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,
- Lam, *CST*, 2007: considers CSP for reaction-diffusion coupling.

Motivation

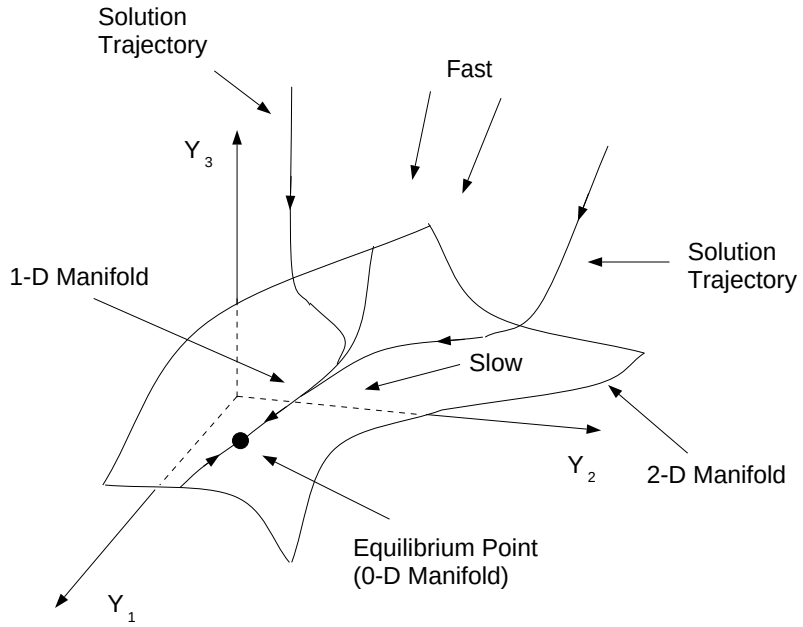
- Severe stiffness in reactive flow systems with detailed gas phase chemical kinetics renders fully resolved simulations of many systems to be impractical.
- ILDM method can reduce computational time while retaining essential fidelity of full detailed kinetics.
- The ILDM is only an approximation of 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:

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

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



Eigenvalues and Eigenvectors from Decomposition of Jacobian

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

$$\mathbf{V} = \left(\begin{array}{c:c} \mathbf{V}_s & \mathbf{V}_f \end{array} \right),$$

$$\mathbf{\Lambda} = \left(\begin{array}{c:c} \mathbf{\Lambda}_{(s)} & 0 \\ \hdashline 0 & \mathbf{\Lambda}_{(f)} \end{array} \right).$$

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

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

- By equilibrating the fast dynamics

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

- Slow dynamics approximated from differential algebraic equations on the ILDM

$$\tilde{\mathbf{V}}_s \frac{d\mathbf{y}}{dt} = \tilde{\mathbf{V}}_s \mathbf{f}, \qquad \mathbf{0} = \tilde{\mathbf{V}}_f \mathbf{f}.$$

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.

Comparison of the SIM with the ILDM

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

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

- The ILDM for this system is given by

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

- while the SIM is given by

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

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,
- thermodynamic data from Sonntag, *et al.*, 2003.

Zel'dovich Mechanism: ODEs

$$
\begin{aligned}
\frac{d[NO]}{dt} &= r_2 - r_1 = \dot{\omega}_{[NO]}, \quad [NO](t=0) = [NO]_o, \\
\frac{d[N]}{dt} &= -r_1 - r_2 = \dot{\omega}_{[N]}, \quad [N](t=0) = [N]_o, \\
\frac{d[N_2]}{dt} &= r_1 = \dot{\omega}_{[N_2]}, \qquad [N_2](t=0) = [N_2]_o, \\
\frac{d[O]}{dt} &= r_1 + r_2 = \dot{\omega}_{[O]}, \qquad [O](t=0) = [O]_o, \\
\frac{d[O_2]}{dt} &= -r_2 = \dot{\omega}_{[O_2]}, \qquad [O_2](t=0) = [O_2]_o, \\
r_1 &= k_1[N][NO]\left(1 - \frac{1}{K_{eq1}}\frac{[N_2][O]}{[N][NO]}\right), \; K_{eq1} = \exp\left(\frac{-\Delta G_1^o}{\Re T}\right) \\
r_2 &= k_2[N][O_2]\left(1 - \frac{1}{K_{eq2}}\frac{[NO][O]}{[N][O_2]}\right), \; K_{eq2} = \exp\left(\frac{-\Delta G_2^o}{\Re T}\right).
\end{aligned}
$$

