On the Computation of Approximate Slow Invariant Manifolds

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Major Issues in Reduced Modeling of Reactive Flows

- How to construct a Slow Invariant Manifold (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

- Davis and Skodje, *JCP*, 1999: demonstration that (Intrinsic Low Dimensional Manifold) ILDM is not SIM in simple non-linear ODEs, finds SIM in simple ODEs,

- Singh, Powers, and Paolucci, *JCP*, 2002: use ILDM to construct Approximate SIM (ASIM) in simple and detailed PDEs,

- Ren and Pope, *C&F*, 2006: show conditions for chemical manifold to approximate reaction-diffusion system,

- Davis, *JPC*, 2006: systematic development of manifolds for reaction-diffusion,

Motivation

• Severe stiffness in reactive flow systems with detailed gas phase chemical kinetics renders fully resolved simulations of many systems to be impractical.

• ILDM method can reduce computational time while retaining essential fidelity of full detailed kinetics.

• The ILDM is only an approximation of the SIM.

• Using ILDM in systems with diffusion can lead to large errors at boundaries and when diffusion time scales are comparable to those of reactions.

• An Approximate Slow Invariant Manifold (ASIM) is developed for systems where reactions couple with diffusion.
Chemical Kinetics Modeled as a Dynamical System

- ILDM developed for spatially homogeneous premixed reactor:

\[
d\frac{y}{dt} = f(y), \quad y(0) = y_0, \quad y \in \mathbb{R}^n, \\
y = (h, p, Y_1, Y_2, \ldots, Y_{n-2})^T.
\]
Eigenvalues and Eigenvectors from Decomposition of Jacobian

\[ f_y = J = V \Lambda \tilde{V}, \quad \tilde{V} = V^{-1}, \]
\[ V = \begin{pmatrix} V_s & V_f \end{pmatrix}, \]
\[ \Lambda = \begin{pmatrix} \Lambda(s) & 0 \\ 0 & \Lambda(f) \end{pmatrix}. \]

• 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 $z = \tilde{V} y$ and $g = f - f_y y$

$$
\frac{1}{\lambda(i)} \left( \frac{dz_i}{dt} + \tilde{v}_i \sum_{j=1}^{n} \frac{dv_j}{dt} z_j \right) = z_i + \frac{\tilde{v}_i g}{\lambda(i)}, \quad i = 1, \ldots, n,
$$

• By equilibrating the fast dynamics

$$
z_i + \frac{\tilde{v}_i g}{\lambda(i)} = 0, \quad i = m + 1, \ldots, n. \quad \Rightarrow \tilde{V}_f f = 0. \quad \text{ILDM}
$$

• Slow dynamics approximated from differential algebraic equations on the ILDM

$$
\tilde{V}_s \frac{dy}{dt} = \tilde{V}_s f, \quad 0 = \tilde{V}_f f.
$$
**SIM vs. ILDM**

- An invariant manifold is defined as a subspace $S \subset \mathbb{R}^n$ if for any solution $y(t), y(0) \in S$, implies that for some $T > 0$, $y(t) \in S$ 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.
Comparison of the SIM with the ILDM

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

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

- The ILDM for this system is given by

\[
\tilde{V}_f f = 0, \quad \Rightarrow \quad y_2 = \frac{y_1}{1+y_1} + \frac{2y_1^2}{\gamma(\gamma-1)(1+y_1)^3},
\]

- while the SIM is given by

\[
y_2 = y_1 (1 - y_1 + y_1^2 - y_1^3 + y_1^4 + \ldots) = \frac{y_1}{1+y_1}.
\]
Construction of the SIM via Trajectories

- An exact SIM can be found by identifying *all* critical points and connecting them with trajectories (Davis, Skodie, 1999; Creta, *et al.* 2006).
- Useful for ODEs.
- Equilibrium points at infinity must be considered.
- Not all invariant manifolds are attracting.
Zel’dovich Mechanism for $NO$ Production

\[ N + NO \rightleftharpoons N_2 + O \]
\[ N + O_2 \rightleftharpoons NO + O \]

