

Model Reduction for Reaction-Diffusion Systems: Bifurcations in Slow Invariant Manifolds

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50th AIAA Aerospace Sciences Meeting

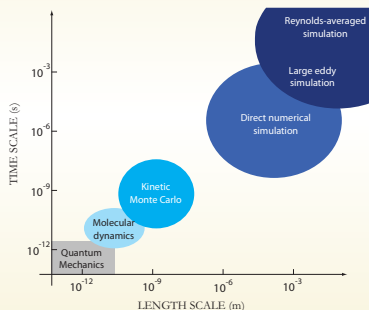
Nashville, Tennessee
January 10, 2012



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Motivation and Background

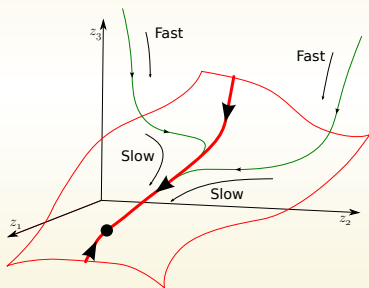
- Detailed kinetics are essential for accurate modeling of reactive systems
- Reactive systems induce a wide range of spatial and temporal scales, and subsequently severe stiffness occurs
- The spatial and temporal scales are coupled by the underlying physics of the problem
- Verification of a simulation's accuracy requires resolution of all scales
- The computational cost for reactive flow simulations increases with the range of scales present, the number of reactions and species, and the size of the spatial domain.
- Manifold methods provide a potential for computational savings.



“Research needs for future internal combustion engines,” *Physics Today*, Nov. 2008, pp. 47–52.

Motivation and Background

- Manifold methods are typically spatially homogeneous, yet most engineering applications require spatial variation.
- Diffusion is often modeled with a correction to the spatially homogeneous methods in the long wavelength limit.
- However, for thin regions of flames, reaction is fast relative to diffusion, and the short wavelength limit is more appropriate.
- Al-Khateeb, et al. 2009, *Journal of Chemical Physics*, provides details on construction of spatially homogeneous SIMs.



Assumptions

Model a system of N species reacting in J reactions with diffusion in one spatial dimension

- Ideal mixture
- Ideal gases
- Isochoric
- Isothermal
- Negligible advection
- Single constant mass diffusivity

- Evolution of species

$$\rho \frac{\partial Y_i}{\partial t} + \frac{\partial j_i^m}{\partial x} = M_i \dot{\omega}_i(Y_n, T), \quad \text{for } i, n \in [1, N]$$

- Boundary conditions

$$\left. \frac{\partial Y_i}{\partial x} \right|_{x=0} = \left. \frac{\partial Y_i}{\partial x} \right|_{x=\ell} = 0, \quad \text{for } i \in [1, N]$$

- Initial conditions

$$Y_i(x, t = 0) = \tilde{Y}_i(x), \quad \text{for } i \in [1, N]$$

Constitutive Equations

- Fick's law of diffusion

$$j_i^m = -\rho D \frac{\partial Y_i}{\partial x}, \quad \text{for } i \in [1, N]$$

- Ideal gas equation of state

$$P = \rho \bar{\mathcal{R}} T \sum_{i=1}^N \frac{Y_i}{M_i}$$

- Molar production rate

$$\dot{\omega}_i = \sum_{j=1}^J \nu_{ij} r_j, \quad \text{for } i \in [1, N]$$

$$r_j = k_j \left(\prod_{i=1}^N \left(\frac{\rho Y_i}{M_i} \right)^{\nu'_{ij}} - \frac{1}{K_j^c} \prod_{i=1}^N \left(\frac{\rho Y_i}{M_i} \right)^{\nu''_{ij}} \right), \quad \text{for } j \in [1, J]$$

$$k_j = a_j T^{\beta_j} \exp \left(\frac{-\bar{E}_j}{\mathfrak{R}T} \right), \quad \text{for } j \in [1, J]$$

$$K_j^c = \exp \left(\frac{-\sum_{i=1}^N \bar{g}_i^o \nu_{ij}}{\mathfrak{R}T} \right), \quad \text{for } j \in [1, J]$$

- Certain linear combinations of molar production rate sum to zero,

$$\frac{\partial}{\partial t} \left(\sum_{i=1}^N \varphi_{li} \frac{Y_i}{M_i} \right) = \mathcal{D} \frac{\partial^2}{\partial x^2} \left(\sum_{i=1}^N \varphi_{li} \frac{Y_i}{M_i} \right), \quad \text{for } l \in [1, L]$$