Zel'dovich Mechanism: DAEs

$$
\begin{aligned}
\frac{d[NO]}{dt} &= \dot{\omega}_{[NO]}, \\
\frac{d[N]}{dt} &= \dot{\omega}_{[N]}, \\
[NO] + [O] + 2[O_2] &= [NO]_o + [O]_o + 2[O_2]_o \equiv C_1, \\
[NO] + [N] + 2[N_2] &= [NO]_o + [N]_o + 2[N_2]_o \equiv C_2, \\
[NO] + [N] + [N_2] + [O_2] + [O] &= [NO]_o + [N]_o + [N_2]_o \\
&\quad + [O_2]_o + [O]_o \equiv C_3.
\end{aligned}
$$

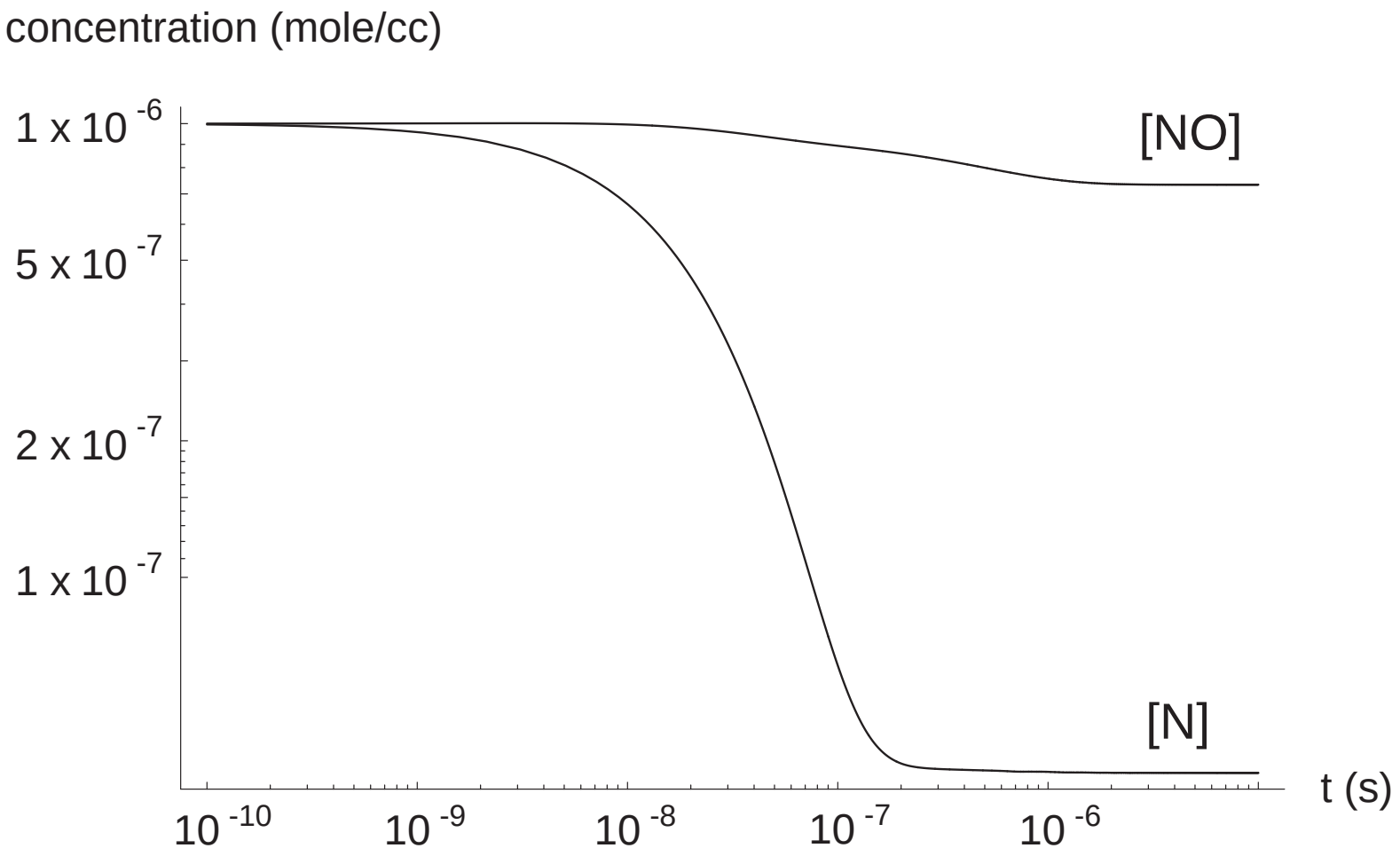
Constraints for element and molecule conservation.

