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***Abstract*— We use a relatively recent nonlinear manifold learning technique (diffusion maps) to parameterize low dimensional attracting manifolds arising in the description of detailed chemical kinetics mechanisms. With no *a priori* knowledge about the shape and dimension of the manifold, such an approach provides a way of solving a reduced (and less stiff) set of equations in terms of automatically detected slow variables. Advantages as well as disadvantages of the approach are discussed.**

I. Introduction

The solution of detailed models for chemical kinetics (either ODE or discretized PDE) often poses severe numerical difficulties mainly due to two aspects: First, the number of degrees of freedom is large; second, the dynamics is characterized by disparate time scales. As a result, reactive flow solvers with detailed chemistry often become intractable even for large clusters of CPUs, especially when dealing with direct numerical simulation (DNS) of turbulent combustion problems. This has motivated the development of several approaches for reducing the complexity of such kinetics models, by expressing them in terms of only a few slow variables. However, there are no generally applicable recipes for selecting a good global parameterization of the reduced model, and the choice of slow variables often relies upon intuition and experience. Clearly, a more systematic approach in this respect would be highly desirable. In this work, we follow a fully automated approach where the low-dimensional attracting manifold is identified, parametrized and a consistent reduced model constructed. The key step is the parameterization, which is obtained by learning the slow manifold through diffusion maps (DMAPs).

II. Diffusion maps

The diffusion maps approach has recently emerged as a powerful tool in data analysis [1], [2], [3]. The basic aim is to provide a nonlinear extension of the Principal Component Analysis (PCA) in order to construct a low-dimensional embedding for a given set of M points (X_1,...,X_M) in a high-dimensional space, if such an embedding exists. To this end, a distance d_{ij} between a pair of states (X_i and X_j) is needed. Based on d_{ij}, a pairwise affinity function can be established such that $W_{ij} = W_{ji} \geq 0$, with the heat kernel being a popular option:

$$W_{ij} = \exp\left[-\left(\frac{d_{ij}}{\varepsilon}\right)^2\right]. \tag{1}$$

Although, for data in $\Re^N$, an obvious choice for d_{ij} is the standard Euclidean distance, this is not always the best option. For instance, a weighted Euclidean norm may be necessary when the different coordinates of a generic point X_i are characterized by disparate orders of magnitude. This is indeed the case encountered in many combustion problems, where data are likely points in concentration space and major species (i.e. reactants and products) arise in much higher concentrations compared to minor species (i.e. radicals). The notion of locality is introduced through the model parameter ε which defines the width of a small neighborhood, where the chosen distance d can be assumed as a good measure of proximity. Based on the symmetric matrix $W = \{W_{ij}\}$, a diagonal matrix $D = \{D_{ii}\}$ can be defined such that: $D_{ii} = \sum_{k=1}^{M} W_{ik}$. Following the DMAPs approach, if the initial data points are located on a low dimensional manifold with dimension k, a gap appears between k nontrivial eigenvalues of the Markov matrix $K = D^{-1}W$ and the remaining ones. Moreover, the components in the corresponding k eigenvectors establish a projection of the high-dimensional points (X_1,...,X_M) into a k-dimensional space.

III. Application to combustion

We will demonstrate the feasibility of constructing reduced kinetics models for combustion applications, by extracting the slow dynamics on a manifold globally parameterized by diffusion maps. To this end, preliminary results are shown for a homogeneous reactive mixture of hydrogen and air at stoichiometric proportions under fixed total enthalpy ($H = 300[kJ/kg]$) and pressure ($P = 1[bar]$). Time evolution of the chemical species follows the Li mechanism [4], and can be generally formulated as follows:

$$\frac{d\vec{y}}{dt} = \vec{f}(\vec{y}), \tag{2}$$

with $\vec{y}$ representing the state in terms of mass fractions of the nine participating chemical components (H_2, N_2, H, O, OH, O_2, H_2O, HO_2, H_2O_2). Equations (2) are further complemented by an implicit algebraic equation for temperature, stipulating the constancy of total enthalpy.

The first step of the proposed method requires the identification of the low-dimensional attracting manifold. While many possible constructions have been suggested in the literature (see, e.g., [5], [6], [7], [8]) here, in the spirit of the *equation free* framework [9], [10], we assume that only the rates $\vec{f}(\vec{y})$ are accessible and do not rely upon any prior knowledge about a good parameterization of the manifold.