- Some evolution PDEs can be integrated to yield algebraic constraints if these quantities are
 - Initially spatially homogeneous, and
 - Not perturbed at the boundaries,

$$\sum_{i=1}^N \varphi_{li} \frac{Y_i}{M_i} = \sum_{i=1}^N \varphi_{li} \frac{\tilde{Y}_i}{M_i}, \quad \text{for } l \in [1, L]$$

Reduced Variables

- The L algebraic constraints can be used to reduce N PDEs to $N - L$ PDEs
- Transform to reduced variables: specific mole concentrations

$$z_i = \frac{Y_i}{M_i}, \quad \text{for } i \in [1, N - L]$$

- Evolution of remaining L species are coupled to these reduced variables by the algebraic constraints

$$\frac{\partial z_i}{\partial t} = \frac{\dot{\omega}_i(z_n, T)}{\rho} + \mathcal{D} \frac{\partial^2 z_i}{\partial x^2}, \quad \text{for } i, n \in [1, N - L]$$

Galerkin Reduction to ODEs

- Assume a spectral decomposition

$$z_i(x, t) = \sum_{m=0}^{\infty} z_{i,m}(t) \phi_m(x), \quad \text{for } i \in [1, N - L]$$

- Orthogonal basis functions, $\phi_m(x)$, are eigenfunctions of diffusive operator that match boundary conditions

$$\frac{\partial^2 \phi_m}{\partial x^2} = -\mu_m^2 \phi_m$$

- Complete orthogonal basis,

$$\phi_m(x) = \cos\left(\frac{m\pi x}{\ell}\right), \quad \text{for } m \in [0, \infty)$$

Galerkin Reduction to ODEs

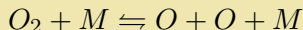
$$\frac{\partial}{\partial t} \left(\sum_{n=0}^{\infty} z_{i,n} \phi_n \right) = \frac{\dot{\omega}_i \left(\sum_{\hat{n}=0}^{\infty} z_{i,\hat{n}} \phi_{\hat{n}} \right)}{\rho} + \mathcal{D} \frac{\partial^2}{\partial x^2} \left(\sum_{n=0}^{\infty} z_{i,n} \phi_n \right)$$

- Finite system of ODEs for amplitude evolution are recovered by taking the inner product with ϕ_m , and truncated at M

$$\frac{dz_{i,m}}{dt} = \underbrace{\frac{\left\langle \phi_m, \dot{\omega}_i \left(\sum_{\hat{n}=0}^{\infty} z_{i,\hat{n}} \phi_{\hat{n}} \right) / \rho \right\rangle}{\langle \phi_m, \phi_m \rangle}}_{\dot{\Omega}_{i,m}} - \mathcal{D} \mu_m^2 z_{i,m}, \quad \begin{array}{l} \text{for } i \in [1, N - L], \\ \text{and } m \in [0, M] \end{array}$$

- Projection modifies reaction eigenvalues, $\lambda_{i,m} = \lambda_{0,m} - \mathcal{D} \mu_m^2$
- Diffusion time scales defined as $\tau_{\mathcal{D},m} \equiv \frac{1}{\mu_m^2 \mathcal{D}}$

Oxygen dissociation reaction:



- $N = 2$ species
- $J = 1$ reaction
- $L = 1$ constraint
- $N - L = 1$ reduced variable
 $z = \frac{Y_O}{M_O}$
- Isochoric,
 $\rho = 1.6 \times 10^{-4} \text{ g/cm}^2$
- Isothermal,
 $T = 5000 \text{ K}$

Spatially Homogeneous System

For domain lengths small enough that diffusion is much faster than reaction

- Galerkin truncation at $M = 0$ is appropriate
- Spatially homogeneous system is recovered

$$\frac{dz}{dt} = \underbrace{\left(249.8 \frac{\text{mol}}{\text{g s}}\right) - \left(7.473 \times 10^4 \frac{\text{g}}{\text{mol s}}\right) z^2 - \left(1.724 \times 10^5 \frac{\text{g}^2}{\text{mol}^2 \text{s}}\right) z^3}_{\dot{\Omega}}$$