Classical Dynamic Systems Form

$$\begin{aligned}
\frac{d[NO]}{dt} &= \hat{\dot{\omega}}_{[NO]} = 0.72 - 9.4 \times 10^5 [NO] + 2.2 \times 10^7 [N] \\
&\quad - 3.2 \times 10^{13} [N][NO] + 1.1 \times 10^{13} [N]^2, \\
\frac{d[N]}{dt} &= \hat{\dot{\omega}}_{[N]} = 0.72 + 5.8 \times 10^5 [NO] - 2.3 \times 10^7 [N] \\
&\quad - 1.0 \times 10^{13} [N][NO] - 1.1 \times 10^{13} [N]^2.
\end{aligned}$$

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

Species Evolution in Time



Dynamical Systems Approach to Construct SIM

Finite equilibria and linear stability:

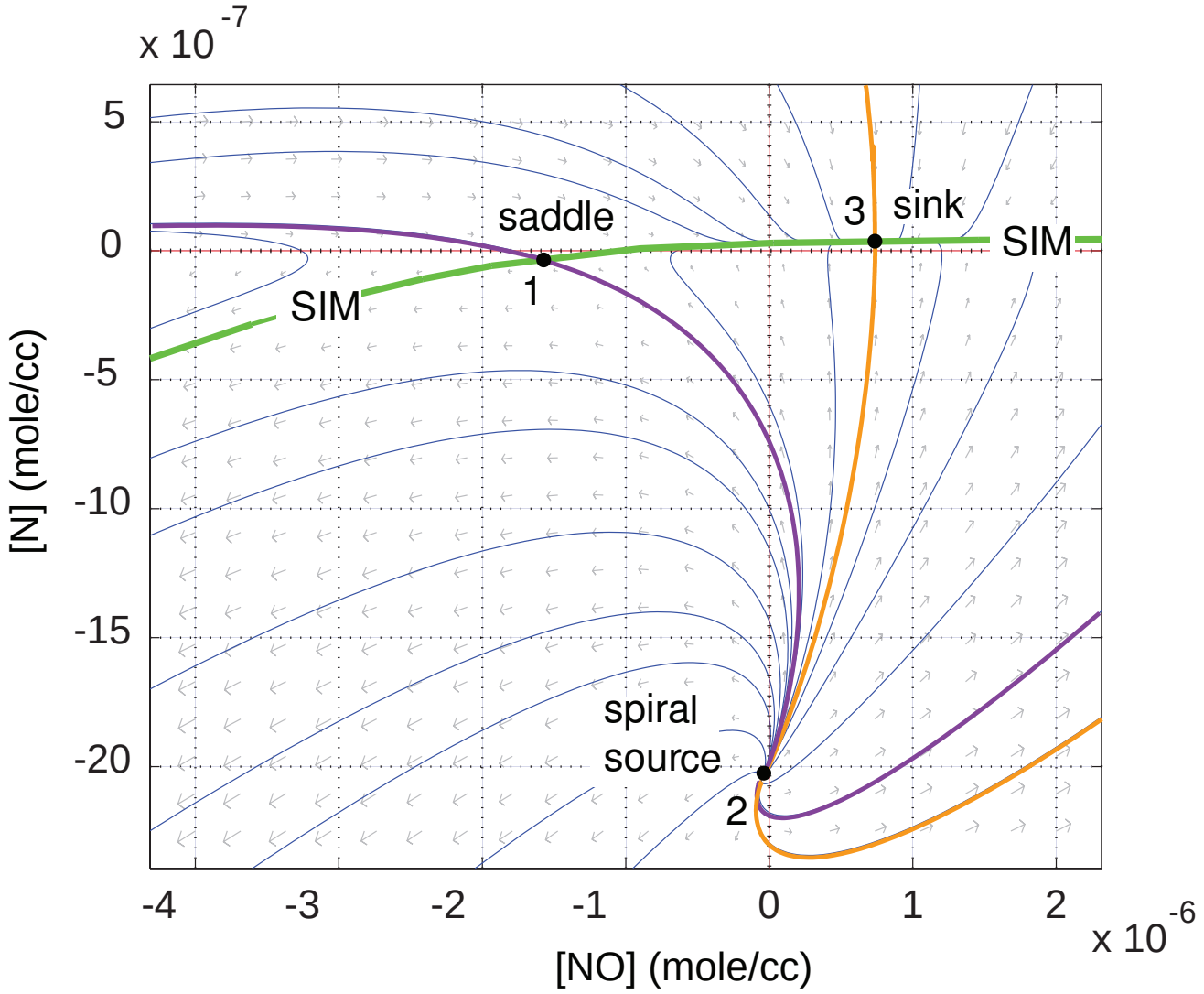
$$
\begin{aligned}
1.\ ([NO],[N]) &= (-1.6\times10^{-6}, -3.1\times10^{-8}),\\
(\lambda_1,\lambda_2) &= (5.4\times10^{6}, -1.2\times10^{7}) \quad \text{saddle (unstable)}\\
2.\ ([NO],[N]) &= (-5.2\times10^{-8}, -2.0\times10^{-6}),\\
(\lambda_1,\lambda_2) &= (4.4\times10^{7} \pm 8.0\times10^{6} i) \quad \text{spiral source (unstable)}\\
3.\ ([NO],[N]) &= (7.3\times10^{-7}, 3.7\times10^{-8}),\\
(\lambda_1,\lambda_2) &= (-2.1\times10^{6}, -3.1\times10^{7}) \quad \text{sink (stable, physical)}
\end{aligned}
$$

