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On the Computation of Approximate Slow Invariant Manifolds

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***Abstract*— Approximate Slow Invariant Manifolds (ASIMs) in reactive flow systems are described by an elliptic system of partial differential equations. This work addresses the efficient construction of these manifolds and their coupling to the slow dynamics. Results are given for a simple benchmark system and for more realistic systems.**

I. Introduction

A wide variety of combustion processes involve a large number of elementary reactions occurring simultaneously within a complex flow field. These processes are modeled by a large number of partial differential equations (PDEs) representing the evolution of numerous reactive chemical species, coupled with the full Navier-Stokes equations. Fully resolved solution of these equations, which incorporate detailed finite rate chemical kinetics, often requires a prohibitive amount of computational resources. Hence, there is a need to develop methods which rationally reduce the model equations such that accurate numerical simulations can be accomplished in a reasonable amount of computational time.

Elementary chemical reactions occur over a wide range of scales which is manifested as stiffness in the model equations, and subsequently high computational costs. For stable systems, this stiffness can be reduced by systematically equilibrating the fast time scale chemical processes and resolving only the relevant slow time scales. The reduced model equations describe the slow dynamics under the assumption that the fast dynamics can be neglected. Most chemical time scales are faster than time scales typically used to model continuum phenomena such as advection and diffusion. Nevertheless, it is important that the reduced model equations maintain the coupling of the flow processes with those chemical processes which occur at similar time scales. Singh, *et al.* [1] address how the coupling of fluid and chemical processes can be maintained such that an approximate and less expensive numerical solution of the reduced model equations is consistent with the more accurate and expensive numerical solution of the full model equations.

In realistic problems it is important to achieve computational efficiency for simulating spatially inhomogeneous reactive systems which are modeled by PDEs and which have infinite dimensional invariant manifolds. The present work addresses the construction of ASIMs as described by Singh, *et al.* [1]. In their construction, the full model equations are projected onto the fast and slow basis vectors associated with chemistry. A set of elliptic PDEs is obtained by equilibrating the fast dynamics. These elliptic PDEs are analogous to algebraic equations describing the commonly used Intrinsic Low Dimensional Manifold (ILDM), [1]. The elliptic PDEs describe the infinite-dimensional ASIM to which the reactive flow system relaxes before reaching steady state. The ASIM accounts for the effects of advection and diffusion in the reactive flow system. When using the ASIM, a set of elliptic PDEs in physical space, coupled with time-dependent reduced PDEs associated with the slow dynamics, is solved. The present work addresses the efficient construction of these manifolds and their coupling to the slow dynamics. Results are given for a simple benchmark system and for more realistic systems.

II. Reactive Flow Equations

The governing equations for a reacting flow system can be written in the following compact form:

$$\frac{\partial \mathbf{y}}{\partial t} = \mathbf{f}(\mathbf{y}) - \nabla \cdot \mathbf{h}(\mathbf{y}), \tag{1}$$

where $\mathbf{y} \in \mathbb{R}^n$ represents a set of dependent variables, $\mathbf{h}(\mathbf{y})$ represents the advective and diffusive flux vectors, and $\mathbf{f}(\mathbf{y})$ represents the reaction source term. The independent time and space variables are t and $\mathbf{x}$, respectively.

We rewrite the advection-diffusion-reaction equations in terms of a new set of variables defined by $\mathbf{z} = \tilde{\mathbf{V}} \cdot \mathbf{y}$, where

$$\tilde{\mathbf{V}} = \mathbf{V}^{-1} = \begin{pmatrix} \tilde{\mathbf{V}}_s \\ \tilde{\mathbf{V}}_f \end{pmatrix} \tag{2}$$

and

$$\mathbf{V} = \begin{pmatrix} \mathbf{V}_s & \mathbf{V}_f \end{pmatrix} \tag{3}$$

is the eigenvector matrix of the Jacobian of the source term $\mathbf{f}$. Assuming m slow variables, then $\tilde{\mathbf{V}}_s$ is of size $m \times n$, while $\tilde{\mathbf{V}}_f$ is of size $(n-m) \times n$. We note that the basis $\mathbf{V}$ is derived solely from the chemistry of a spatially homogeneous system. While this will eventually lead to an improved estimate of the system's behavior, a better basis on which to project would take account of the infinite-dimensional eigenfunctions associated with the advection-diffusion operator. This, however, is difficult.

