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)
- Wavelet Adaptive Multilevel Representation (WAMR) technique (Vasilyev & Paolucci, *Journal of Computational Physics*, 1996)
- 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

$$\frac{\partial y_1}{\partial t} = \underbrace{-y_1}_{\text{reaction}} + \underbrace{\epsilon \frac{\partial^2 y_1}{\partial x^2}}_{\text{diffusion}},$$

$$\frac{\partial y_2}{\partial t} = \underbrace{-\gamma y_2 + \frac{(\gamma - 1)y_1 + \gamma y_1^2}{(1+y_1)^2}}_{\text{reaction}} + \underbrace{\epsilon \frac{\partial^2 y_2}{\partial x^2}}_{\text{diffusion}},$$

$$y_1(x,0) = x, \qquad y_1(0,t) = 0, \qquad y_1(1,t) = 1,$$

$$y_2(x,0) = 0.55x \qquad y_2(0,t) = 0, \qquad y_2(1,t) = 0.55.$$

- $\gamma >> 1$ for chemical stiffness; $\epsilon << 1$ 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:

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

- $y_{10}(x)$ 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

$$\frac{\partial w_s}{\partial t} = -y_{10}(x) - w_s + \underbrace{\epsilon\left(\frac{d^2 y_{10}}{dx^2} + \frac{\partial^2 w_s}{\partial x^2}\right)}_{\text{convection-diffusion correction}} + H.O.T.,$$

$$\frac{\partial w_f}{\partial t} = \underbrace{\text{Maas-Pope ILDM term}}_{=0} - \gamma w_f + \\ + \underbrace{\epsilon\left(g_1(y_{10}(x)) + w_s g_2(y_{10}(x)) + \frac{\partial w_s}{\partial x} g_3(y_{10}(x)) + \frac{\partial^2 w_f}{\partial x^2}\right)}_{\text{convection-diffusion correction}} \\ + H.O.T.$$

Center manifold-motivated correction for small convection-diffusion

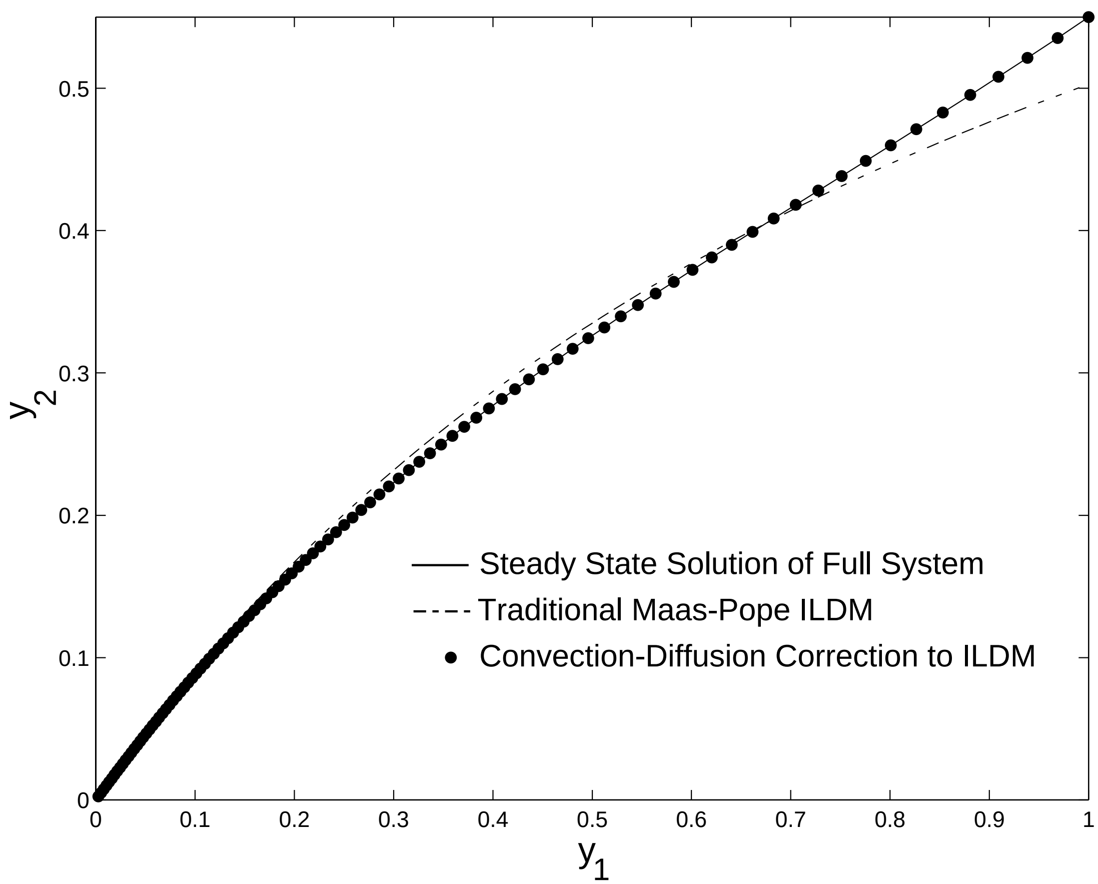
- equilibrate fast variables: $\frac{\partial w_f}{\partial t} = 0$, giving an elliptic equation