stiffness ratio = $\lambda_2/\lambda_1 = 14.7$

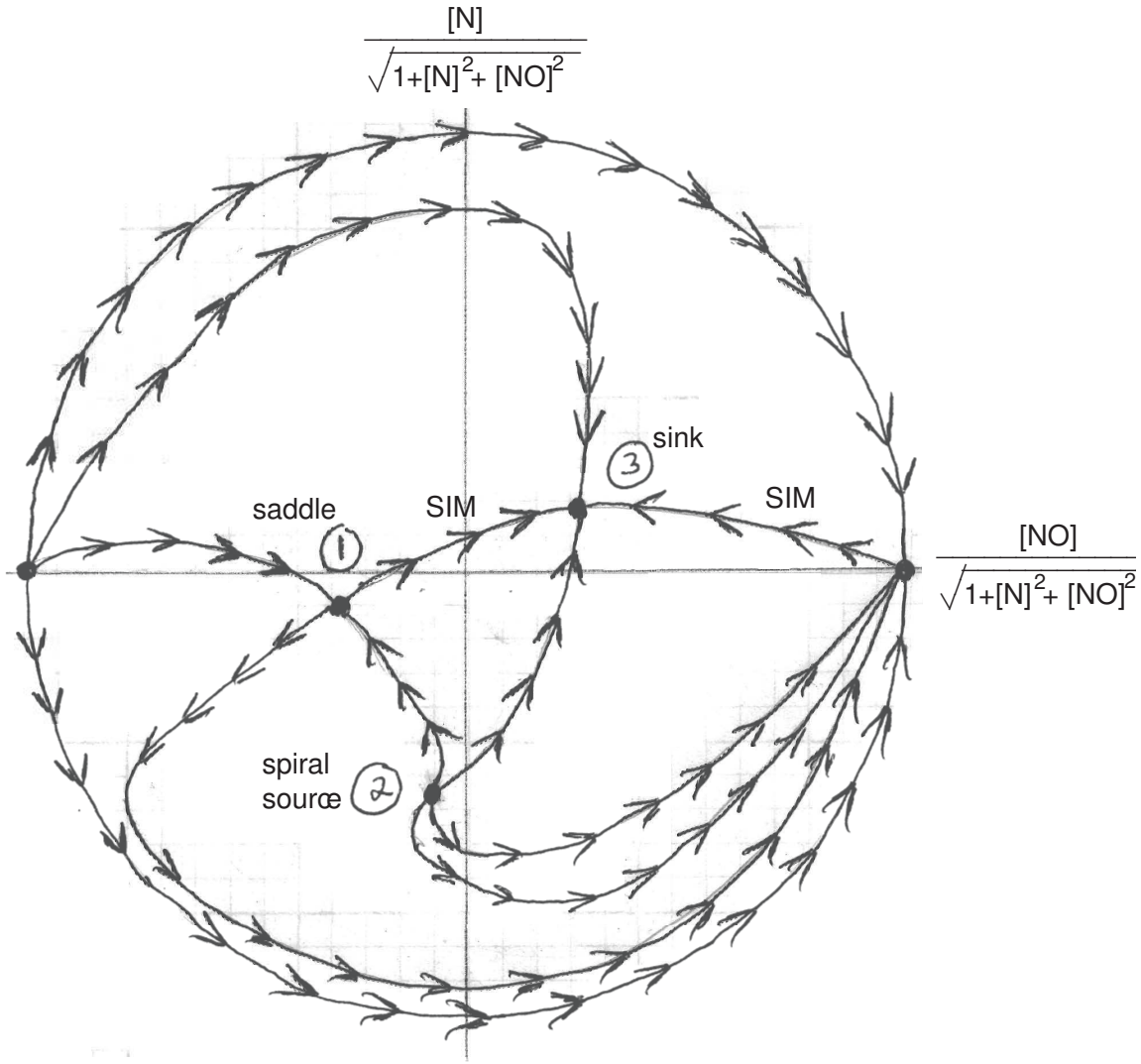
Equilibria at infinity and non-linear stability

$$
\begin{aligned}
1.\ ([NO],[N]) &\rightarrow (+\infty, 0) \quad \text{sink/saddle (unstable),}\\
2.\ ([NO],[N]) &\rightarrow (-\infty, 0) \quad \text{source (unstable).}
\end{aligned}
$$

Detailed Phase Space Map with All Finite Equilibria



Projected Phase Space from Poincaré's Sphere



ASIM for Reaction-Diffusion PDEs

- Slow dynamics can be approximated by the ASIM

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

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

$$\begin{aligned} \tilde{\mathbf{V}}_{si} \frac{d\mathbf{y}_i}{dt} &= \tilde{\mathbf{V}}_{si} \mathbf{f}_i - \tilde{\mathbf{V}}_{si} \frac{\mathbf{h}_{i+1} - \mathbf{h}_{i-1}}{2\Delta x}, \\ \mathbf{0} &= \tilde{\mathbf{V}}_{fi} \mathbf{f}_i - \tilde{\mathbf{V}}_{fi} \frac{\mathbf{h}_{i+1} - \mathbf{h}_{i-1}}{2\Delta x}. \end{aligned}$$

- Solve numerically with DASSL
- $\tilde{V}_s$, $\tilde{V}_f$ computed *in situ*; easily fixed for *a priori* computation

Davis-Skodje Example Extended to Reaction-Diffusion

$$\frac{\partial \mathbf{y}}{\partial t} = \mathbf{f}(\mathbf{y}) - \mathcal{D}\frac{\partial \mathbf{h}}{\partial x}$$