SIM Construction

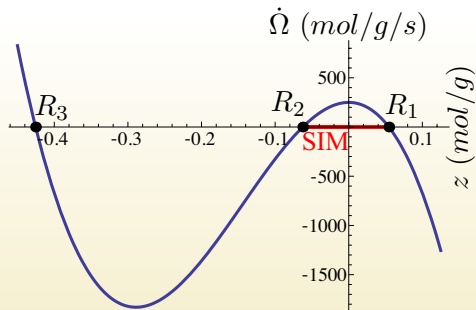
- Identify equilibria
- Characterize equilibria by eigenvalues of their Jacobian matrix (slopes)

$$J_{ij} = \frac{\partial \dot{\Omega}_i}{\partial z_j}$$

- Reaction time scale is the reciprocal of the eigenvalue

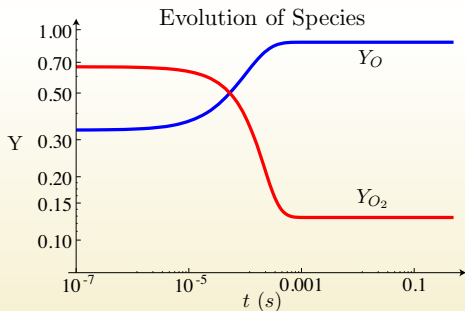
$$\tau_{\mathcal{R}} = |\lambda|^{-1}$$

- SIM is a heteroclinic orbit from R_2 to R_1



Spatially Homogeneous Evolution

- Use z to reconstruct mass fractions of O and O_2
- Only one time scale present
 $\tau_{\mathcal{R}} \sim 10^{-4} \text{ s}$
- Time scale corresponds to reciprocal of equilibrium eigenvalue



Reaction-Diffusion System

For larger domain lengths where diffusion is not much faster than reaction

- Additional terms in Galerkin projection are retained
- We examine the truncation at $M = 1$

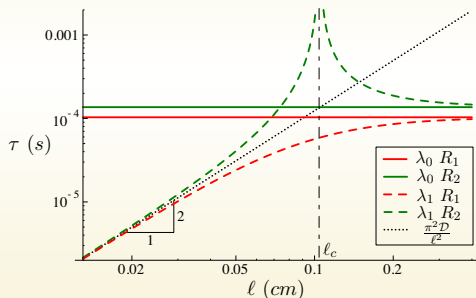
$$\begin{aligned}\frac{dz_0}{dt} &= \left(249.8 \frac{\text{mol}}{g \text{ s}}\right) - \left(7.473 \times 10^4 \frac{g}{\text{mol s}}\right) \left(z_0^2 + \frac{z_1^2}{2}\right) \\ &\quad - \left(1.724 \times 10^5 \frac{g^2}{\text{mol}^2 \text{ s}}\right) \left(z_0^3 + \frac{3z_0 z_1^2}{2}\right) \\ \frac{dz_1}{dt} &= - \left(7.473 \times 10^4 \frac{g}{\text{mol s}}\right) 2z_0 z_1 \\ &\quad - \left(1.724 \times 10^5 \frac{g^2}{\text{mol}^2 \text{ s}}\right) \left(3z_0^2 z_1 + \frac{3z_1^3}{4}\right) - \frac{\pi^2 \mathcal{D}}{\ell^2} z_1\end{aligned}$$

Local Timescales

- Time-scale coupling between reaction and diffusion

$$\frac{1}{\tau_C} = \frac{1}{\tau_R} + \frac{1}{\tau_D}$$

- R_3 is a sink; diffusion keeps it stable

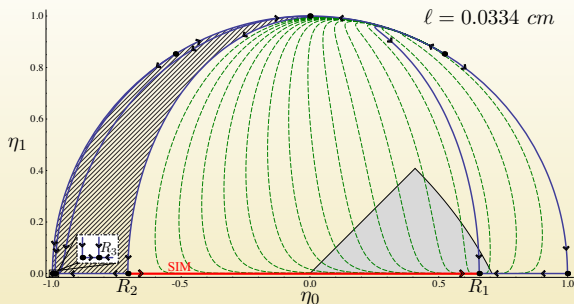


- R_2 is a source, diffusion changes its stability
- Critical wavelength, ℓ_c , where stable diffusion time-scale is equal to unstable reaction time-scale

Poincaré Sphere

- Map variables into a space where infinity is on the unit circle
- We can see the dynamics of the entire system
- What changes occur in the SIM as we vary ℓ ?

