncertainty in rate parameters (e.g., pre-exponential factors, activation energies, temperature exponents, etc) gives rise to uncertainty in these importance indices. Given a probabilistic description of the rate parameter uncertainties, the importance indices are naturally endowed with a joint probability distribution.

The importance indices calculated here are normalized for each species. Additionally, we consider only the time average of each normalized importance index; averages are calculated over the time trajectory of each ignition process. Monte Carlo simulation of homogeneous autoignition, over the space of uncertain rate parameters, is used to construct the probability distribution of the importance indices. (Polynomial chaos approximations to the importance indices are, of course, a viable and potentially far more efficient alternative to Monte Carlo; we shall explore this avenue in future work.) We consider eight uncertain parameters; all are pre-exponential factors endowed with log-normal probability distributions. These pre-exponential factors correspond to elementary reactions involved in hydrogen oxidation. The resulting marginal probability distribution of a particular fast importance index is shown in Figure 3.

Deterministic CSP simplification employs a user-defined threshold on normalized importance indices to decide which reactions influence the evolution of a particular species, and which reactions may be neglected. The retained reactions enlarge the set of retained species, and the algorithm iterates to convergence. Here, we replace the hard threshold on importance index with a probabilistic criterion. In particular, we consider the conditional value-at-risk (CVaR). As depicted in Figure 3, the CVaR is the expected value of the importance index given that the importance index exceeds a particular level:

$$\mathrm{CVaR} \equiv \mathbb{E}\left[I_{km} | I_{km} > \mu\right] \tag{3}$$

where μ is determined by $\mathbb{P}\left\{I_{km} > \mu\right\} = \alpha$. In this definition, $1-\alpha$ is known as the confidence level while μ is the value-at-risk (VaR). Compared to VaR, numerical evaluation of CVaR is less sensitive to sampling error. Moreover, using CVaR avoids the difficulties of arbitrary threshold selection, and naturally captures the notion that exceeding a threshold by a large amount is undesirable.

Beginning with the importance index distributions calculated above, we use a CVaR threshold in the simplification algorithm to construct simplified mechanisms of various sizes. We then use Monte Carlo simulation with each simplified mechanism to evaluate a probability density for the predicted ignition delay. Figure 4 shows probability densities resulting from several simplified models (colored solid line), compared to the probability density produced by the full detailed model (dashed line). Agreement is quite good, even for a 20-species mechanism. Figure 5, on the other hand, shows ignition delay probability densities calculated with a different set of simplified mechanisms—mechanisms constructed via the usual deterministic CSP simplification algorithm. In this case, the simplified mechanisms do a much poorer job replicating the output probability density of the detailed model.

2.2 Rank reduction for parametric partial differential equations

In a parallel effort at MIT, we have developed preconditioning techniques to reduce the solution rank of parametric partial differential equation (PDEs). By applying these techniques, efficient integration of the PDE can be achieved through classical tensor methods. Although our abstract formulation is quite general, we have focused on time dependent problems. In particular, we study a preconditioner based on a nonlinear change of the time coordinate, which is determined as the solution of an optimal control problem for rank minimization.

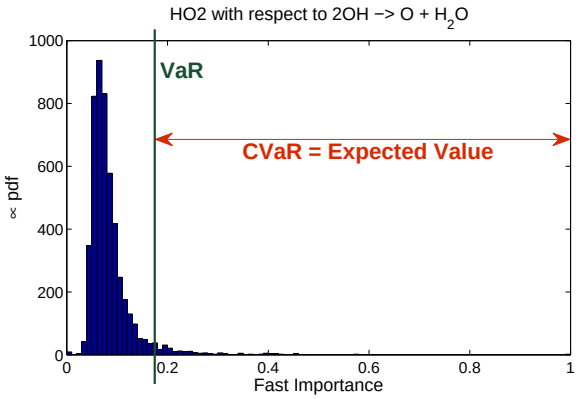

Figure 3: Probability density function of the fast importance index of $\{2OH \rightarrow O + H_2O\}$ to HO_2. Also shown are the VaR and CVaR at a 95% confidence level.

