Reactive Flow Calculations with Intrinsic Low Dimensional Manifold Corrections for Convection and Diffusion [1]

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1. Summary

A method is described which rationally corrects the method of intrinsic low dimensional manifolds (ILDM) to account for the effects of small convection and diffusion. The ILDM method is well suited for spatially homogeneous problems and provides a systematic way to overcome the severe stiffness which is associated with full models of detailed kinetics and thus significantly improves computational efficiency. Significant errors can arise however when the ILDM method is applied to systems which have convection and diffusion. Motivated by techniques from center manifold theory, and using the ILDM as a reference manifold, we project our entire system of equations onto a new basis, which is segregated into fast and slow sets of equations. The fast scale equations are equilibrated, requiring the solution of an elliptic equation in space. The slow equations are allowed to temporally evolve. Improvements in predictions relative to those of the traditional IDLM method are shown for a simple model problem.

2. Background

It is well known that in order to accurately simulate a wide variety of thermochemical phenomena, the effects of detailed finite rate chemistry must be incorporated into models. The development of these detailed models over the past decades has provided a strong link between traditional collision-based gas phase chemistry and fundamental fluid mechanics. However, implementation of fully detailed chemistry models with the obligatory numerical resolution has proven to require a prohibitive amount of computational resources for all but the simplest of flows. While the addition of species and reaction mechanisms induces an increase in computational time required to simulate a given event, a more serious problem is often the severe stiffness associated with the differential equations which model the chemistry. In general, the time scales of reaction, found by eigensystem analysis of locally linearized systems, are often widely disparate; for example in a hydrogen/air system, their ratio is as large as 10^7. This leads to computations which routinely take hundreds of hours on supercomputers; such efforts are often impractical.

Consequently, it becomes necessary to implement some strategy to reduce the stiffness introduced by the chemistry. The simplest, full equilibrium, is effectively an ILDM of dimension zero; however, this approach will necessarily miss the coupling of events which occur on time scales of chemical reaction. Simple and often useful strategies which capture some of the kinetic time scales employ explicit one- and two-step models, e.g. Westbrook and Dryer, 1981. Also useful are the commonly employed partial equilibrium and steady state modeling assumptions. As shown by Maas and Pope, 1992, such assumptions are often not robust. While they may be useful in the range in which they have been calibrated, it is often easy to find scenarios where such models cannot accurately reproduce the results of full kinetic models. As a consequence, Maas and Pope and simultaneously Goussis and Lam, 1992, have advocated methods which systematically reduce chemical kinetic models in such a way that consistency with full model equations is maintained to a user-specified precision. A number of studies have appeared in recent years advancing the technique and some variants, Lam, 1993; Schmidt, *et al.*, 1996; Eggels, *et al.*, 1997; Pope, 1997; Hamiroune, *et al.*, 1998; Norris, 1998; Schmidt, *et al.*, 1998; Yang and Pope, 1998a,b, Davis and Skodje, 1999; Lowe and Tomlin, 2000; and Singh, *et al.*, 2001.

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Here, the method of Maas and Pope, 1992, as we apply it in this study to find one-dimensional manifolds, is summarized. The adiabatic, isochoric combustion of a well-stirred system of N species with L elements leads to $N-L$ non-linear ordinary differential equations, which evolve in an $N-L$ dimensional composition space. The ILDM method identifies M-dimensional subspaces ($M < N-L$) on which slower time scale events evolve. For example, for a one-dimensional manifold, we take $M = 1$. Fast time scale events rapidly move onto the manifold, and can be projected onto it avoiding costly explicit time integration. The manifold is determined prior to actual calculations which may use the method. One first determines the equilibrium point of the system and the local real Schur decomposition, which gives local eigenvalues and associated orthonormal Schur vectors for a system linearized about the equilibrium point. One then perturbs M of the species away from equilibrium to prescribed values to form M algebraic equations; these are solved simultaneously with $N-L-M$ algebraic equations which arise from considering the combination of the forcing term of length $N-L$ projected onto the basis defined by the $N-L-M$ orthonormal Schur vectors associated with the $N-L-M$ fastest time scales. These equations are solved with a predictor-corrector technique coupled with a Newton's method iteration to obtain the mass fractions at a new point on the manifold. The new manifold point is used as a seed for calculation of further points. An arc-length parameterization of the manifold is employed to overcome difficulties associated with turning points of the manifold in composition space.

The ILDM method has been extensively developed for closed, spatially homogeneous systems with temporal but not spatial dependencies due to such processes as convection and diffusion. When considering application of the ILDM method to such systems, a typical technique is to employ operator splitting. In this approach, after discretization, each spatial point is first allowed to evolve due to convection and diffusion only. Next, convection and diffusion are suppressed, and each spatial point evolves due to chemistry. The reactive step is effectively a series of closed homogeneous reactors at each spatial point, and the ILDM technique can be used effectively. Other approaches are used as well.

