Computational methods for multiscale reactive fluid mechanics: Intrinsic low dimensional manifolds coupled with a wavelet adaptive multilevel representation

by

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Outline

• Motivation for multiscale methods

• Intrinsic Low Dimensional Manifold (ILDM) technique (Maas and Pope, *Combustion and Flame* 1992)


• Results for one-dimensional viscous $H_2/O_2/Ar$ detonation with detailed kinetics (Singh, Rastigejev, Paolucci, & Powers, *Combustion Theory and Modeling*, 2001)

• Systematic correction to ILDM method for convection and diffusion (Singh, Paolucci, & Powers, to be submitted to *Journal of Chemical Physics*, 2001)

• Conclusions
Center manifold-motivated correction for small convection-diffusion

- Consider system of Davis and Skodje, 1999, extended for diffusion

\[
\frac{\partial y_1}{\partial t} = -y_1 + \epsilon \frac{\partial^2 y_1}{\partial x^2}, \\
\frac{\partial y_2}{\partial t} = -\gamma y_2 + \frac{(\gamma - 1)y_1 + \gamma y_1^2}{(1 + y_1)^2} + \epsilon \frac{\partial^2 y_2}{\partial x^2},
\]

\[
y_1(x, 0) = x, \quad y_1(0, t) = 0, \quad y_1(1, t) = 1,
\]

\[
y_2(x, 0) = 0.55x \quad y_2(0, t) = 0, \quad y_2(1, t) = 0.55.
\]

- \( \gamma \gg 1 \) for chemical stiffness; \( \epsilon \ll 1 \) for small diffusion

- Maas-Pope ILDM:

\[
y_2 = \frac{y_1}{1 + y_1} + \frac{2y_1^2}{\gamma(\gamma - 1)(1 + y_1)^3}.
\]

- *Purely* reactive system has equilibrium *point* in phase space at \( y_1 = 0, y_2 = 0 \) at \( t \to \infty \).

- System with convection-diffusion approaches steady state *manifold*, not ILDM, as \( t \to \infty \) given by solution of ODEs:

\[
0 = -y_1 + \epsilon \frac{d^2 y_1}{dx^2}; \quad y_1(0) = 0; \quad y_1(1) = 1,
\]

\[
0 = -\gamma y_2 + \frac{(\gamma - 1)y_1 + \gamma y_1^2}{(1 + y_1)^2} + \epsilon \frac{d^2 y_2}{dx^2}; \quad y_2(0) = 0; \quad y_2(1) = 0.55.
\]
Center manifold-motivated correction for small convection-diffusion

- Assume convection-diffusion acts as a small perturbation

- Define fast \((w_f)\) and slow \((w_s)\) variables based on analytic Jacobian of chemical source term:

\[
\begin{pmatrix}
  w_s(x, t) \\
  w_f(x, t)
\end{pmatrix} =
\begin{pmatrix}
  1 & 0 \\
  -\alpha(y_{10}(x)) & 1
\end{pmatrix}
\begin{pmatrix}
  y_1(x, t) - y_{10}(x) \\
  y_2(x, t) - h(y_{10}(x))
\end{pmatrix}
\]

- \(y_{10}(x)\) is solution for \(y_1(x)\) at previous time step,

- \(h(y_{10}(x))\) is the ILDM.

- Project original PDEs onto the slow and fast basis near ILDM to get

\[
\frac{\partial w_s}{\partial t} = -y_{10}(x) - w_s + \epsilon \left( \frac{d^2 y_{10}}{dx^2} + \frac{\partial^2 w_s}{\partial x^2} \right) + H.O.T.,
\]

\[
\text{convection-diffusion correction}
\]

\[
\frac{\partial w_f}{\partial t} = \text{Maas-Pope ILDM term} - \gamma w_f + 0
\]

\[
+ \epsilon \left( g_1(y_{10}(x)) + w_s g_2(y_{10}(x)) + \frac{\partial w_s}{\partial x} g_3(y_{10}(x)) + \frac{\partial^2 w_f}{\partial x^2} \right)
\]

\[
+ H.O.T.
\]

\[
\text{convection-diffusion correction}
\]
Center manifold-motivated correction for small convection-diffusion

- equilibrate fast variables: $\frac{\partial w_f}{\partial t} = 0$, giving an elliptic equation

$$0 = -\gamma w_f +$$

$$+ \epsilon \left( g_1(y_{10}(x)) + w_sg_2(y_{10}(x)) + \frac{\partial w_s}{\partial x} g_3(y_{10}(x)) + \frac{\partial^2 w_f}{\partial x^2} \right)$$

convection–diffusion correction

$$+ H.O.T.$$ 

- Use method of lines, combined with simultaneous solution of elliptic equation, to advance slow variables using large time step,

- Analogous to solving elliptic equation for pressure when time advancing incompressible Navier-Stokes equations.
Center Manifold-Motivated Correction for Convection-Diffusion

- Long time solution does not approach Maas and Pope ILDM,
- Convection-diffusion correction gives more accurate predictions

![Graph showing comparison between Steady State Solution of Full System, Traditional Maas-Pope ILDM, and Convection-Diffusion Correction to ILDM.]

- $H_2/O_2/Ar$ ILDM results accurate because restricted to near equilibrium regions
- arbitrary use of ILDM can give inaccurate results
Center Manifold-Motivated Correction for Convection-Diffusion

- The corrected method gives more accurate predictions of intermediate and long times.
Work in progress

- Extension of WAMR method to three dimensions
- Implementation of method in parallel architectures
- Convection-diffusion ILDM correction for ozone and methane laminar flames