Low-Dimensional Manifolds in Reaction-Diffusion Systems

by

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Major Issues in Reduced Modeling of Reactive Flows

- Intrinsic Low Dimensional Manifold (ILDM) is not a Slow Invariant Manifold (SIM).
- How to construct an ILDM and a SIM?
- SIM for ODEs is different than SIM for PDEs.
- How to construct a SIM for PDEs?

Partial Review of Manifold Methods in Reactive Systems

- Fraser, *JCP*, 1988: clarification of steady state and partial equilibrium and discussion of SIM in ODEs, algebraic functional iteration to find SIM in simple ODEs
- Roussel and Fraser, *JCP*, 1991: extension of algebraic functional iteration to find SIM in simple ODEs,
- Maas and Pope, *C & F*, 1992: identification of ILDM in ODEs resulting from detailed mass action kinetics,
- Maas and Pope, *25th Comb. Symp.*, 1994: application of ILDM to PDEs with detailed kinetics; linear approximation for boundary condition errors,
- Davis and Skodje, *JCP*, 1999: demonstration that ILDM is not SIM in simple non-linear ODEs, numerical iteration and further extensions to find SIM in simple ODEs,
- Singh, Powers, and Paolucci, *JCP*, 2002: show ILDM is not a SIM for general ODEs, use ILDM to construct ASIM in simple and detailed PDEs,
- Kaper and Kaper, *Phys. D*, 2002: show ILDM is not a SIM for general ODEs,
- Nafe and Maas, *CTM*, 2002: use iteration to find SIM for ODEs with detailed kinetics.

Outline

- Motivation.
- Comparison of ILDM and Slow Invariant Manifold (SIM) for spatially homogeneous premixed reactive systems.
- Theoretical development of the Approximate Slow Invariant Manifold (ASIM) for the extension of the ILDM method to couple convection and diffusion with reaction.
- Comparison of the ASIM with the Maas and Pope projection (MPP) for a simple reaction diffusion model problem.
- Use of ASIM in premixed laminar flames for ozone decomposition and methane combustion.
- Conclusions.

Motivation

- Severe stiffness in reactive fluid mechanical systems with detailed gas phase chemical kinetics renders fully resolved simulations of many systems to be impractical.
- ILDM method of Maas and Pope, 1992, offers a systematic robust method to equilibrate fast time scale phenomena for spatially homogeneous premixed reactive systems with widely disparate reaction time scales.
- ILDM method can reduce computational time while retaining essential fidelity of full detailed kinetics.
- ILDM method effectively reduces large n-species reactive system to user-defined low order m-dimensional system by replacing differential equations with algebraic constraints.
- The ILDM is only an approximation of the SIM, and contains a small intrinsic error for large stiffness.
- Using ILDM in systems with convection and diffusion can lead to large errors when convection and diffusion time scales are comparable to those of reactions.
- An Approximate Slow Invariant Manifold (ASIM) is developed for systems where reactions couple with convection and diffusion.
- Full details in Singh, Powers, Paolucci, *Journal of Chemical Physics*, 2002.

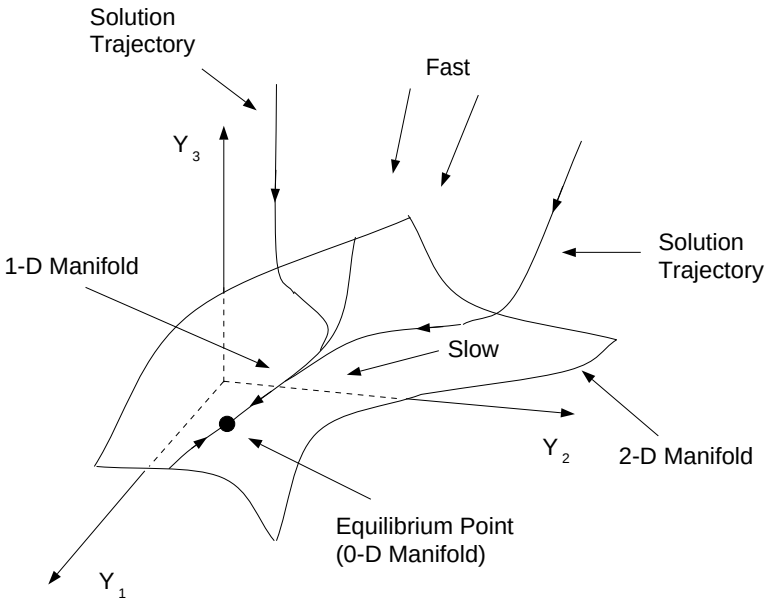
Chemical Kinetics Modeled as a Dynamical System

- ILDM developed for spatially homogeneous premixed reactor:

$$\frac{d\mathbf{y}}{dt} = \mathbf{f}(\mathbf{y}), \quad \mathbf{y}(0) = \mathbf{y}_0, \quad \mathbf{y} \in \mathbb{R}^n,$$

$$\mathbf{y} = (h, p, Y_1, Y_2, ..., Y_{n-2})^T.$$

- $\mathbf{f}(\mathbf{y})$ from Arrhenius kinetics.
- Closed with equation of state.



Eigenvalues and Eigenvectors from Decomposition of Jacobian

$$\mathbf{f_y} = \mathbf{J} = \mathbf{V}\mathbf{\Lambda}\tilde{\mathbf{V}}, \qquad \tilde{\mathbf{V}} = \mathbf{V}^{-1},$$

$$\mathbf{V} = \left(\begin{array}{ccc:ccc} | & & | & | & & | \\ \mathbf{v}_1 & \cdots & \mathbf{v}_m & \mathbf{v}_{m+1} & \cdots & \mathbf{v}_n \\ | & & | & | & & | \end{array}\right) = \left(\begin{array}{c:c} \mathbf{V}_s & \mathbf{V}_f \end{array}\right),$$

$$\mathbf{\Lambda} = \left(\begin{array}{ccc:ccc} \lambda_{(1)} & & 0 & & & \\ & \ddots & & & 0 & \\ 0 & & \lambda_{(m)} & & & \\ \hdashline & & & \lambda_{(m+1)} & & 0 \\ & 0 & & & \ddots & \\ & & & 0 & & \lambda_{(n)} \end{array}\right) = \left(\begin{array}{c:c} \mathbf{\Lambda}_{(s)} & 0 \\ \hdashline 0 & \mathbf{\Lambda}_{(f)} \end{array}\right),$$

$$\tilde{\mathbf{V}} = \left(\begin{array}{ccc} - & \tilde{\mathbf{v}}_1 & - \\ & \vdots & \\ - & \tilde{\mathbf{v}}_m & - \\ \hdashline - & \tilde{\mathbf{v}}_{m+1} & - \\ & \vdots & \\ - & \tilde{\mathbf{v}}_n & - \end{array}\right) = \left(\begin{array}{c} \tilde{\mathbf{V}}_s \\ \hdashline \tilde{\mathbf{V}}_f \end{array}\right).$$

The time scales associated with the dynamical system are the reciprocal of the eigenvalues:

$$\tau_i = \frac{1}{|\lambda_{(i)}|}.$$

Mathematical Model for ILDM

- With $\mathbf{z} = \mathbf{V}^{-1}\mathbf{y}$

$$\frac{1}{\lambda_{(i)}}\left(\frac{dz_i}{dt} + \tilde{\mathbf{v}}_i \sum_{j=1}^{n} \frac{d\mathbf{v}_j}{dt} z_j\right) = z_i + \frac{\tilde{\mathbf{v}}_i \mathbf{g}}{\lambda_{(i)}}, \text{ for } i = 1, \ldots, n,$$

  where $\mathbf{g} = \mathbf{f} - \mathbf{f}_\mathbf{y}\mathbf{y}$.

- $\frac{1}{\lambda_{(m+1)}}, \ldots, \frac{1}{\lambda_{(n)}}$ are the small parameters, as in singularly perturbed systems.