However, the inclusion of convection and diffusion fundamentally alters the dynamics of the relaxation. This is because the manifold of the resulting PDEs is infinite dimensional, while the ILDMs are obtained from a finite dimensional system of ODEs. We extend the traditional ILDM approach to a first order correction to account for the effects of small convection and diffusion. Here we briefly describe the method.

The equations of combustion can be written as

$$\frac{\partial \mathbf{u}}{\partial t} = \mathbf{G}(\mathbf{u}) - \epsilon \frac{\partial}{\partial x_i} \mathbf{F}(\mathbf{u}). \tag{1}$$

Here, we take $\epsilon << 1$ so that the effects of convection and diffusion are locally small compared to those of reaction. With small ϵ, the Maas-Pope ILDM captures the leading order dynamics of the system, and identifies fast and slow variables as linear combinations of primitive variables. In a procedure similar to that used in the technique of center manifold projection, we project the original system onto a new basis so as to get time evolution equations for fast and slow variables. These equations also involve spatial derivatives of coupled fast and slow variables. The proper extension of the traditional ILDM method is to then equilibrate the fast variables, which gives rise to an elliptic equation in space that must be solved in a coupled iterative fashion with the time evolution equation for the slow variable. This procedure is completely analogous to that used in solving the incompressible Navier-Stokes equations, in which the incompressibility assumption effectively filters the fast acoustic time scales. This comes at the expense of solving an elliptic equation at each time step.

3. Results

We consider a simple model problem which is an extension to the system studied by Davis and Skodje, 1999, to include diffusion:

$$\begin{aligned}
\frac{\partial y_1}{\partial t} &= -y_1 + \epsilon \frac{\partial^2 y_1}{\partial x^2}, && (2)\\
\frac{\partial y_2}{\partial t} &= -\gamma y_2 + \frac{(\gamma - 1) y_1 + \gamma y_1^2}{(1 + y_1)^2} + \epsilon \frac{\partial^2 y_2}{\partial x^2}, && (3)\\
y_1(x,0) &= x, \qquad y_1(0,t) = 0, \qquad y_1(1,t) = 1, && (4)
\end{aligned}$$

$$y_2(x,0) \quad = \quad 0.55x \qquad y_2(0,t) = 0, \qquad y_2(1,t) = 0.55. \tag{5}$$

We take $\epsilon << 1$ for small diffusion. The terms not involving ϵ are taken to represent a reaction process. We take $\gamma >> 1$ to represent a system, which in the limit where diffusion is completely neglected, is stiff due to chemical source terms. Now it can be shown that for $\epsilon \to 0$ the ILDM is given by

$$y_2 = \frac{y_1}{1+y_1} + \frac{2y_1^2}{\gamma(\gamma-1)(1+y_1)^3}. \tag{6}$$

When we consider a problem with $\epsilon = 0.1$ and $\gamma = 10$, it is found that the actual long time solution is close to the ILDM, but is much better captured by the corrected manifold method described by the above procedure. This is shown in Figure 1. On the scales shown in Figure 1, there is actually no discernible difference between the predictions of the corrected manifold method and that of a full numerical solution. The actual differences along with an improvement relative to that of the traditional ILDM method can be seen in Figure 2. To obtain Figure 2, we first calculate a full solution using a traditional method of lines approach. We then compute approximations to this solution using a traditional ILDM method with operator splitting and by using our new convection diffusion correction. At each time, we compute the maximum $L_\infty[0,1]$ error throughout the spatial domain. The error for each method is plotted on a logarithmic scale. As the traditional ILDM method is always attracted to the ILDM for long time, the effect of the spatial boundary condition at $x = 1$ not lying on the ILDM is manifested in the relatively large error for the traditional method at late time. We see however that the error is always decreasing when the convection-diffusion correction is applied.