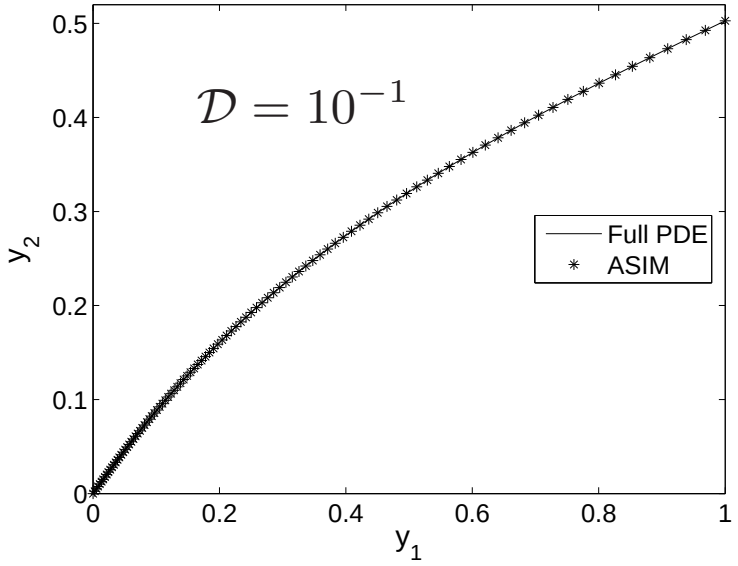
- Boundary conditions are chosen on the SIM

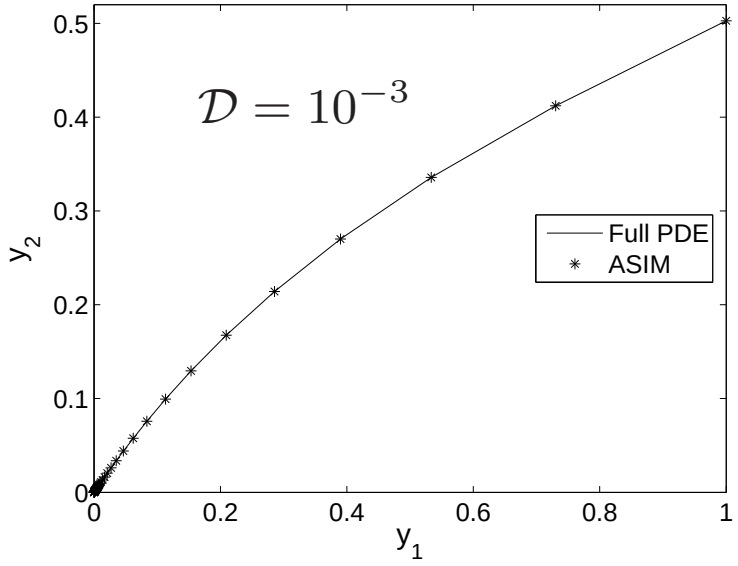
$$\mathbf{y}(t,0) = \mathbf{0}, \qquad \mathbf{y}(t,1) = \begin{pmatrix} 1 \\ \frac{1}{2} + \frac{1}{4\gamma(\gamma-1)} \end{pmatrix}.$$

- Initial conditions

$$\mathbf{y}(0,x) = \begin{pmatrix} x \\ \left(\frac{1}{2} + \frac{1}{4\gamma(\gamma-1)}\right) x \end{pmatrix}.$$