- Equilibrating the fast dynamics

$$\underbrace{z_i + \frac{\tilde{\mathbf{v}}_i \mathbf{g}}{\lambda_{(i)}} = 0,}_{\text{ILDM}} \text{ for } i = m+1, \ldots, n.$$

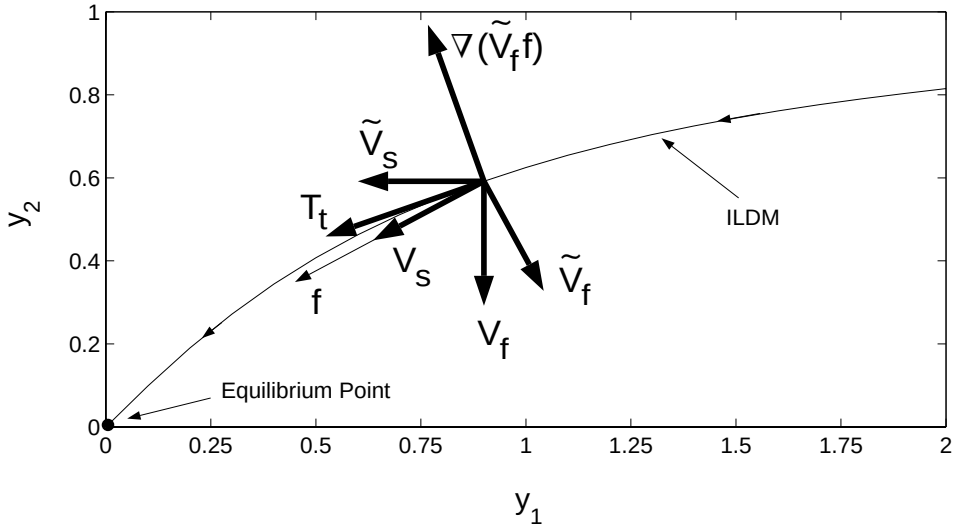
$$\Rightarrow \quad \underbrace{\tilde{\mathbf{V}}_f \mathbf{f} = \mathbf{0}}_{\text{ILDM}}.$$

- Slow dynamics approximated from differential algebraic equations on the ILDM

$$\begin{aligned} \tilde{\mathbf{V}}_s \frac{d\mathbf{y}}{dt} &= \tilde{\mathbf{V}}_s \mathbf{f}, \\ \mathbf{0} &= \tilde{\mathbf{V}}_f \mathbf{f}. \end{aligned}$$

SIM vs. ILDM

- An invariant manifold is defined as a subspace $S \subset \mathbb{R}^n$ if for any solution $\mathbf{y}(t)$, $\mathbf{y}(0) \in S$, implies that for some $T > 0$, $\mathbf{y}(t) \in S$ for all $t \in [0, T]$.
- Slow Invariant Manifold (SIM) is a trajectory in phase space, and the vector $\mathbf{f}$ must be tangent to it.
- *ILDM is an approximation of the SIM and is not a phase space trajectory.*



- ILDM approximation gives rise to an intrinsic error which decreases as stiffness increases.

Demonstration that ILDM is not a trajectory in phase space.

- Normal vector to the ILDM is given by

$$\nabla(\underbrace{\tilde{\mathbf{V}}_f \mathbf{f}}_{\text{ILDM}}) = \tilde{\mathbf{V}}_f \mathbf{J} + (\nabla \tilde{\mathbf{V}}_f)\mathbf{f}$$

$$= \lambda_{(f)} \tilde{\mathbf{V}}_f + (\nabla \tilde{\mathbf{V}}_f)\mathbf{f},$$

  where in two dimensions $\lambda_{(f)} = \lambda_{(2)}$.

- If $\mathbf{f}$ is linear, $\nabla \tilde{\mathbf{V}}_f = \mathbf{0}$. Normal to the ILDM is parallel to $\tilde{\mathbf{V}}_f$ and orthogonal to $\mathbf{f}$ in two dimensions. ILDM is a trajectory.

- If $\mathbf{f}$ is non-linear, $\nabla \tilde{\mathbf{V}}_f \neq \mathbf{0}$. Normal to the ILDM is not parallel to $\tilde{\mathbf{V}}_f$ and not orthogonal to $\mathbf{f}$ in two dimensions. ILDM is not a trajectory.

- The second term on RHS is a local measure of the curvature of the manifold. ILDM approximates the SIM well for small curvatures of the manifold.

- In the limit of large $\lambda_{(f)}$ the deviation of the ILDM from a phase space trajectory, and the SIM is small.

Comparison of the SIM with the ILDM

- Example from Davis and Skodje, J. Chem. Phys. 1999:

$$\frac{d\mathbf{y}}{dt} = \frac{d}{dt}\begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} -y_1 \\ -\gamma y_2 + \frac{(\gamma-1)y_1+\gamma y_1^2}{(1+y_1)^2} \end{pmatrix} = \mathbf{f}(\mathbf{y}),$$

- $$\mathbf{f_y} = \begin{pmatrix} -1 & 0 \\ \frac{\gamma-1+(\gamma+1)y_1}{(1+y_1)^3} & -\gamma \end{pmatrix}, \qquad \text{Jacobian}$$

$$\tilde{\mathbf{v}}_1 = \tilde{\mathbf{V}}_s = \begin{pmatrix} 1 & 0 \end{pmatrix}, \qquad \lambda_{(1)} = \lambda_{(s)} = -1, \qquad \text{slow}$$
$$\tilde{\mathbf{v}}_2 = \tilde{\mathbf{V}}_f = \begin{pmatrix} -\frac{\gamma-1+(\gamma+1)y_1}{(\gamma-1)(1+y_1)^3} & 1 \end{pmatrix}, \qquad \lambda_{(2)} = \lambda_{(f)} = -\gamma, \qquad \text{fast}$$

- The ILDM for this system is given by

$$\tilde{\mathbf{V}}_f\mathbf{f} = 0 \quad \Rightarrow \quad y_2 = \frac{y_1}{1+y_1} + \frac{2y_1^2}{\gamma(\gamma-1)(1+y_1)^3}.$$

Comparison of the SIM with the ILDM

- SIM assumed to be a polynomial

$$y_2 = \sum_{k=0}^{\infty} c_k y_1^k.$$

- Substituting the polynomial in the following equation

$$-\gamma y_2 + \frac{(\gamma - 1)y_1 + \gamma y_1^2}{(1 + y_1)^2} = -y_1 \frac{dy_2}{dy_1}.$$

- SIM is given by

$$y_2 = y_1(1 - y_1 + y_1^2 - y_1^3 + y_1^4 + \ldots) = \frac{y_1}{1 + y_1}.$$

- ILDM

$$\tilde{\mathbf{V}}_f \mathbf{f} = 0 \quad \Rightarrow \quad y_2 = \frac{y_1}{1 + y_1} + \frac{2y_1^2}{\gamma(\gamma - 1)(1 + y_1)^3}.$$

- For large γ or stiffness, the ILDM approaches the SIM.
- For even a slightly more complicated systems we have to resort to a numerical computation of the SIM using the method of Roussel and Fraser, 1992.
- In our experience the numerical computation of the ILDM is more tractable than that for the SIM.

Comparison of the SIM with the ILDM

- Projection of the system on the slow and fast basis.

$$\text{Slow:} \quad \tilde{\mathbf{V}}_s \frac{d\mathbf{y}}{dt} = \tilde{\mathbf{V}}_s \mathbf{f} \;\Rightarrow\; \frac{dy_1}{dt} = -y_1$$

$$\text{Fast:} \quad \tilde{\mathbf{V}}_f \frac{d\mathbf{y}}{dt} = \tilde{\mathbf{V}}_f \mathbf{f} \;\Rightarrow$$

$$\frac{1}{\gamma}\left(-\frac{\gamma - 1 + (\gamma+1)y_1}{(\gamma-1)(1+y_1)^3}\frac{dy_1}{dt} + \frac{dy_2}{dt}\right) = -y_2 + \frac{y_1}{1+y_1} + \frac{2y_1^2}{\gamma(\gamma-1)(1+y_1)^3}$$

Order of terms in the fast equation:

$$\mathcal{O}\left(\frac{1}{\gamma}\right) + \mathcal{O}\left(\frac{1}{\gamma^2}\right) + \ldots = \mathcal{O}(1) + \mathcal{O}\left(\frac{1}{\gamma}\right) + \mathcal{O}\left(\frac{1}{\gamma^2}\right) + \ldots$$

- The ILDM approximation neglects all terms on the LHS while retaining all terms on RHS of the fast equation.
- Systematic matching of terms of all orders in a singular perturbation scheme correctly leads to the SIM.

$$y_2 = \frac{y_1}{1+y_1}.$$

- The ILDM approximates the SIM well for large γ or stiffness and is a more practical method for complicated systems such as chemical kinetics.