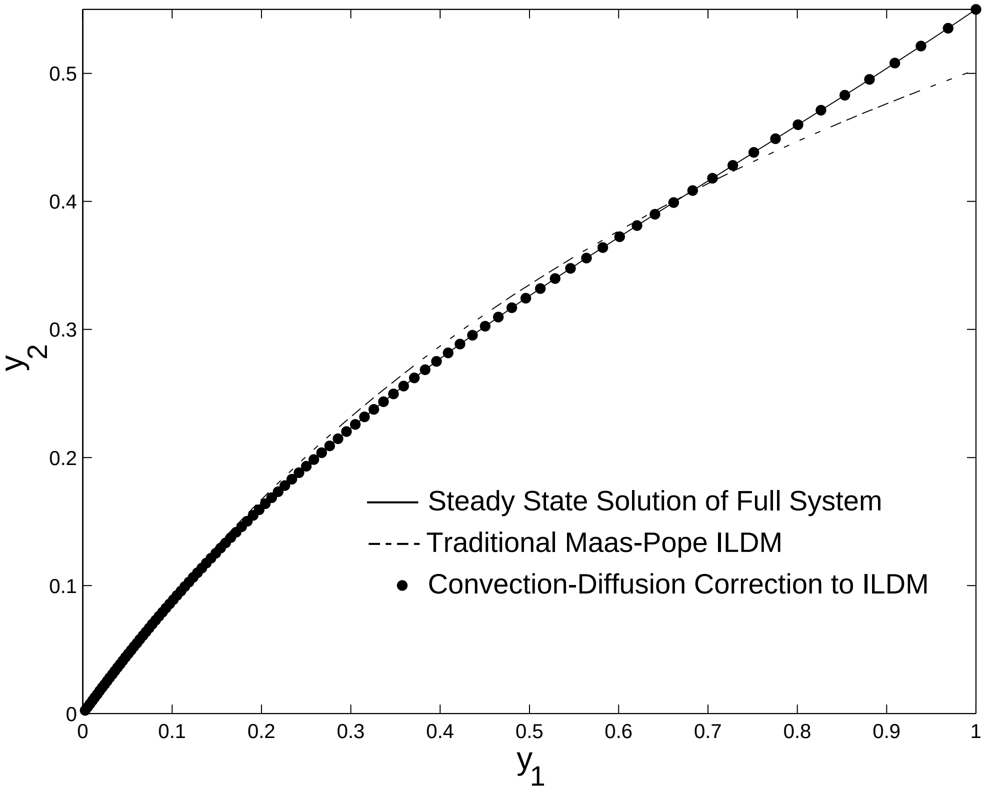

Figure 1: Long time predictions of solution to the diffusive extension of Davis and Skodje's, 1999, model problem via full numerical solution of model problem (solid line), traditional Maas-Pope ILDM implementation (dashed line), and convection-diffusion correction (dots), $\gamma = 10$, $\epsilon = 0.1$.

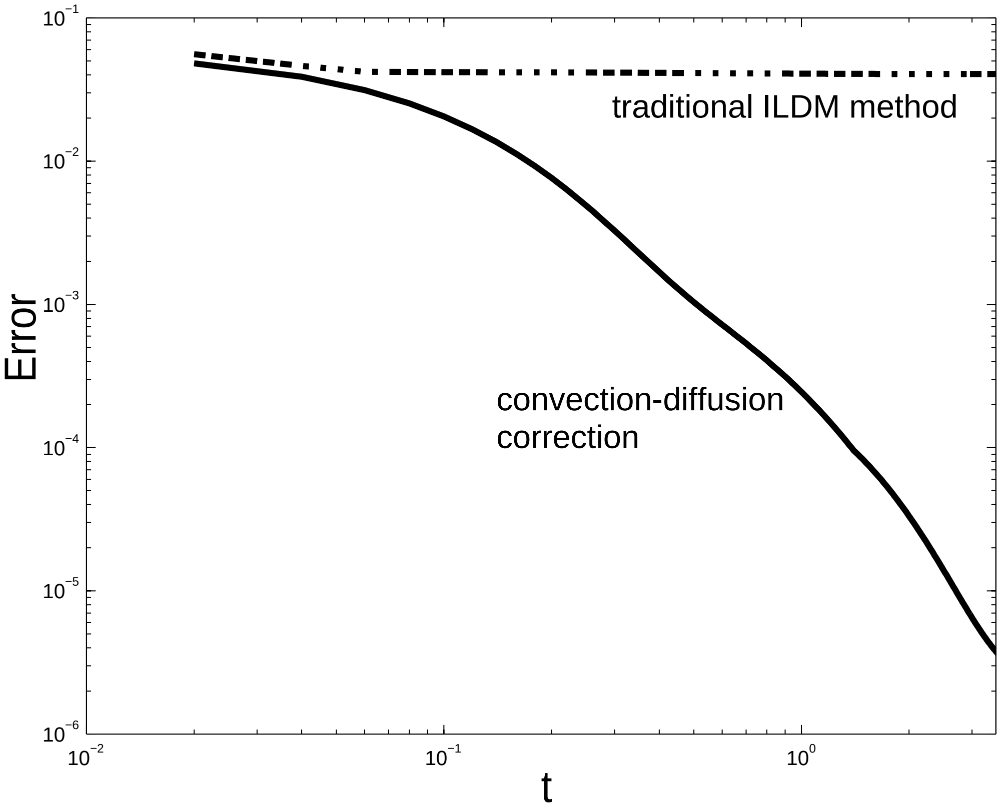

Figure 2: $L_\infty[0,1]$ error over the spatial domain as a function of time for the traditional ILDM method (dashed line) and the method with the correction for convection-diffusion (solid line), $\gamma = 10$, $\epsilon = 0.1$.

It can be shown that a similar improvement in accuracy occurs for more relevant combustion problems.

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