Under some assumptions, Singh, *et al.* [1] have shown that the slow dynamics are described by

$$\tilde{\mathbf{V}}_s \cdot \frac{\partial \mathbf{y}}{\partial t} = \tilde{\mathbf{V}}_s \cdot \mathbf{f} - \tilde{\mathbf{V}}_s \cdot \nabla \cdot \mathbf{h}, \tag{4}$$

and this evolution equation couples with the equation for the infinite-dimensional manifold which accounts for the

effects of advection and diffusion:

$$\mathbf{0} = \tilde{\mathbf{V}}_f \cdot \mathbf{f} - \tilde{\mathbf{V}}_f \cdot \nabla \cdot \mathbf{h}. \quad (5)$$

Equation (5) represents the *infinite-dimensional* ASIM on which the slow dynamics evolve. For two- and three-dimensional reactive flows, the ASIM is described by a set of elliptic partial differential equations. Upon spatial discretization of Eqs. (4) and (5), the slow dynamics are described by a system of differential algebraic equations (DAEs) which have to be solved together with prescribed boundary conditions.

III. Results

The basic problem is to efficiently and accurately compute an approximation to the slow invariant manifold embedded in the infinite-dimensional space. In order to test the accuracy of the numerical construction of the ASIM we first use the generalized Davis-Skodje model (see [1] and [2]) which includes diffusion effects and is defined in the domain $x \in [0, 1]$:

$$\frac{\partial y_1}{\partial t} = -y_1 + D_1 \frac{\partial^2 y_1}{\partial x^2}, \quad (6)$$

$$\frac{\partial y_2}{\partial t} = -\gamma y_2 + \frac{(\gamma - 1)y_1 + \gamma y_1^2}{(1 + y_1)^2} + D_2 \frac{\partial^2 y_2}{\partial x^2}, \quad (7)$$

with boundary conditions

$$y_1(t, 0) = y_2(t, 0) = 0, \text{ and }, y_1(t, 1) = a, \, y_2(t, 1) = b. \quad (8)$$

where $\gamma > 1$ gives a measure of stiffness for the system, $D_1 > 0$ and $D_2 > 0$ are diffusion coefficients, and a and b are arbitrary constants. If γ is increased, the stiffness of the system will increase.

In addition to discussing the accuracy of the construction, we characterize the attractiveness of the slow manifold as a function of γ, D_1, D_2, a, and b, and given arbitrary initial conditions, provide an efficient strategy to determine approximately the time it takes for the solution trajectory to be sufficiently close to the slow manifold and the corresponding location near the manifold.

Subsequently, we demonstrate the the efficiency of the algorithm by solving a reaction-diffusion problem which describes the NO formation using the Zel'dovich mechanism, and other more complex systems.

IV. Conclusion

While no robust analysis exists to determine advection and diffusion time scales *a priori*, we find that in reactive flow systems, in which advection and diffusion have time scales comparable to those of reactions, the ASIM provides a better approximation of the slow dynamics compared to most other reduction strategies. Most importantly, we demonstrate that the ASIM can in general be efficiently computed and subsequently we show that the slow dynamics of relevant advection-diffusion-reaction systems can be modeled with a substantial reduction in computational cost.

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References

[1] Singh, S., Powers, J.M., Paolucci, S., 2002, On slow manifolds of chemically reactive systems. *Journal of Chemical Physics*, **117**, pp. 1482-1496.

[2] Davis, M.J., Skodje, R.T., 1999, Geometric investigation of low-dimensional manifolds in systems approaching equilibrium. *Journal of Chemical Physics*, **111**, pp. 859-874.