A priori computation of m-dimensional ILDM

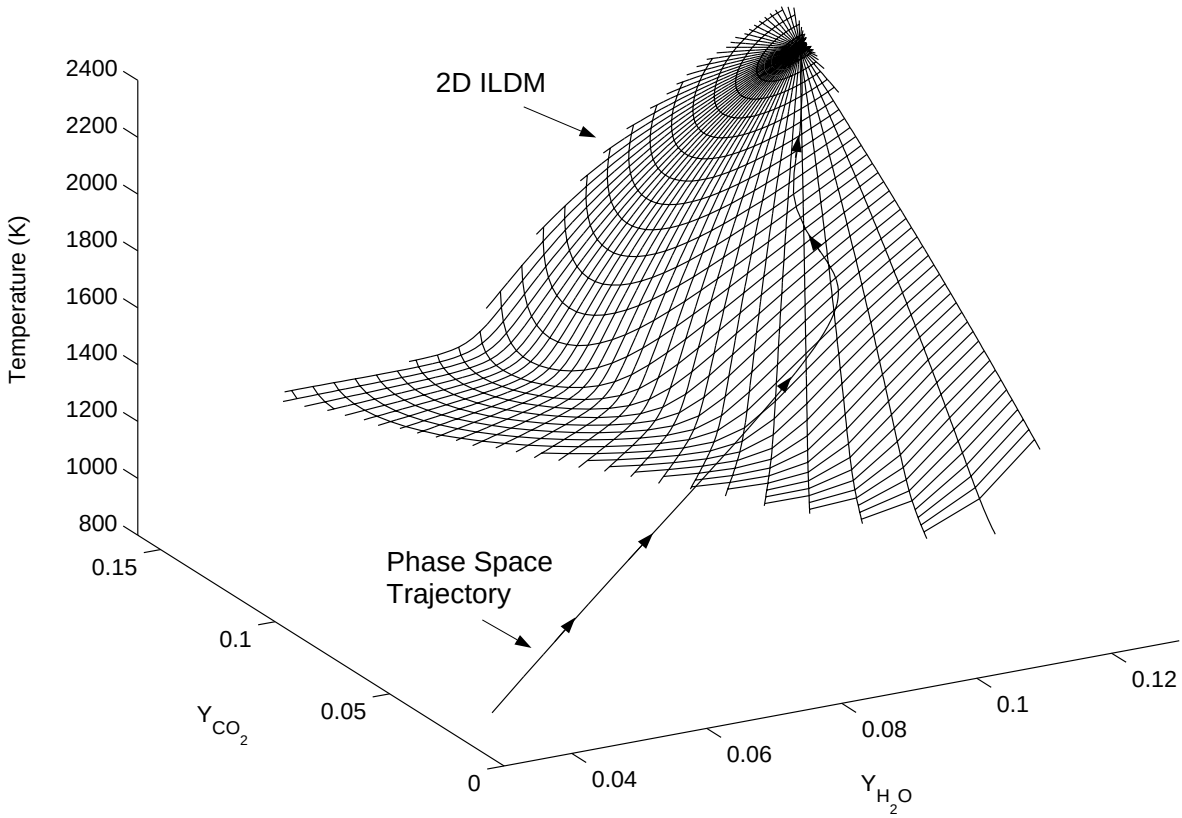
- $n-m$ algebraic equations are solved coupled with m parametric equations

$$\underbrace{\tilde{\mathbf{V}}_f \mathbf{f} = \mathbf{0}}_{n-m \text{ algebraic equations}}$$

$$\underbrace{\mathbf{R} \cdot \mathbf{P} \begin{pmatrix} y_1 - y_{10} \\ \vdots \\ y_n - y_{n0} \end{pmatrix} = \mathbf{R} \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_m \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ r \end{pmatrix}}_{m \text{ parametric equations}}$$

- $\mathbf{R}$ is m dimensional rotational matrix, $\mathbf{P}$ is $m \times n$ parametric matrix.
- $\mathbf{y}_0 = (y_{10}, \ldots, y_{n0})^T$ is the chemical equilibrium point.
- $(\alpha_1, \ldots, \alpha_m)^T$ are the m parameters.
- r is the radial distance of a point on the m dimensional ILDM from $\mathbf{y}_0$.
- Radial slices of m-dimensional ILDM are computed in the parametric space, by changing the rotation matrix $\mathbf{R}$.
- Tangent predictor and Newton's method corrector is used.

Sample 2D-ILDM for CH_4 combustion



2D-ILDM for isobaric adiabatic combustion of reactive mixture of CH_4 for $T = 298\ K$, $p = 1\ atm$, $Y_{CH_4} = 0.055$, $Y_{O_2} = 0.22$ and $Y_{N_2} = 0.725$, $17(=n-2)$ species, 58 reaction system.

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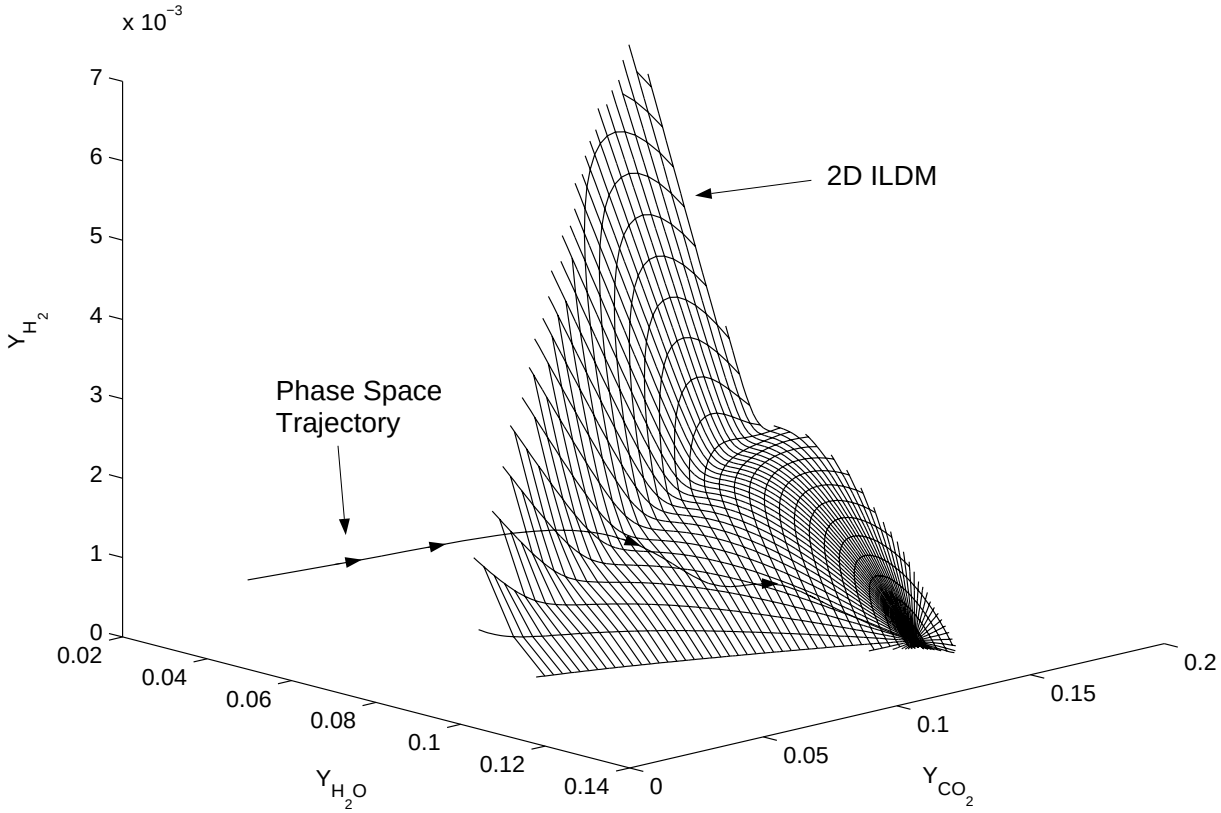

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Reaction Convection Diffusion Equations

- In one spatial dimension

$$\frac{\partial \mathbf{y}}{\partial t} = \underbrace{\mathbf{f}(\mathbf{y})}_{\text{reaction}} - \underbrace{\frac{\partial}{\partial x}\mathbf{h}(\mathbf{y})}_{\text{convection-diffusion}} .$$

- Substituting $\mathbf{z} = \mathbf{V}^{-1}\mathbf{y}$

$$\underbrace{\frac{1}{\lambda_{(i)}}\left(\frac{dz_i}{dt} + \tilde{\mathbf{v}}_i \sum_{j=1}^{n} \frac{d\mathbf{v}_j}{dt} z_j\right)}_{=0 \text{ for i=m+1,...,n}} = z_i + \frac{\tilde{\mathbf{v}}_i \mathbf{g}}{\lambda_{(i)}} - \frac{1}{\lambda_{(i)}}\left(\tilde{\mathbf{v}}_i \frac{\partial \mathbf{h}}{\partial x}\right) \text{ for } i = 1, \ldots, n.$$

- Equilibrating the fast dynamics, we get the elliptic equations

$$z_i + \frac{\tilde{\mathbf{v}}_i \mathbf{g}}{\lambda_{(i)}} - \frac{1}{\lambda_{(i)}}\left(\tilde{\mathbf{v}}_i \frac{\partial \mathbf{h}}{\partial x}\right) = 0, \text{ for } i = m+1, \ldots, n.$$

- For diffusion time scales which are of the order of the chemical time scales

$$z_i + \frac{\tilde{\mathbf{v}}_i \mathbf{g}}{\lambda_{(i)}} - \frac{1}{\lambda_{(i)}}\left(\tilde{\mathbf{v}}_i \frac{\partial \mathbf{h}}{\partial x}\right) = 0, \text{ for } i = m+1, \ldots, p.$$

- For fast chemical time scales we obtain the ILDM

$$z_i + \frac{\tilde{\mathbf{v}}_i \mathbf{g}}{\lambda_{(i)}} = 0, \text{ for } i = p+1, \ldots, n.$$

Approximate Slow Invariant Manifold (ASIM)

- Slow dynamics can be approximated by the ASIM

$$\begin{aligned}
\tilde{\mathbf{V}}_s \frac{\partial \mathbf{y}}{\partial t} &= \tilde{\mathbf{V}}_s \mathbf{f} - \tilde{\mathbf{V}}_s \frac{\partial \mathbf{h}}{\partial x}, \\
\mathbf{0} &= \tilde{\mathbf{V}}_{fs} \mathbf{f} - \tilde{\mathbf{V}}_{fs} \frac{\partial \mathbf{h}}{\partial x}, \\
\mathbf{0} &= \tilde{\mathbf{V}}_{ff} \mathbf{f}.
\end{aligned}$$

where $\tilde{\mathbf{V}}_{fs} = \begin{pmatrix} - & \tilde{\mathbf{v}}_{m+1} & - \\ & \vdots & \\ - & \tilde{\mathbf{v}}_p & - \end{pmatrix}$, $\tilde{\mathbf{V}}_{ff} = \begin{pmatrix} - & \tilde{\mathbf{v}}_{p+1} & - \\ & \vdots & \\ - & \tilde{\mathbf{v}}_n & - \end{pmatrix}$

- The diffusion term can be neglected only if the following term is small

$$\frac{1}{\lambda_{(i)}} \left(\tilde{\mathbf{v}}_i \frac{\partial \mathbf{h}}{\partial x} \right).$$

- Difficult to determine appropriate p, which is spatially dependent!