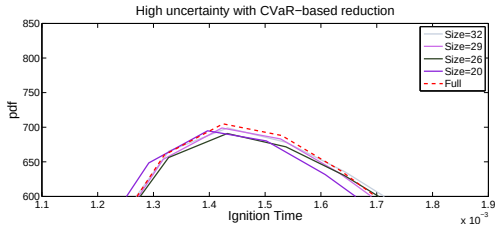

Figure 4: Probability densities of ignition delay as predicted by simplified mechanisms constructed with risk-based thresholding. Detailed mechanism predictions are depicted with the dashed red line.

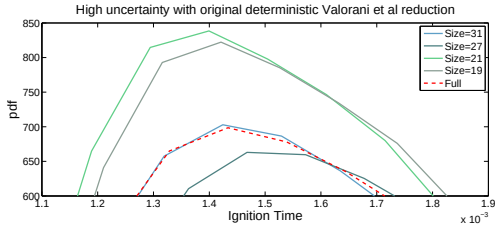

Figure 5: Probability densities of ignition delay as predicted by simplified mechanisms constructed with the deterministic CSP simplification algorithm. Detailed mechanism predictions are shown with the dashed red line.

2.2.1 Motivation

Let $u(\boldsymbol{x}, \xi) : X \times \Xi \to \mathbb{R}$ be the solution field of a well-posed parametric equation:

$$\mathcal{G}(u; \xi) = f(\boldsymbol{x}, \xi) \tag{4}$$

where $\mathcal{G}(\cdot; \xi)$ is a possibly nonlinear partial differential operator parameterized by ξ and $f(\boldsymbol{x}, \xi)$ is a forcing term. X is the range of the physical variable $\boldsymbol{x}$ and Ξ represents the range of the parametric variable ξ. We can introduce a suitable function space $\Omega_{X\times\Xi}$ of functionals defined over $X \times \Xi$ to characterize a solution of (4) in a weak sense. In practice, we always assume $\Omega_{X\times\Xi}$ to be a separable Hilbert space. Since $\Omega_{X\times\Xi} \sim \Omega_X \otimes \Omega_\Xi$, any function in $\Omega_{X\times\Xi}$ can be written as a possibly infinite converging series of separable functions defined over X and Ξ:

$$h(\boldsymbol{x}, \xi) = \sum_{i=1}^{r} w_i(\boldsymbol{x})\lambda_i(\xi) \tag{5}$$

where $w_i \in \Omega_X$, $\lambda_i \in \Omega_\Xi$, and the cardinality of the sum is said to be the rank of h, possibly infinite. The convergence of (5) is with respect to a metric of $\Omega_X \otimes \Omega_\Xi$. In numerical applications, it is often more convenient the notion of ϵ-rank defined as the minimal cardinality of a series like (5) needed to approximate h with relative precision of at least ϵ. For ease of notation and without loss of generality, we always refer to the numerical ϵ-rank whenever dealing with the notion of rank.

Efficient numerical techniques to solve parametric equations exploit linear separability (5) of the solution. In this case, the solution is low rank and its realizations $\{u(\boldsymbol{x}, \xi_i)\}_i$ lie in a low dimensional subspace of Ω_X. Thus, the rank is a crucial quantity that measures both the dimensionality of a representation of the solution, and the complexity of solving the associated equation. Ideally, we want a low rank solution. Unfortunately, this is not always the case. When the solution is high rank, classical linear reduction techniques such as PGD, POD, and RB are not numerically efficient in terms of CPU and memory requirements and one has to resort on expensive classical simulations. The key observation is that even though the solution is high rank, there might exist a low dimensional map of a low rank field y which yields the solution: $u = \Phi(y)$. We seek the map $\Phi(\cdot)$ and we call it: the preconditioner.

One might wonder how a such a low dimensional map could possibly exist. The reason is straightforward: high rank does not necessarily correspond to a high degree of information content. We give a simple example to clarify this point. Consider the identity matrix $\mathbf{I} \in \mathbb{R}^{n\times n}$. This matrix is full rank despite its simplicity. Any attempt to represent $\mathbf{I}$ in a classical low rank fashion without loss of information is doomed to failure. However, we can certainly write the identity $\mathbf{I}$ as a low dimensional map of a low rank matrix. Namely:

$$\mathbf{I} = \begin{bmatrix} 1 & & \\ & \ddots & \\ & & 1 \end{bmatrix} = \Phi\left(\begin{bmatrix} & 1 & \\ & \vdots & \\ & 1 & \end{bmatrix}\right) \tag{6}$$

where Φ suitably shifts the entries of each row of the input matrix to yield the identity (6). The shift is uniquely defined once we assign a scalar for each row of the input matrix. Hence, the linear invertible map Φ can be represented by an element of $\mathbb{R}^n$ and thus, it is low dimensional.