- spatially homogeneous,
- isothermal and isobaric, $T = 6000 \, K$, $P = 2.5 \, bar$,
- law of mass action with reversible Arrhenius kinetics,
- kinetic data from Baulch, et al., 2005,
Zel’dovich Mechanism: ODEs

\[
\begin{align*}
\frac{d[NO]}{dt} &= r_2 - r_1 = \dot{\omega}_{[NO]}, \quad [NO](t = 0) = [NO]_o, \\
\frac{d[N]}{dt} &= -r_1 - r_2 = \dot{\omega}_{[N]}, \quad [N](t = 0) = [N]_o, \\
\frac{d[N_2]}{dt} &= r_1 = \dot{\omega}_{[N_2]}, \quad [N_2](t = 0) = [N_2]_o, \\
\frac{d[O]}{dt} &= r_1 + r_2 = \dot{\omega}_{[O]}, \quad [O](t = 0) = [O]_o, \\
\frac{d[O_2]}{dt} &= -r_2 = \dot{\omega}_{[O_2]}, \quad [O_2](t = 0) = [O_2]_o,
\end{align*}
\]

\[
\begin{align*}
r_1 &= k_1[N][NO] \left(1 - \frac{1}{K_{eq1} [N][NO]} \right), \quad K_{eq1} = \exp \left( \frac{-\Delta G_{1}^o}{\mathcal{R}T} \right) \\
r_2 &= k_2[N][O_2] \left(1 - \frac{1}{K_{eq2} [N][O_2]} \right), \quad K_{eq2} = \exp \left( \frac{-\Delta G_{2}^o}{\mathcal{R}T} \right).
\end{align*}
\]
Zel’dovich Mechanism: DAEs

\[
\frac{d[NO]}{dt} = \dot{\omega}_{[NO]},
\]

\[
\frac{d[N]}{dt} = \dot{\omega}_{[N]},
\]

\[
[NO] + [O] + 2[O_2] = [NO]_o + [O]_o + 2[O_2]_o \equiv C_1,
\]

\[
[NO] + [N] + 2[N_2] = [NO]_o + [N]_o + 2[N_2]_o \equiv C_2,
\]

\[
[NO] + [N] + [N_2] + [O_2] + [O] = [NO]_o + [N]_o + [N_2]_o
+ [O_2]_o + [O]_o \equiv C_3.
\]

Constraints for element and molecule conservation.
Classical Dynamic Systems Form

\[ \frac{d[NO]}{dt} = \hat{\omega}_{[NO]} = 0.72 - 9.4 \times 10^5[NO] + 2.2 \times 10^7[N] \\
- 3.2 \times 10^{13}[N][NO] + 1.1 \times 10^{13}[N]^2, \]

\[ \frac{d[N]}{dt} = \hat{\omega}_{[N]} = 0.72 + 5.8 \times 10^5[NO] - 2.3 \times 10^7[N] \\
- 1.0 \times 10^{13}[N][NO] - 1.1 \times 10^{13}[N]^2. \]

Constants evaluated for \( T = 6000 \text{ } K, P = 2.5 \text{ } \text{bar}, C_1 = C_2 = 4 \times 10^{-6} \text{mole/cc}, \Delta G_1^o = -2.3 \times 10^{12} \text{erg/mole}, \Delta G_2^o = -2.0 \times 10^{12} \text{erg/mole}. \) Algebraic constraints absorbed into ODEs.
Species Evolution in Time

concentration (mole/cc)

$[NO]$

$[N]$
Dynamical Systems Approach to Construct SIM

Finite equilibria and linear stability:

1. \((\begin{bmatrix} NO \\ N \end{bmatrix}, \begin{bmatrix} N \end{bmatrix}) = (-1.6 \times 10^{-6}, -3.1 \times 10^{-8}),\) 
   \((\lambda_1, \lambda_2) = (5.4 \times 10^6, -1.2 \times 10^7)\) saddle (unstable)

2. \((\begin{bmatrix} NO \\ N \end{bmatrix}, \begin{bmatrix} N \end{bmatrix}) = (-5.2 \times 10^{-8}, -2.0 \times 10^{-6}),\) 
   \((\lambda_1, \lambda_2) = (4.4 \times 10^7 \pm 8.0 \times 10^6 i)\) spiral source (unstable)