- It is difficult to determine *a priori* the diffusion length scales and hence the diffusion time scales.

Davis Skodje Example Extended to Reaction Diffusion

$$\frac{\partial \mathbf{y}}{\partial t} = \frac{\partial}{\partial t}\begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} -y_1 \\ -\gamma y_2 + \frac{(\gamma-1)y_1+\gamma y_1^2}{(1+y_1)^2} \end{pmatrix} - \frac{\partial}{\partial x}\begin{pmatrix} -\mathcal{D}\frac{\partial y_1}{\partial x} \\ -\mathcal{D}\frac{\partial y_2}{\partial x} \end{pmatrix} = \mathbf{f}(\mathbf{y}) - \frac{\partial}{\partial x}\mathbf{h}(\mathbf{y})$$

- Boundary conditions are chosen on the ILDM

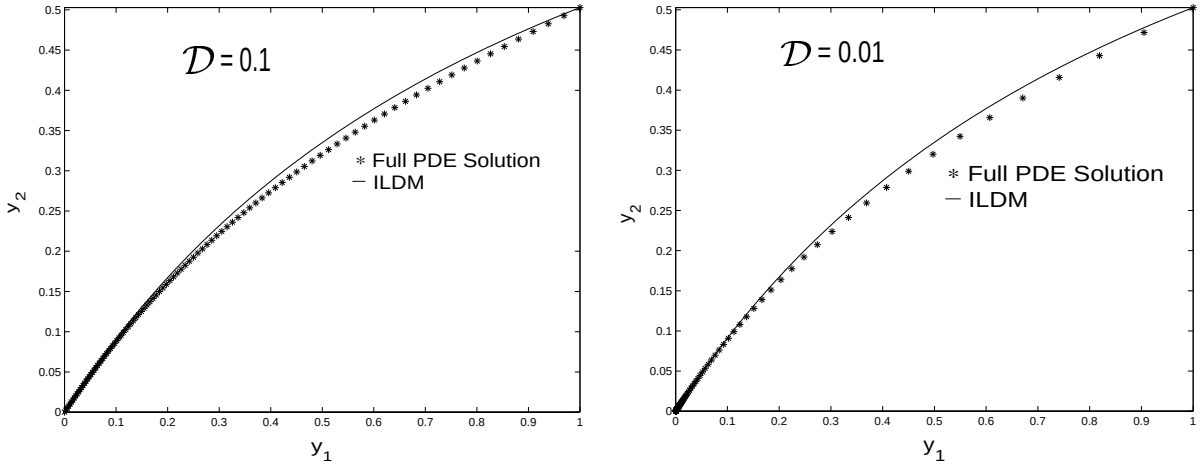
$$y_1(t,0) = 0, \;\; y_1(t,1) = 1,$$

$$y_2(t,0) = 0, \;\; y_2(t,1) = \tfrac{1}{2} + \tfrac{1}{4\gamma(\gamma-1)}.$$

- Initial conditions

$$y_1(0,x) = x, \quad y_2(0,x) = \left(\frac{1}{2} + \frac{1}{4\gamma(\gamma-1)}\right) x$$

Reaction Diffusion Example Results: Low Stiffness

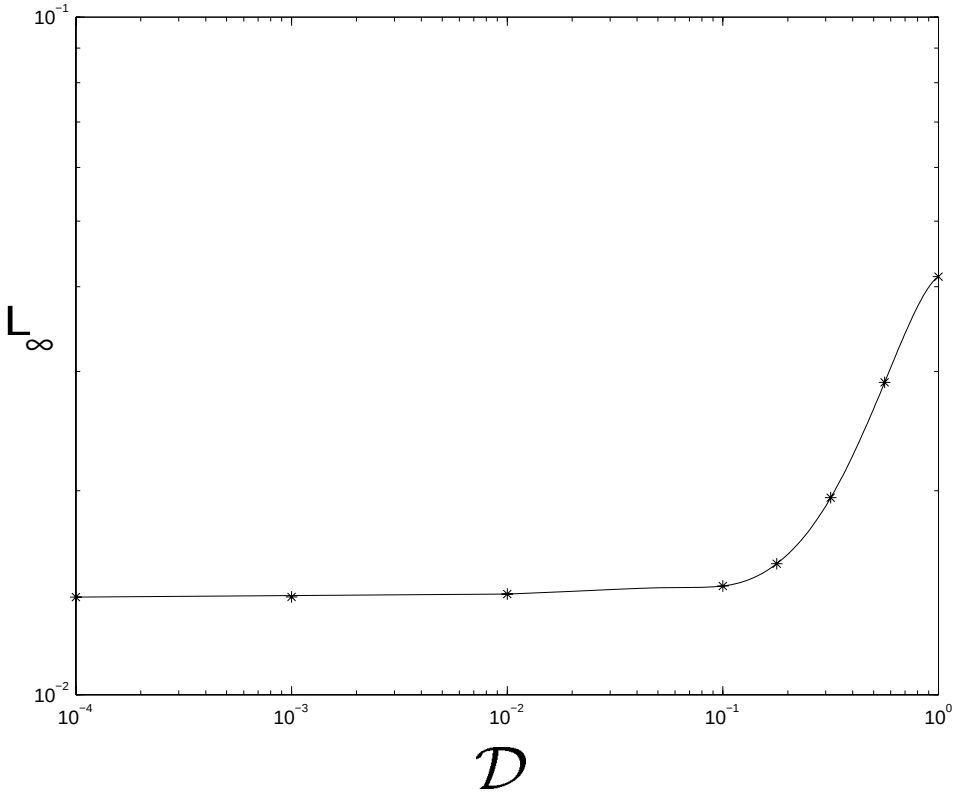


(a) (b)

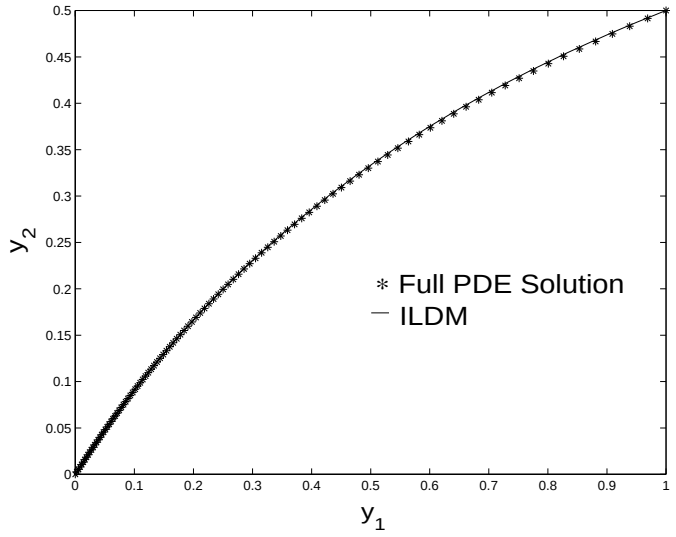
- Solution at $t = 5$, for $\gamma = 10$ with varying $\mathcal{D}$.
- PDE solution fully resolved; no ILDM or convection-diffusion correction.
- Forcing the solution onto the ILDM will induce large errors.

Reaction Diffusion Example Results: Low Stiffness

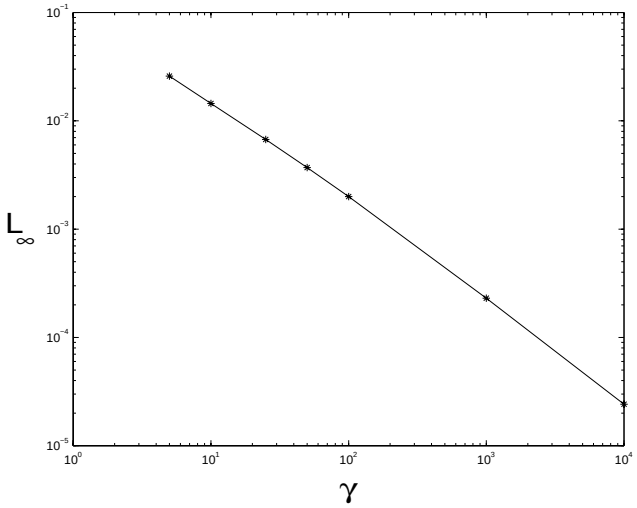
- Modification of $\mathcal{D}$ alone for fixed γ does not significantly change the error.