For data collection, Eqs. (2) are integrated starting from a rich enough set of random states within the admissible phase-space (convex polytope defined by elemental conservation constraints and concentration positivity) and, after sufficient time to approach a neighborhood of the manifold, samples are collected from each trajectory. As a result, a set of points $\{X_i, i = 1, ..., M\}$ in $\Re^N$ (hopefully dense enough within the region of interest) becomes available for defining the manifold.

As a second step, the diffusion maps approach is performed as outlined in Section II. Due to a disparity of the magnitudes of species concentrations, d_{ij} is taken as the Euclidean distance between properly rescaled points $\tilde{X}_i$ and $\tilde{X}_j$, with $\tilde{X}_i = RX_i$ using the fixed diagonal matrix $R = \{R_{kk}\}$, $R_{kk} = 1/max(X(k))$. Here, $max(X(k))$ represents the largest k-th coordinate among all sample points, whereas the parameter ε in (1) can be chosen as a multiple of the quantity: $\max_j \min_{i \neq j} d_{ij}$ [11], [12], [13]. An example is shown in Fig. 1. Finally, as a third step, following [13], [14], the reduced model of (2) can be constructed as follows:

$$\frac{d\vec{L}}{dt} = \frac{\partial \vec{\psi}\left(\vec{\psi}^{-1}\left(\vec{L}\right)\right)}{\partial \vec{y}} \vec{f}\left(\vec{\psi}^{-1}\left(\vec{L}\right)\right), \qquad (3)$$

where $\vec{L}$ denotes the reduced state, while $\vec{\psi}$ and $\vec{\psi}^{-1}$ represent the *restriction* and *lifting* operators. Clearly, obtaining these operators, for example through Nyström extension [15] and various interpolation approaches, is a crucial step in our model reduction method.

IV. Conclusion

In this work, we provide evidence that the diffusion maps technique is a useful tool for systematically extracting a global parameterization of low-dimensional manifolds arising in combustion problems, while less stiff reduced systems can be expressed in terms of the slow variables parametrizing these manifolds as identified by the process.

Acknowledgment

E.C. acknowledges partial support of the Fulbright commission and the Italian Ministry of Research (FIRB grant RBFR10VZUG). I.G.K. and C.W.G. gratefully acknowledge partial support by the US DOE.

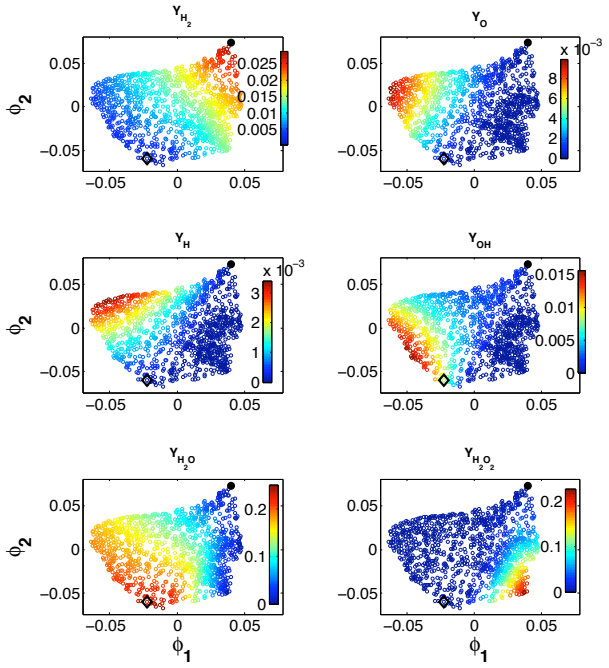

Fig. 1. Homogeneous reactive mixture of hydrogen and air at stoichiometric proportions with fixed enthalpy ($H = 300[kJ/kg]$) and pressure ($P = 1[bar]$). Two dimensional DMAPs parameterization of 1095 points as provided by the two nontrivial leading eigenvectors ϕ_1 and ϕ_2 of the Markov matrix K. Colors represent mass fractions, while black filled circle and black diamond represent the fresh mixture condition and equilibrium state, respectively.

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