- PRF# 59081-DNI9
- **Project Title:** Reduced Order Modeling of Filter Density Function of Reactive Turbulence
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1 Project Description

State of the art approaches reduce the chemical kinetic model in an offline manner, in which unimportant reactions of the detailed model are removed. However, in turbulent reactive flows, this processes are strongly coupled to the turbulent flow, and an offline reduction strategy may remove reactions that otherwise significantly affect the turbulent flow and vice versa. These eliminated reactions may be active for only a short period of time, but they may alter the system dynamics by triggering a different chain of reactions, or nonlinearly activate instabilities in the turbulent flow. Current approaches would require expensive turbulent reactive flows to compute sensitivities required for reducing chemical kinetics model, which is computationally infeasible. The goal of this project is to establish new framework for the real-time reduction of chemical kinetics coupled with turbulent reactive flows. This reduced order modeling approach will then be utilized in solving the high-dimensional partial differential equation of the evolution of the filter density function. Our approach is based on a new time-dependent low-rank basis that instantaneously follows the most important reactions and lead to an adaptive reaction addition/removal scheme. The computational cost of the proposed method scales linearly with the size of the low-rank basis and in general, is independent of the size of the detailed chemical kinetic model.

2 Accomplishments

In the first year we focused on developing the theoretical framework and its validation and demonstration. In the second year we plan to apply this framework to reduced-order modeling of filter density function in the large eddy simulation of turbulent reactive flows. To this end, we considered a stochastic framework in which the dynamical ($d\boldsymbol{\phi}/dt = \mathbf{f}(t)$) system is subject to parameters $\boldsymbol{\xi}$, where $\boldsymbol{\xi} = [\xi_1, \xi_2, \dots, \xi_d] \in \mathbb{R}^d$ are the reaction parameters. We consider the following decomposition:

$$\boldsymbol{\phi}(t;\boldsymbol{\xi}) = \sum_{i=1}^{r} y_i(t;\boldsymbol{\xi})\mathbf{u}_i(t), \tag{1}$$

where $\boldsymbol{\phi} = \left\{\phi_1, \phi_2, \dots, \phi_{N_s}\right\}$ is represents the mass fraction of all species and N_s is the total number of species, $\mathbf{U}(t) = \left\{\mathbf{u}_1(t), \mathbf{u}_2(t), \dots, \mathbf{u}_r(t)\right\} \in \mathbb{R}^{N_s \times r}$ is a set of time-dependent orthonormal modes, referred to as dynamic basis (DB), and $\mathbf{Y}(t;\boldsymbol{\xi}) = \left\{\mathbf{y}_1(t;\boldsymbol{\xi}), \mathbf{y}_2(t;\boldsymbol{\xi}), \dots, \mathbf{y}_r(t;\boldsymbol{\xi})\right\} \in \mathbb{R}^{d \times r}$ represents the coefficients of the corresponding modes. The coefficients are functions of the reaction parameters, and they capture the hidden space of the reactions. The dimension of the hidden space is often much smaller than the number of the species $r < N_s$ and $r < d$, and therefore the above reduction given by equation 1 amounts to a (potentially significant) reduction in representing the solution. To this end, our two main accomplishments during the first year are described below.

1. Variational principle for solving real-time reduced-order model of detailed kinetics: Deriving evolution equations for both $\mathbf{Y}(t;\boldsymbol{\xi})$ and $\mathbf{U}(\boldsymbol{\phi}, t)$ requires particular attention to the fact that both $\mathbf{Y}(t;\boldsymbol{\xi})$ and $\mathbf{U}(t)$ are time-dependent. During the first year, we developed a theoretical framework that leads to closed-form evolution equations for $\mathbf{Y}(t;\boldsymbol{\xi})$ and $\mathbf{U}(t)$. The variational principle is shown in Fig. 1(a), where $\mathbb{E}$ denotes the mean of the sensitivities and $||\ .\ ||$ denotes the second norm induced by the inner product $\langle .\ ,\ . \rangle$ in the mass fraction space, and $\mathbf{f}$ represents nonlinear detailed kinetics. We showed that the first-order optimality condition of the functional with respect to $\dot{\mathbf{U}}$ and $\dot{\mathbf{Y}}$ leads to a closed form evolution equations for the time-dependent basis $\mathbf{U}$ and their coefficients $\mathbf{Y}$ as shown in Fig. 1(a), where $\mathbf{C} = \mathbb{E}[\mathbf{Y}^T\mathbf{Y}]$ is the reduced covariance matrix ($\mathbf{C} \in \mathbb{R}^{r \times r}$), and $\prod_{\perp \mathbf{U}} = \mathbf{I} - \mathbf{U}\mathbf{U}^T$ is the orthogonal projection to the space spanned by the complement of $\mathbf{U}$. More details of the variational principle for a generic case can be found in reference [1], which is currently under revision for being published in the Proceedings of Royal Society (Part A).