Reaction Diffusion Example Results: High Stiffness



- Solution at $t = 5$, for $\gamma = 100$ and $\mathcal{D} = 0.1$.
- Increasing γ moves solution closer to the ILDM.



Comparison of the ASIM and the MPP

- The slow dynamics for the simple system obtained using the ASIM by taking $n = 2$, $m = 1$, $p = n$

$$\begin{aligned} \frac{\partial y_1}{\partial t} &= -y_1 + \mathcal{D}\frac{\partial^2 y_1}{\partial x^2} \\ y_2 - \frac{1}{\gamma}\frac{\partial^2 y_2}{\partial x^2} &= \frac{y_1}{1+y_1} + \frac{2y_1^2}{\gamma(\gamma-1)(1+y_1)^3} - \left(\frac{\gamma - 1 + (\gamma+1)y_1}{\gamma(\gamma-1)(1+y_1)^3}\right)\frac{\partial^2 y_1}{\partial x^2} \end{aligned}$$

- The Maas and Pope projection (MPP) method is given by projecting the convection diffusion term along the local slow subspace on the reaction ILDM, hence, ensuring that the slow dynamics occurs on the ILDM

$$\frac{\partial \mathbf{y}}{\partial t} = \mathbf{f}(\mathbf{y}) - \mathbf{V}_s\tilde{\mathbf{V}}_s\frac{\partial}{\partial x}\left(\mathbf{h}(\mathbf{y})\right).$$

- For the simple system the corresponding equations are given by

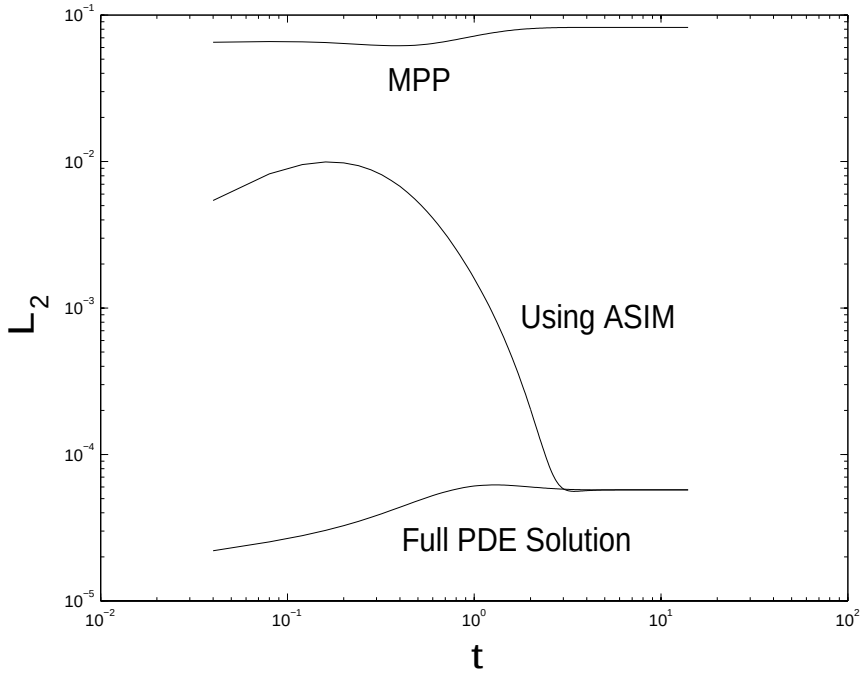
$$\begin{aligned} \frac{\partial y_1}{\partial t} &= -y_1 + \mathcal{D}\frac{\partial^2 y_1}{\partial x^2}, \\ \frac{\partial y_2}{\partial t} &= -\gamma y_2 + \frac{(\gamma-1)y_1 + \gamma y_1^2}{(1+y_1)^2} - \left(\frac{\gamma - 1 + (\gamma+1)y_1}{\gamma(\gamma-1)(1+y_1)^3}\right)\mathcal{D}\frac{\partial^2 y_1}{\partial x^2}. \end{aligned}$$

- The slow dynamics for the simple system obtained using the MPP method by taking $n = 2$ and $m = p = 1$.

$$\begin{aligned} \frac{\partial y_1}{\partial t} &= -y_1 + \mathcal{D}\frac{\partial^2 y_1}{\partial x^2}, \\ y_2 &= \frac{y_1}{1+y_1} + \frac{2y_1^2}{\gamma(\gamma-1)(1+y_1)^3}. \end{aligned}$$

Comparison of the ASIM and the MPP

- Solutions obtained by the MPP, the ASIM, and full equations, all calculated on a fixed grid with 100 points.
- All results compared to solution of full equations at high spatial resolution of 10000 grid points.
- $\gamma = 10$ and $\mathcal{D} = 0.1$.
- Forcing the solution onto the ILDM leads to large errors in the MPP method.
- Overall the error when using the ASIM is lower than the error when using the MPP, and is similar to that incurred by the full equations near steady state.



1D Premixed Laminar Flame for Ozone Decomposition

- Governing equations of one-dimensional, isobaric, premixed laminar flame for ozone decomposition in Lagrangian coordinates for low Mach number flows, Margolis, 1978.

$$\begin{aligned}
\frac{\partial T}{\partial t} &= -\frac{1}{\rho c_p}\sum_{k=1}^{3}\dot{\omega}_k M_k h_k + \frac{1}{c_p}\frac{\partial}{\partial \psi}\left(\rho\lambda\frac{\partial T}{\partial \psi}\right), \\
\frac{\partial Y_k}{\partial t} &= \frac{1}{\rho}\dot{\omega}_k M_k + \frac{\partial}{\partial \psi}\left(\rho^2 \mathcal{D}_k \frac{\partial Y_k}{\partial \psi}\right), \text{ for } k = 1, 2, 3,
\end{aligned}$$

- Equation of state

$$p_0 = \rho \Re T \sum_{k=1}^{3}\frac{Y_k}{M_k},$$

- $Le = 1$.
- $c_p = 1.056 \times 10^7$ erg/(g-K).
- $\rho\lambda = 4.579 \times 10^{-2}$ g^2/(cm^2-s^3-K).
- $\mathcal{D}_1 = \mathcal{D}_2 = \mathcal{D}_3 = \mathcal{D}$.
- $\rho^2\mathcal{D} = 4.336 \times 10^{-7}$ g^2/(cm^4-s).
- $Y_1 = Y_O$, $Y_2 = Y_{O_2}$, $Y_3 = Y_{O_3}$.
- $p_0 = 8.32 \times 10^5$ dynes/cm^2.

1D Premixed Laminar Flame for CH_4 combustion

- Governing equations of one-dimensional, isobaric, premixed laminar flame for methane combustion for low Mach number flows