3. \((\begin{bmatrix} NO \\ N \end{bmatrix}, \begin{bmatrix} N \end{bmatrix}) = (7.3 \times 10^{-7}, 3.7 \times 10^{-8}),\) 
   \((\lambda_1, \lambda_2) = (-2.1 \times 10^6, -3.1 \times 10^7)\) sink (stable, physical)

   Stiffness ratio = \(\lambda_2/\lambda_1 = 14.7\)

Equilibria at infinity and non-linear stability

1. \((\begin{bmatrix} NO \\ N \end{bmatrix}, \begin{bmatrix} N \end{bmatrix}) → (+\infty, 0)\) sink/saddle (unstable),
2. \((\begin{bmatrix} NO \\ N \end{bmatrix}, \begin{bmatrix} N \end{bmatrix}) → (-\infty, 0)\) source (unstable).
Detailed Phase Space Map with All Finite Equilibria

-4 -3 -2 -1 0 1 2

\[ \times 10^{-7} \]

-20
-15
-10
-5
0
5
\[ \times 10^{-6} \]

\[ [N] \text{ (mole/cc)} \]

\[ [\text{NO}] \text{ (mole/cc)} \]

saddle
1
sink
3
saddle
3
sink
1

source
2

sink
3

sink
3

sink
3
Projected Phase Space from Poincaré’s Sphere

\[ \frac{[N]}{\sqrt{1+[N]^2+[NO]^2}} \]

sink

saddle

spiral source

SIM

sink

SIM

\[ \frac{[NO]}{\sqrt{1+[N]^2+[NO]^2}} \]
ASIM for Reaction-Diffusion PDEs

• Slow dynamics can be approximated by the ASIM

\[
\tilde{V}_s \frac{\partial y}{\partial t} = \tilde{V}_s f - \tilde{V}_s \frac{\partial h}{\partial x},
\]

\[
0 = \tilde{V}_f f - \tilde{V}_f \frac{\partial h}{\partial x}.
\]

• Spatially discretize to form differential-algebraic equations (DAEs):

\[
\tilde{V}_{si} \frac{dy_i}{dt} = \tilde{V}_{si} f_i - \tilde{V}_{si} \frac{h_{i+1} - h_{i-1}}{2\Delta x},
\]

\[
0 = \tilde{V}_{fi} f_i - \tilde{V}_{fi} \frac{h_{i+1} - h_{i-1}}{2\Delta x}.
\]

• Solve numerically with DASSL

• \( \tilde{V}_s, \tilde{V}_f \) computed \textit{in situ}; easily fixed for \textit{a priori} computation
Davis-Skodje Example Extended to Reaction-Diffusion

\[ \frac{\partial y}{\partial t} = f(y) - D \frac{\partial h}{\partial x} \]

- Boundary conditions are chosen on the SIM

\[ y(t, 0) = 0, \quad y(t, 1) = \left( \frac{1}{2} + \frac{1}{4\gamma(\gamma-1)} \right). \]

- Initial conditions

\[ y(0, x) = \left( \frac{x}{\left( \frac{1}{2} + \frac{1}{4\gamma(\gamma-1)} \right)x} \right). \]
• Solution at $t = 5$, for $\gamma = 10$ with varying $D$.

• PDE solutions are fully resolved.
Reaction Diffusion Example Results

- The global error when using ASIM is small in general, and is similar to that incurred by the full PDE near steady state.
Production Reaction-Diffusion System

- Isothermal and isobaric, $T = 3500 \, K$, $P = 1.5 \, bar$, with Neumann boundary conditions, and initial distribution:
Production Reaction Diffusion System

- At $t = 10^{-6}$ s.
Conclusions

• No robust analysis currently exists to determine reaction and diffusion time scales \textit{a priori}.

• The ASIM couples reaction and diffusion while systematically equilibrating fast time scales.

• Casting the ASIM method in terms of differential-algebraic equations is an effective way to robustly implement the method.

• At this point the fast and slow subspace decomposition is dependent only on reaction and should itself be modified to include fast and slow diffusion time scales.

• The error incurred in approximating the slow dynamics by the ASIM is small in general.