2.2.2 Abstract formulation

For brevity and generality, we describe here only the abstract formulation of our rank reduction approach. If u is a solution of the parametric equation $\mathcal{G}(u) = f$, we regard any field y satisfying

$\Phi(y) = u$ for some map Φ, as the preconditioned solution field. The preconditioned solution field solves a slightly different equation than (4), namely:

$$(\mathcal{G} \circ \Phi)(y) = f \tag{7}$$

We want to find a preconditioner such that the solution of $(\mathcal{G} \circ \Phi)(\cdot) = f$ is low rank and thus, easy to integrate. Invertibility of the preconditioning map is a desirable property since it guarantees well-posedness of (7) for any given map Φ, but it is definitely not necessary. If Φ is not invertible, we can always relax the constraint (7) as:

$$\|(\mathcal{G} \circ \Phi)(y) - f\| \leq \delta \tag{8}$$

where $\delta > 0$ is a free parameter controlling the norm of the residual. In particular, for a given map Φ, there need not exist a feasible preconditioned field. For the sake of simplicity, we will focus on invertible preconditioners in the rest of the paper.

Our goal is mathematically equivalent to a constrained minimization problem: find an optimal map $\Phi^\star$ and a preconditioned solution field $y^\star$ such that

$$\begin{aligned} \Phi^\star, y^\star \quad \in \quad & \arg\inf_{\Phi,y} \operatorname{rank}[y] \\ & (\mathcal{G} \circ \Phi)(y) = f \\ & \Phi \in \boldsymbol{\Phi}^{\text{adm}} \end{aligned} \tag{9}$$

where $\boldsymbol{\Phi}^{\text{adm}}$ is the constraining set of admissible maps. Namely, $\boldsymbol{\Phi}^{\text{adm}}$ is the set of measurable maps from $\Omega_{X\times\Xi}$ to $\Omega_{X\times\Xi}$, possibly invertible, and need not be a linear space. In practice, we have to constrain the dimensionality of functions in $\boldsymbol{\Phi}^{\text{adm}}$ to retain the benefits of a low rank preconditioned solution. Problem (9) should be contrasted with:

$$\begin{aligned} \Phi^\star \quad \in \quad & \arg\inf_{\Phi} \operatorname{rank}[\Phi(u)] \\ & \mathcal{G}(u) = f \\ & \Phi \in \boldsymbol{\Phi}^{\text{adm}} \end{aligned} \tag{10}$$

In (10), we first solve for a possibly high rank solution field u such that $\mathcal{G}(u) = f$, and then, we look for an invertible map $\Phi(\cdot)$ that minimizes the rank of $\Phi(u)$. This is not what we want. We never want to deal with the high rank original field. The problem we solve is (9), where the preconditioner and a low rank solution field are determined at the same time without never resorting on the solution of the unpreconditioned problem. The existence of a low rank solution of (9) is still an open issue and it is mostly problem dependent. Clearly, the richer the space of admissible maps for the preconditioner, the more likely is a low rank preconditioned field. It should be clear, however, that we are not imposing a low rank ansatz for the solution. We just want to find a preconditioned equation whose solution is intrinsically low rank. There is no loss of information between the original and the preconditioned field, as long as the preconditioner is an invertible map.

Example. As a more concrete example, consider the case of a linear operator $\mathcal{G} = \boldsymbol{G} \in \mathbb{R}^{np\times np}$ over the finite dimensional space $\Omega_X \otimes \Omega_\Xi$, with $\dim \Omega_X = n$ and $\dim \Omega_\Xi = p$. The unfolded solution tensor $u \in \mathbb{R}^{np}$ solves the linear system $\boldsymbol{G}u = \boldsymbol{f}$ where $f \in \mathbb{R}^{np}$ is a forcing term. The rank of the solution field is defined as the matrix rank of a suitable folding of the solution as an element of $\mathbb{R}^{n\times p}$ which is isomorphic to $\Omega_X \otimes \Omega_\Xi$. Restrict the set of admissible maps $\boldsymbol{\Phi}^{\text{adm}}$ to

linear functions, possibly low rank. Thus, our goal is to find a matrix $\boldsymbol{\Phi} \in \boldsymbol{\Phi}^{\text{adm}}$ and a low rank unfolded preconditioned field $y \in \mathbb{R}^{np}$ such that:

$$(\boldsymbol{G}\boldsymbol{\Phi})\, y = \boldsymbol{f} \tag{11}$$

and the rank of y is minimized.