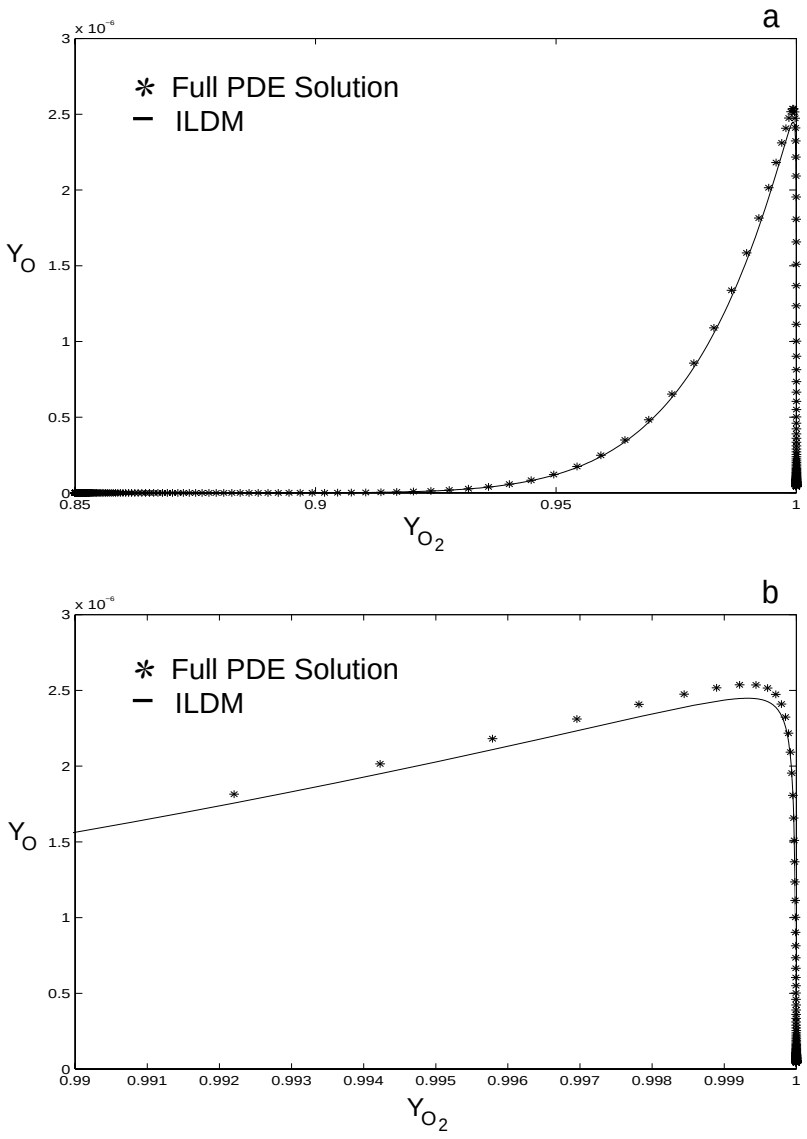
$$
\begin{aligned}
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} &= 0 \\
\rho c_p \frac{\partial T}{\partial t} + \rho u c_p \frac{\partial T}{\partial x} &= -\sum_{k=1}^{17} \dot{\omega}_k M_k h_k + \frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x}\right) \\
&\quad -\rho \sum_{k=1}^{17} \mathcal{D}_k c_{p_k} \frac{\partial Y_k}{\partial x}\frac{\partial T}{\partial x}, \\
\rho \frac{\partial Y_k}{\partial t} + \rho u \frac{\partial Y_k}{\partial x} &= \dot{\omega}_k M_k + \frac{\partial}{\partial x}\left(\rho \mathcal{D}_k \frac{\partial Y_k}{\partial x}\right), \text{ for } k = 1, \ldots, 17
\end{aligned}
$$

- Equation of state

$$
p_0 = \rho \Re T \sum_{k=1}^{17} \frac{Y_k}{M_k},
$$

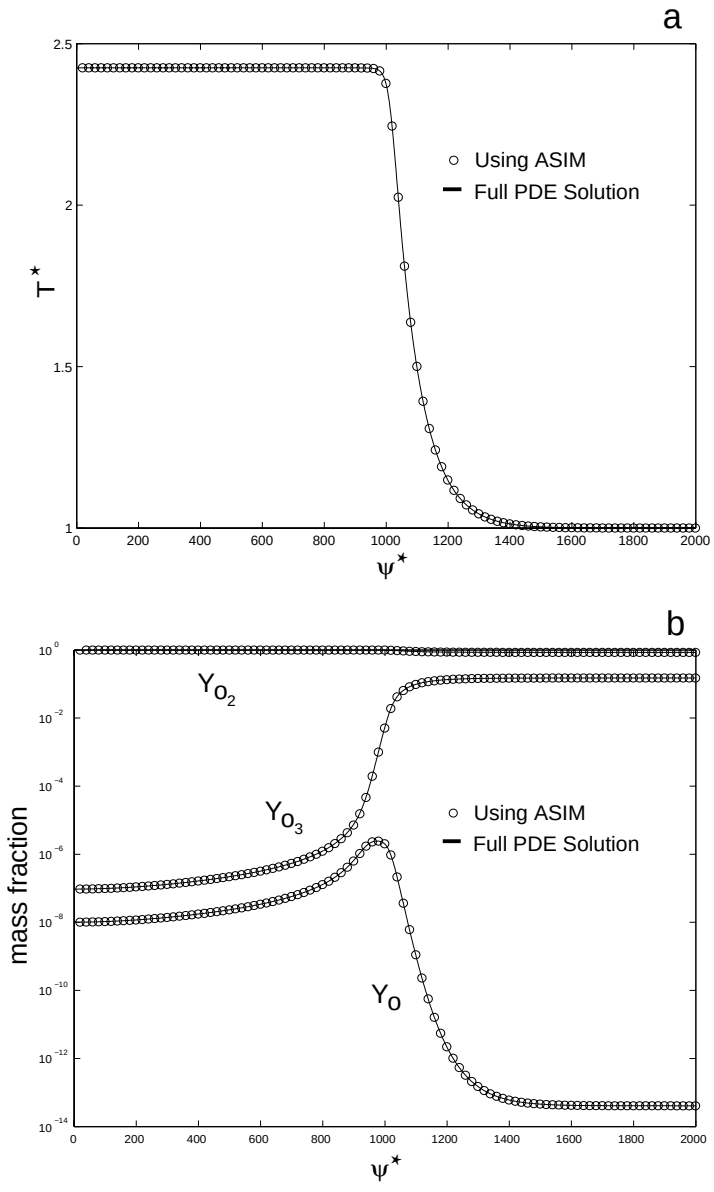
Comparison of the ILDM with the PDE solution for ozone decomposition flame

For unreacted mixture of $Y_{O_2} = 0.85$, $Y_{O_3} = 0.15$ at $T = 300K$



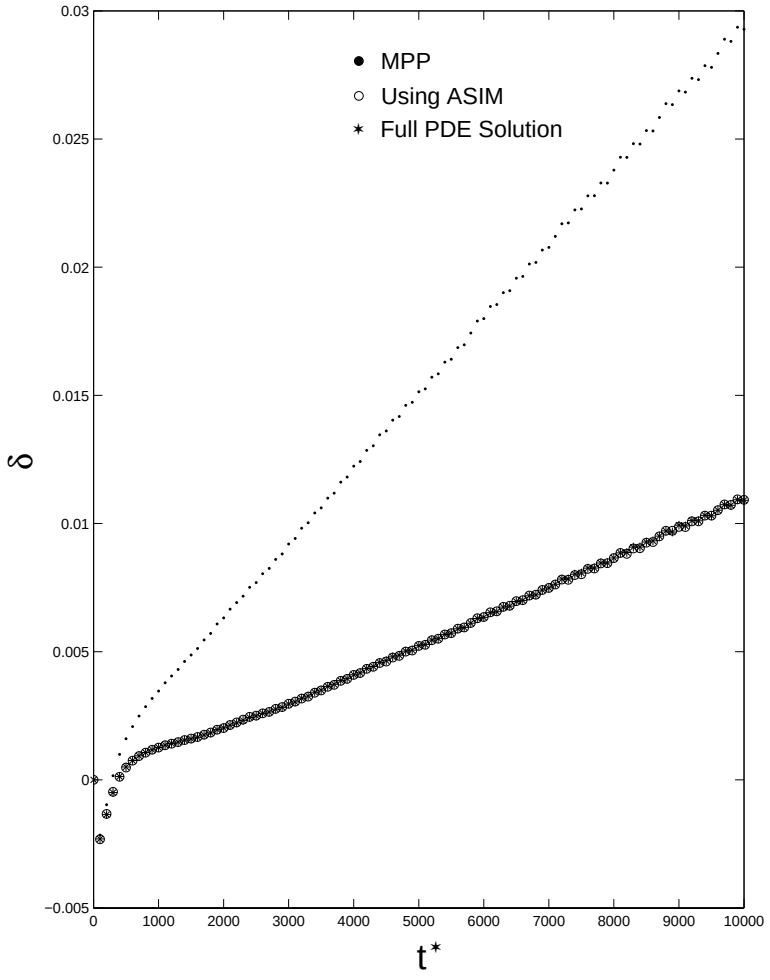
Profiles for 1D Premixed Laminar Flame for Ozone Decomposition