Davis-Skodje Reaction-Diffusion Results

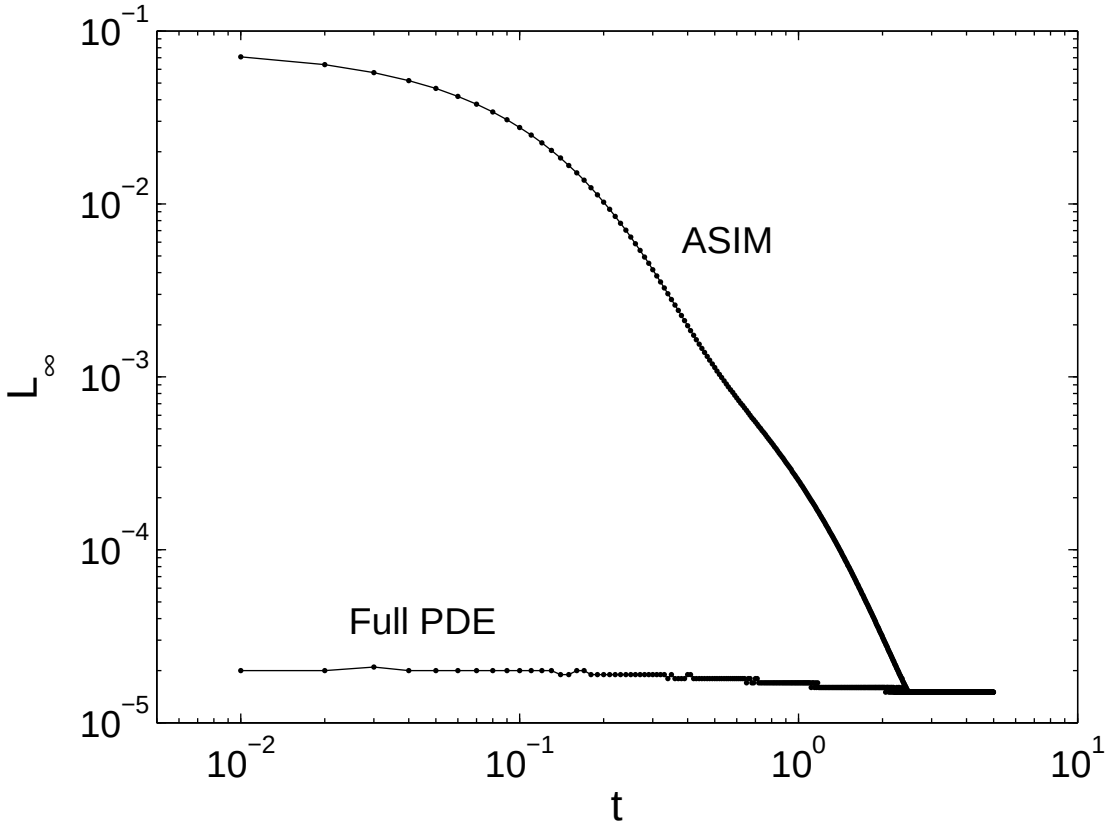




- Solution at $t = 5$, for $\gamma = 10$ with varying $\mathcal{D}$.
- PDE solutions are fully resolved.