2.2.3 Specific instantiations

The framework that we have developed and described above is quite general. But we have focused many of our implementations on time dependent problems for at least two reasons. On the one hand, we have an intuitive notion of preconditioner based on space-time dilations. On the other hand, we can achieve good balance between the cost of determining an optimal preconditioner $\Phi^\star$ and the advantages of integrating a low rank preconditioned field $y^\star$ over a possibly high rank original solution.

Specific instantiations of the framework are therefore as follows:

- A time-dilation preconditioner, applied to advection equations and to the Navier-Stokes equations at moderate Reynolds number, to solve a problem of stochastic vortex shedding behind a cylinder.
- A space-and-time dilation preconditioner, applied to a multi-front advection diffusion problem with multiple distinct stochastic front velocities
- A time-independent problem, solved via the proper generalized decomposition (PGD) method; here we introduced new preconditioners at each iteration, effectively composing multiple preconditioners as we deflated the problem.

3 Personnel Supported

MIT (Marzouk): 2 graduate students, 1 postdoc (partial), PI summer time

4 Publications and Talks

Publications

1. T Coles, "Model simplification of chemical kinetic systems under uncertainty," SM Thesis, MIT, June 2011.
2. T Coles, H Najm, Y Marzouk, "CSP simplification of chemical kinetic systems under uncertainty." International Workshop on Model Reduction in Reacting Flow/13th International Conference on Numerical Combustion (2011).
3. R Berry, H Najm, B Debusschere, Y Marzouk, H Adalsteinsson, "Data-free inference of the joint distribution of uncertain model parameters." *Journal of Computational Physics* 231: 2180–2198 (2012).
4. A Spantini, "Preconditioning techniques for stochastic partial differential equations," SM Thesis, MIT, June 2013.
5. A Spantini, L Mathelin, Y Marzouk, "A rank reduction technique for time-dependent parameterized PDEs." To be submitted to *SIAM Journal on Scientific Computing* (2015).

Talks

1. Y Marzouk,"Analysis and reduction of complex networks under uncertainty." Workshop on Uncertainty Quantification for Multiscale Systems. Johns Hopkins University. Baltimore, MD. July 2010.

2. T Coles, Y Marzouk,"Reduced models of multiscale kinetic systems under uncertainty." SIAM Conference on Computational Science & Engineering (CSE11), invited minisymposium. Reno, NV. March 2011.

3. Y Marzouk, "Simplification of multiscale chemical kinetic systems under uncertainty." Workshop on Uncertainty Quantification in Multiscale/Multiphysics Systems, University of Southern California. Los Angeles, CA. March 2011.

4. T Coles, Y Marzouk, "Model simplification of chemical kinetic systems under uncertainty." International Conference on Chemical Kinetics. Cambridge, MA. July 2011.

5. Y Marzouk, University of Southern California, Department of Aerospace and Mechanical Engineering. Los Angeles, CA. April 2012.

6. Y Marzouk, University of Colorado at Boulder, Department of Applied Mathematics. Boulder, CO. April 2012.

7. Y Marzouk, UOP/Honeywell Invitational Lecture Series. Chicago, IL. May 2012.

8. A Spantini, L Mathelin, Y Marzouk, "Preconditioning techniques for stochastic conservation laws." SIAM Conference on Computational Science and Engineering (CSE13), invited minisymposium. Boston, MA. February 2013.

9. L Tosatto, Y Marzouk, "Simplifying chemical kinetic systems under uncertainty using Markov chains." Fourth International Workshop on Model Reduction in Reacting Flow. San Francisco, CA. June 2013.

10. A Spantini, L Mathelin, Y Marzouk, "Rank reduction of parameterized time- dependent PDEs." SIAM Conference on Uncertainty Quantification (UQ14), invited minisymposium. Savannah, GA. April 2014.