For unreacted mixture of $Y_{O_2} = 0.85$, $Y_{O_3} = 0.15$ at $T = 300K$

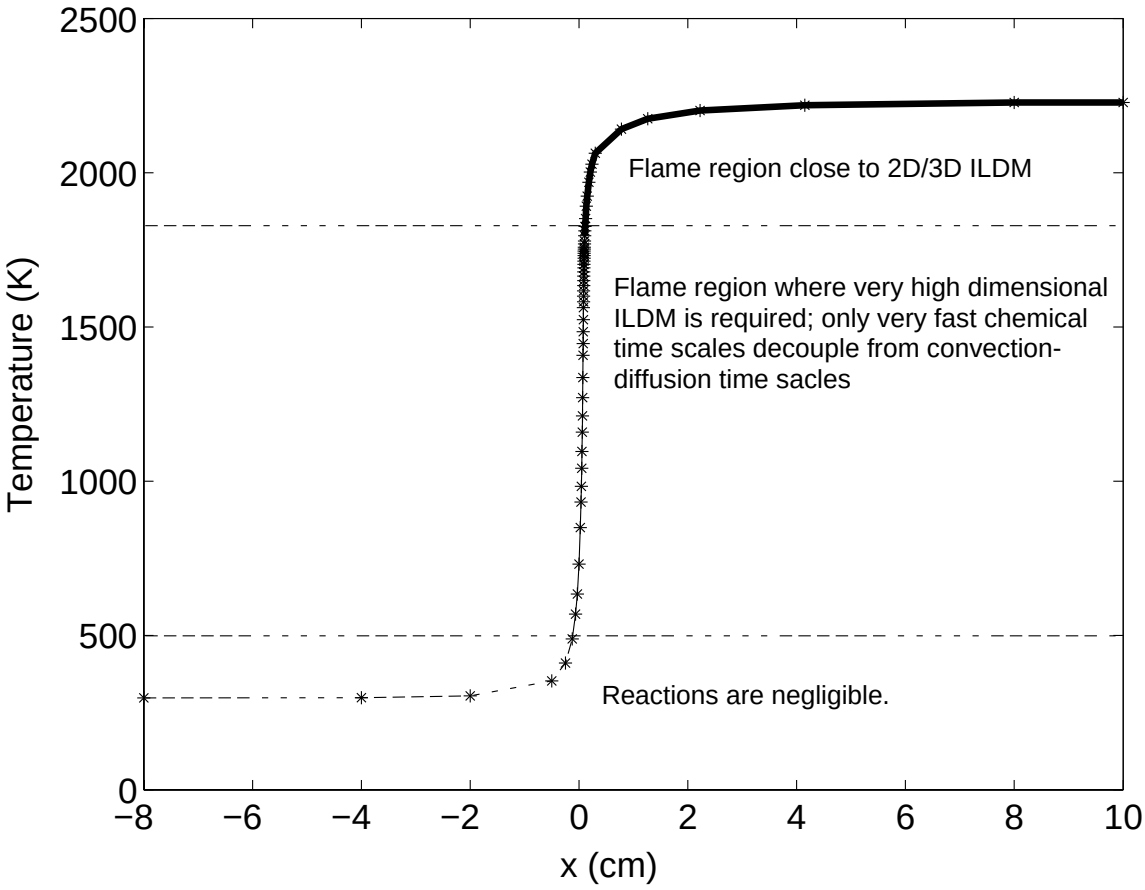


Comparison of phase errors incurred by the MPP, the ASIM and full integration.

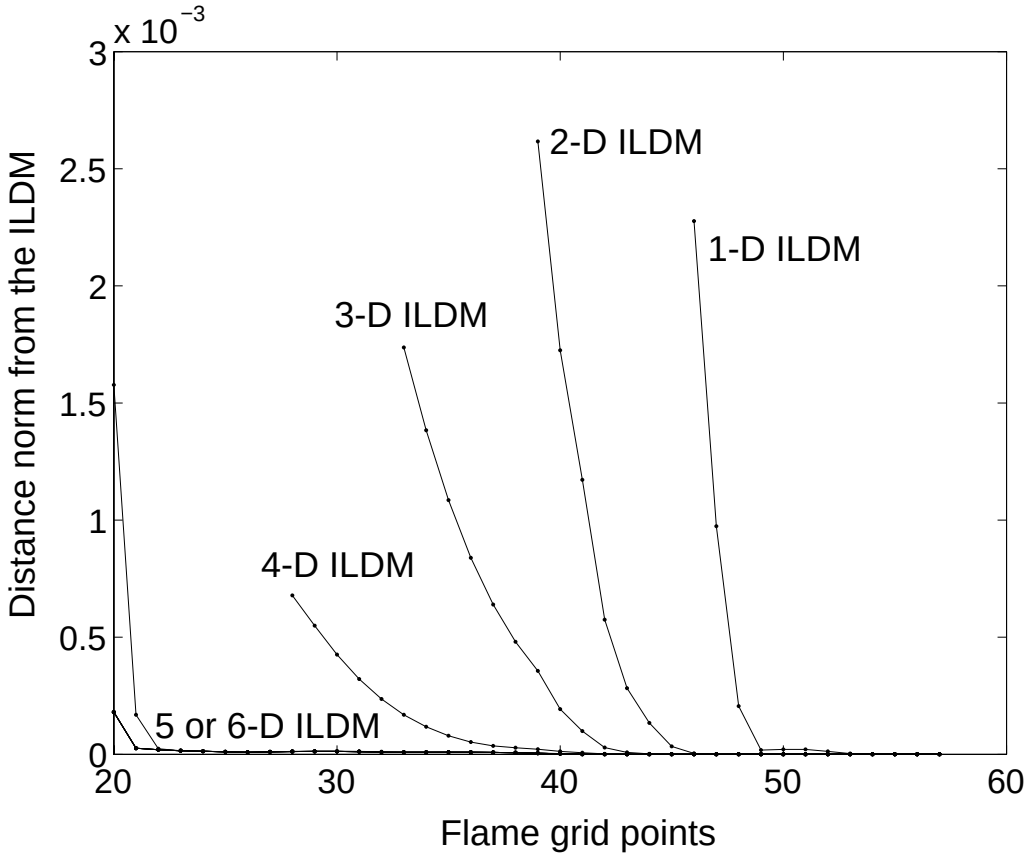
- For unreacted mixture of $Y_{O_2} = 0.85$, $Y_{O_3} = 0.15$ at $T = 300K$.
- The phase error δ is measured as the Lagrangian distance between the location within the flame front where the mass fraction of O_3 is 0.075, for the solution obtained by the three methods, for 1000 grid points, and the full integration solution at 10000 grid points.