$$
\begin{aligned}
0 &= -\gamma w_f + \\
&+ \underbrace{\epsilon \left(g_1(y_{10}(x)) + w_s g_2(y_{10}(x)) + \frac{\partial w_s}{\partial x} g_3(y_{10}(x)) + \frac{\partial^2 w_f}{\partial x^2} \right)}_{\text{convection}-\text{diffusion correction}} \\
&+ H.O.T.
\end{aligned}
$$

- 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

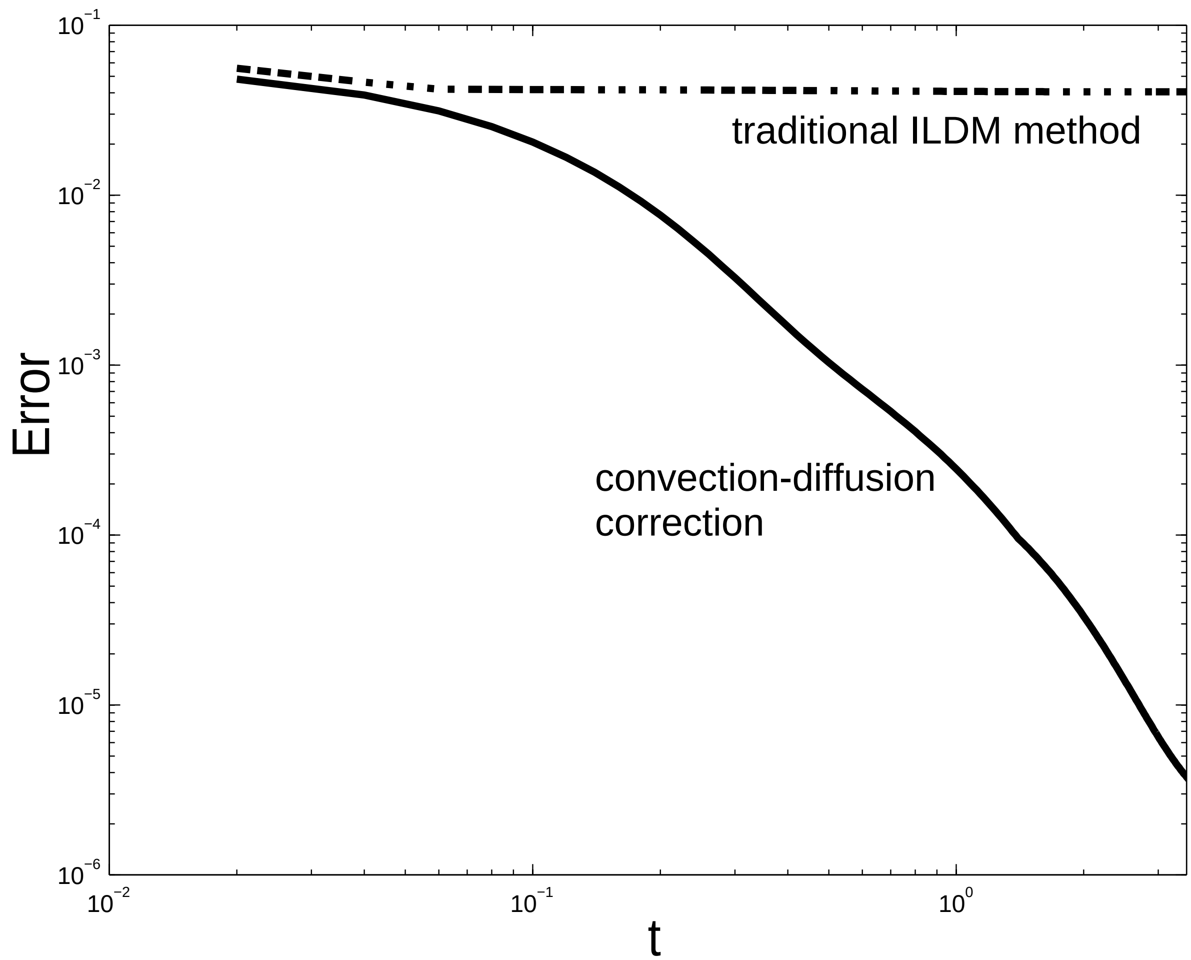
- Long time solution does not approach Maas and Pope ILDM,
- Convection-diffusion correction gives more accurate predictions



- $H_2/O_2/Ar$ 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
- Implemetnation of method in parallel architechtures
- Convection-diffusion ILDM correction for ozone and methane laminar flames