2. Reduced-order modeling of chemical reaction for large number of species: During the first year of this project, we applied the reduced order modeling strategies to a diverse set of systems to study the effectiveness of the our framework for obtaining real-time reduced order models. In this report we show results for reduced-order modeling of USC Mech II chemical kinetic

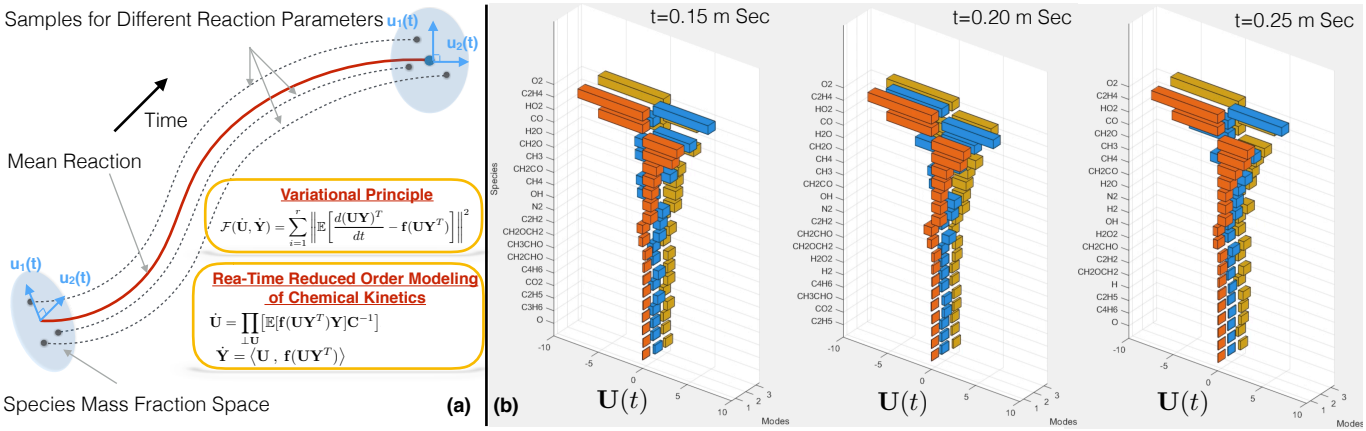

Figure 1: (a) Schematic of the framework, the variational principle and the resulting reduced order model. (b) Real-time reduced order modeling of USC Mech II chemical kinetic model that contains 111 species and 784 reactions. The time-dependent modes $\mathbf{U}(t)$ at three times are shown. Each mode has $N_s = 111$ elements. Only the first 20 most important species are shown. The ranking of the 20 species changes in time based on their values on the the vector $\mathbf{u}_1(t)$. For more details on the methodology, please see reference [1].

model, which contains 111 species and 784 reactions. Here we consider a reduction of order $r = 4$, which amounts to a reduction from $N_s = 111$ to $r = 4$. For this demonstration, we used a non-intrusive data-driven counterpart of the above reduced order modeling strategy. Please see reference [1] for more details and more demonstration cases. We have shown mathematically that the data-driven approach is equivalent to the model-driven reduced-order modeling. However, the data-driven approach allows us to quickly test the reduced order modeling strategy on a variety of problems. For the USC Mech II chemical kinetic model, we generated a skeletal reaction model and compare it against the outcome of published results in the literature. We analyzed the stoichiometric ethylene-air ignition, prepare data with changing pre-exponential factors, and our target functions are species mass fractions. The results are shown in Fig. 1(b). In each time step, the most subspace $\mathbf{U}(t)$ determines which species are dominant. This would constitute a *real-time ranking* of the most important species. We set a threshold on the values of each component (species) of $\mathbf{u}_i$. The species that are above threshold 0.01 are shown for three time instants. For more details please see reference [1].

3 Impact

PI: The developed framework for the real-time reduced order modeling has already generated significant interest in several US government agencies for similar and different applications. The PI has already received significant funding from NASA in further developing this framework for computing sensitivities in chaotic flows. The PI is also in consultation with Dr. Jackie Chen from the Department of Energy to further expand on this work to develop reduced-order model for ignition and extinction in turbulent reactive flows. The PI has also received significant interest from the Combustion and Fire Systems at NSF and is currently preparing a proposal for that program. **Students:** The PI is currently funding one PhD student, who is in her third year and is responsible for further development and implementation of the proposed research. She is in final stages of preparing a manuscript on her work that is funded by this program. An undergraduate student also worked on data-driven version of this approach. He is currently a graduate student at the University of Pennsylvania. **Dissemination:** The PI has developed a new graduate level course titled *Reduced Order Modeling for Engineering*. The course is currently offered for the second time at MEMS Department at the University of Pittsburgh this semester (Fall 2019). We anticipate to have several more publications in the coming year as the implementation of methodology progresses for the filter density function. We are planning to attend at least three conferences in the coming year.

4 References

[1] H. Babaee, "A scalable observation-driven time-dependent basis for a reduced description of transient systems," *arXiv e-prints*, p. arXiv:1904.09846, Apr 2019.