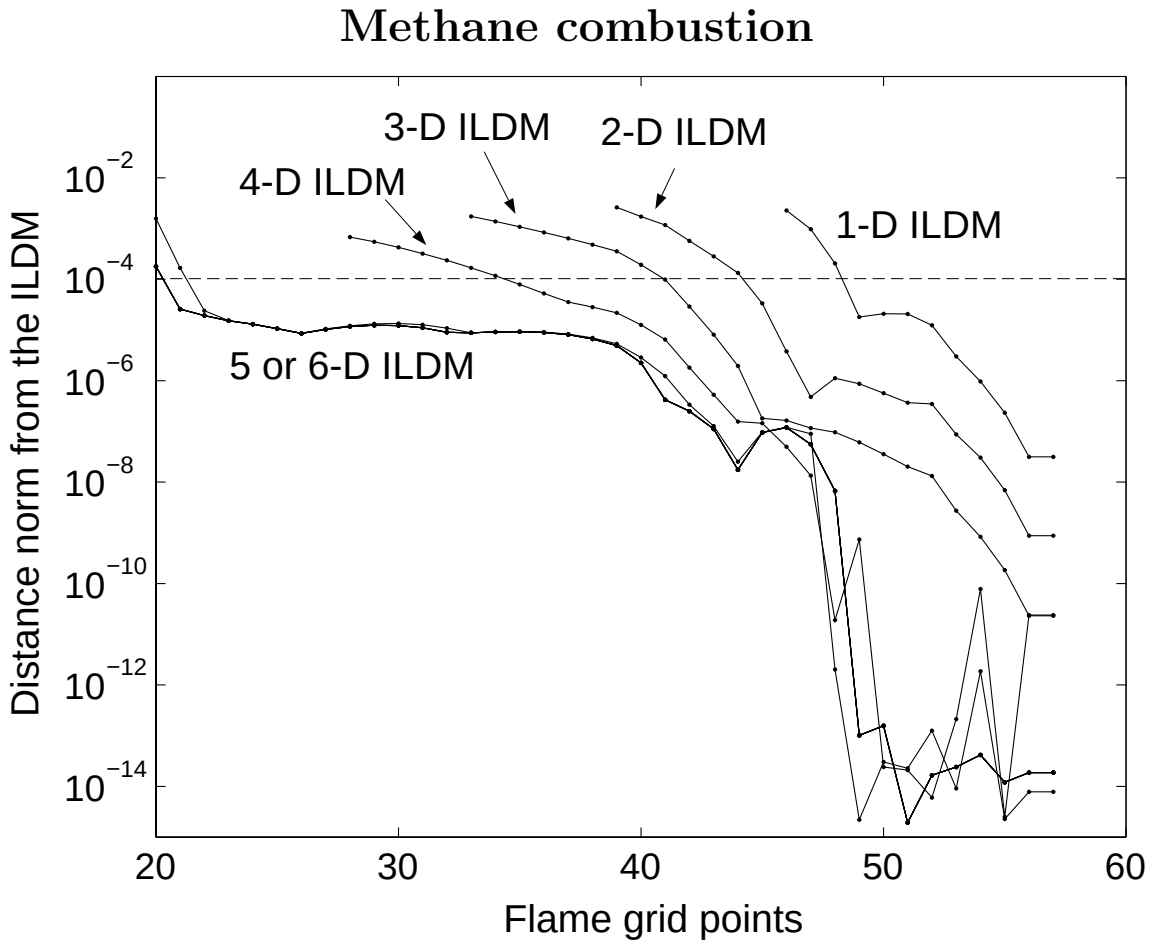


Methane combustion

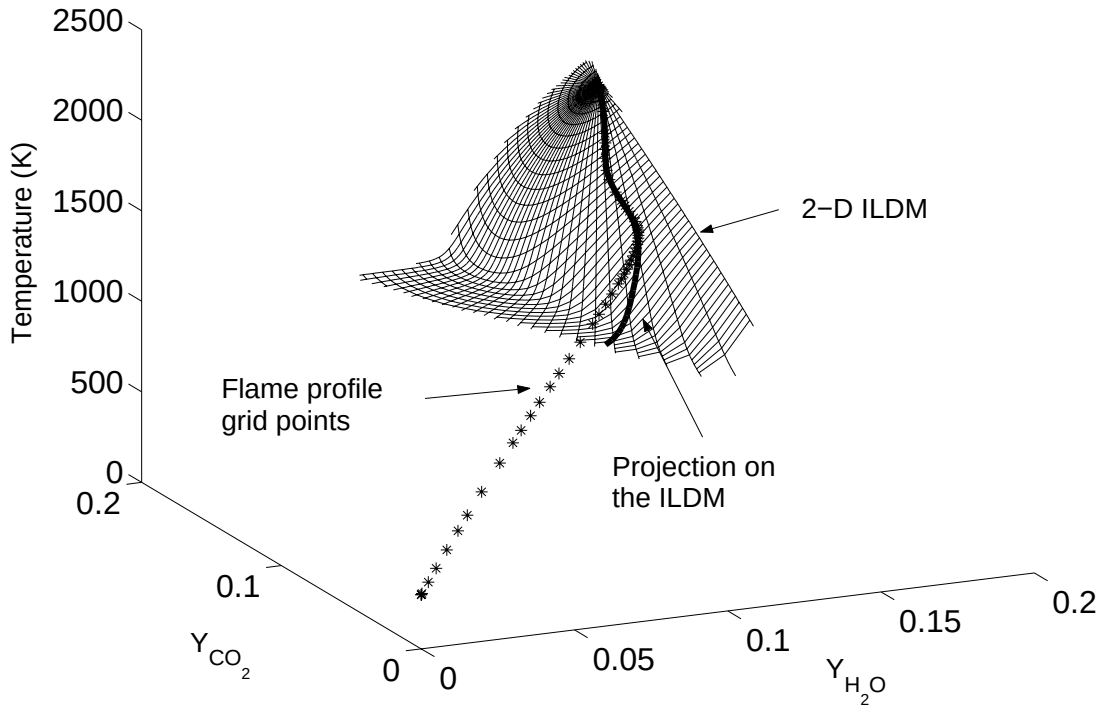


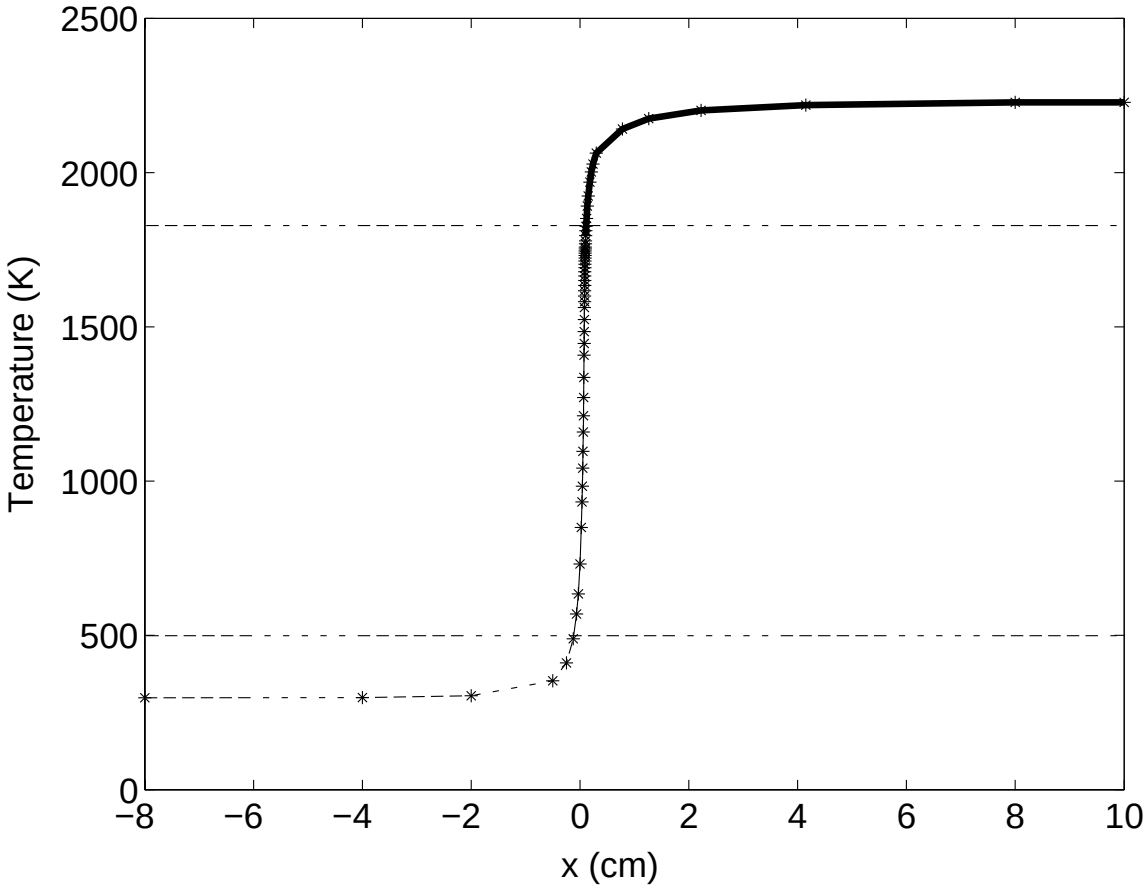
Methane combustion




Methane combustion
3-D ILDM
2-D ILDM
4-D ILDM
1-D ILDM
5 or 6-D ILDM
Distance norm from the ILDM
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
20
30
40
50
60
Flame grid points

Methane combustion




2500
2000
1500
1000
500
0
Temperature (K)
−8
−6
−4
−2
0
2
4
6
8
10
x (cm)

Conclusions

- ILDM approaches SIM in the limit of large stiffness for spatially homogeneous systems.
- Difficult to use SIM in practical combustion calculations while ILDM works well.
- No robust analysis currently exists to determine convection and diffusion time scales *a priori*.
- For systems in which convection and diffusion have time scales comparable to those of reaction, MPP method can lead to a large transient and steady state error.
- The ASIM couples reaction, convection and diffusion while systematically equilibrating fast time scales.
- At this point the fast and slow subspace decomposition is dependent only on reaction and should itself be modified to include fast and slow convection-diffusion time scales.
- The error incurred in approximating the slow dynamics by the ASIM is smaller than that incurred by the MPP; in general this error can be primarily attributed to the failure of MPP to satisfy boundary condtions.

Linearization of ASIM about the ILDM

$$\begin{pmatrix} \tilde{\mathbf{V}}_{s0}\frac{\partial \mathbf{y}}{\partial t} \\ \mathbf{0} \end{pmatrix} = \begin{pmatrix} \tilde{\mathbf{V}}_{s0}\mathbf{F}(\mathbf{y}_0) \\ \mathbf{0} \end{pmatrix} + \begin{pmatrix} \tilde{\mathbf{V}}_{s0} \\ \tilde{\mathbf{V}}_{f0} \end{pmatrix} \left(\mathbf{J}|_{\mathbf{y}=\mathbf{y}_0}(\mathbf{y}-\mathbf{y}_0) - \frac{\partial}{\partial x}\left(\mathbf{h}(\mathbf{y}_0) + \frac{\partial \mathbf{h}}{\partial \mathbf{y}}|_{\mathbf{y}=\mathbf{y}_0}(\mathbf{y}-\mathbf{y}_0) \right) \right)$$

- $\mathbf{y}_0$ is the solution of the ILDM $\tilde{\mathbf{V}}_s\mathbf{F}(\mathbf{y}) = 0$.
- Expensive computation of the fast and slow basis vectors not required during reactive flow computations, as they stored as a lookup table along the ILDM.

Operator Splitting Method

- Reactive flow equations are solved in two steps using Strang splitting.
  - Equivalent to a spatially homogeneous premixed reactor at every point in the co-ordinate space. Uses the ILDM look up tables and time integration of m ODE (for m dimensional ILDM)

$$\frac{\partial \mathbf{y}}{\partial t} = \mathbf{F}(\mathbf{y}).$$

  - Physical perturbation off the ILDM due to convection and diffusion,

$$\frac{\partial \mathbf{y}}{\partial t} = -\frac{\partial \mathbf{h}(\mathbf{y})}{\partial x}.$$

    Then linear projection back onto the ILDM along the fast subspace.

Maas and Pope Projection (MPP)

- The Maas and Pope projection (MPP) method is given by projecting the convection diffusion term along the local slow subspace on the reaction ILDM, hence, ensuring that the slow dynamics occurs on the ILDM

$$\frac{\partial \mathbf{y}}{\partial t} = \mathbf{f}(\mathbf{y}) - \mathbf{V}_s \tilde{\mathbf{V}}_s \frac{\partial}{\partial x} \left(\mathbf{h}(\mathbf{y}) \right).$$