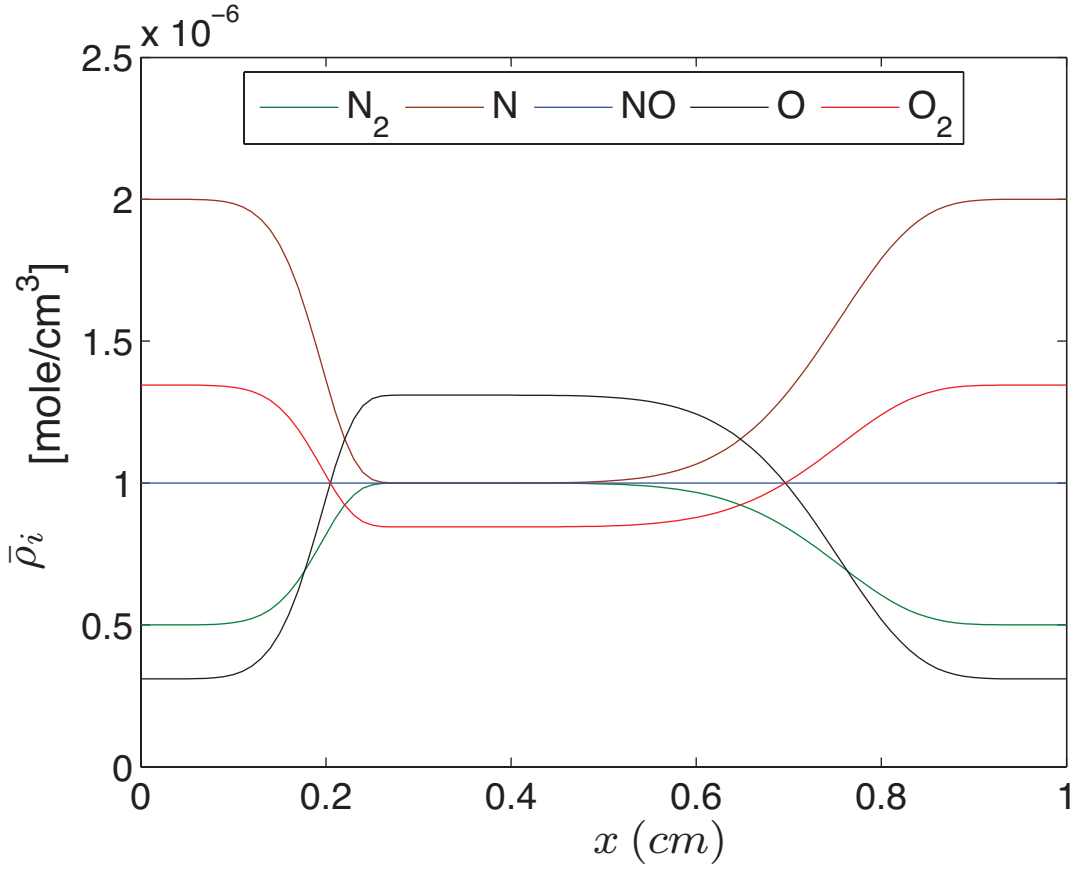
Reaction Diffusion Example Results

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



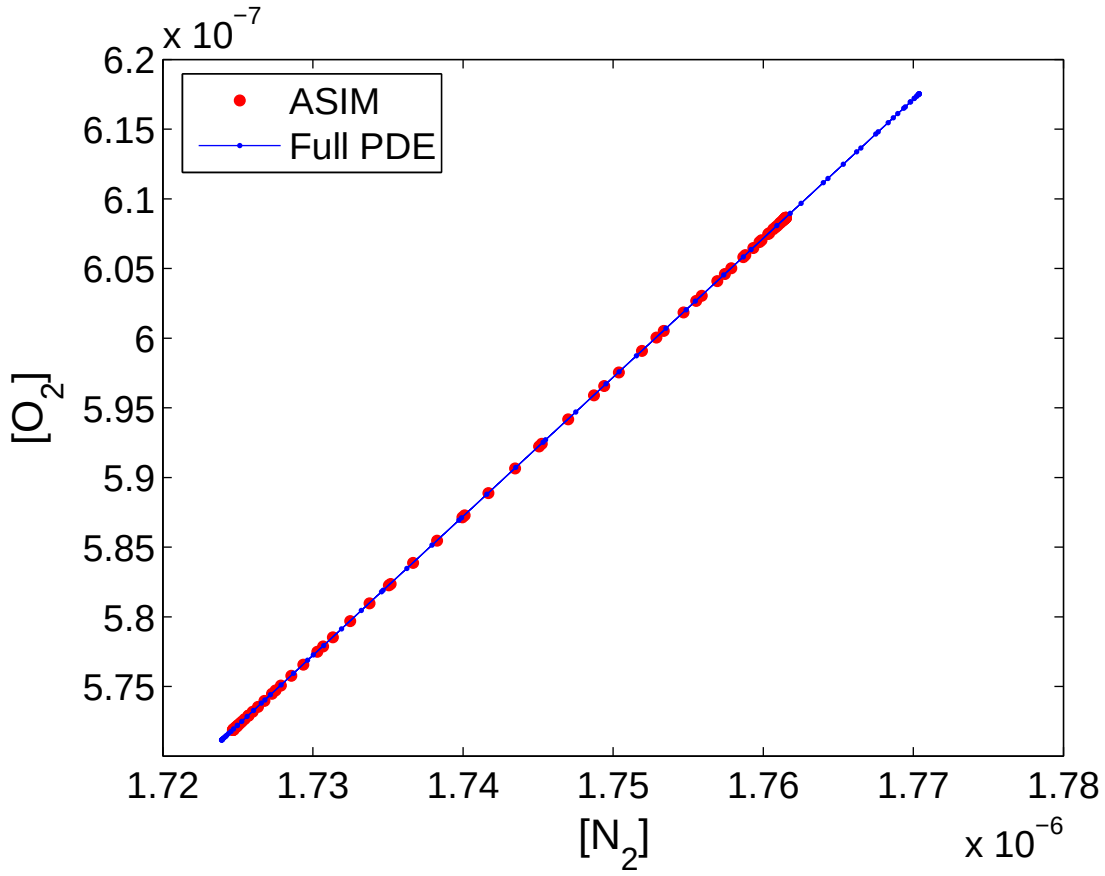
NO Production Reaction-Diffusion System

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



NO Production Reaction Diffusion System

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



Conclusions

- No robust analysis currently exists to determine reaction and diffusion time scales *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.