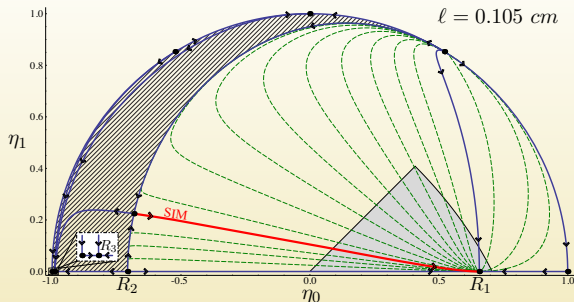
$$\eta_0 = \frac{z_0}{\sqrt{M_O^{-1} + z_0^2 + z_1^2}}$$
$$\eta_1 = \frac{z_1}{\sqrt{M_O^{-1} + z_0^2 + z_1^2}}$$



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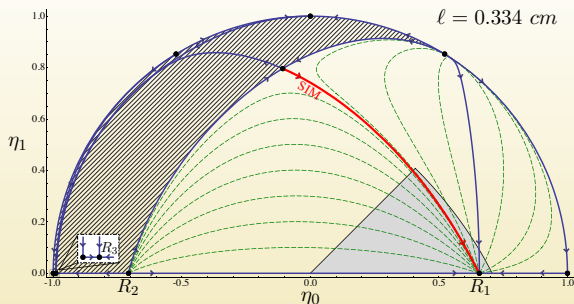
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Poincaré Sphere

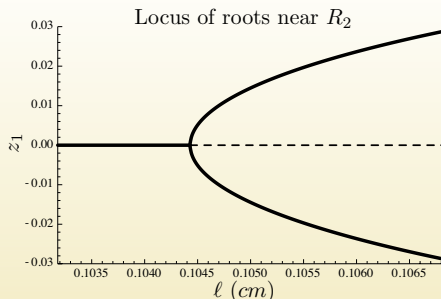
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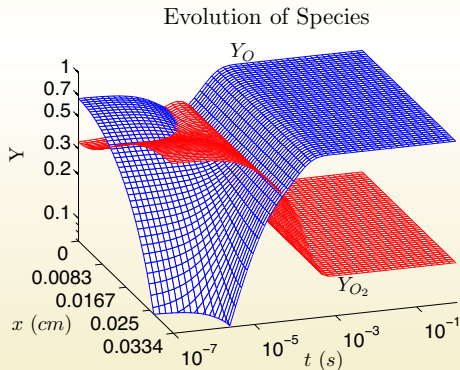
Bifurcation

- The change in stability of the combined Fourier mode at the critical wavelength, ℓ_c , is indicative of a bifurcation
- Bold branches are saddles; dashed branch is source
- This bifurcation changes the starting point of the SIM
- Subsequently, the slow dynamics of the entire system are modified



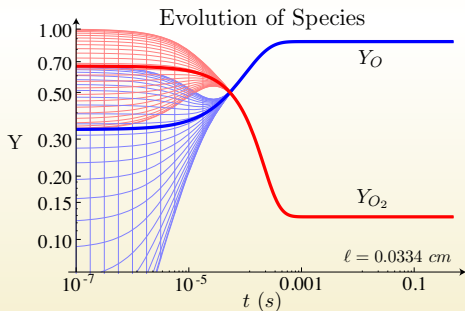
Reaction-Diffusion Evolution

- Use z_0 and z_1 to reconstruct spatial distributions of mass fractions of O and O_2
- For $\ell = 0.0334 \text{ cm} < \ell_c$, diffusion is faster than reaction
- Difficult to segregate into reaction and diffusion contributions



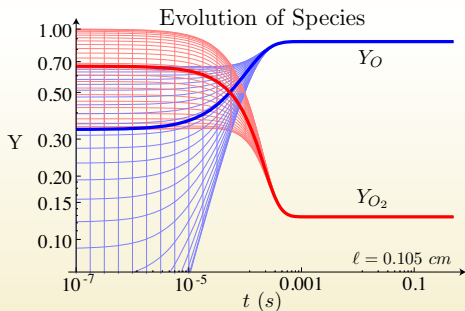
Reaction-Diffusion Evolution

- Project spatial evolution of mass fractions onto $Y - t$ plane to see diffusion time scale.
- Bold line is spatially homogeneous SIM
- Two time scales present:
 - $\tau_R \sim 10^{-4} \text{ s}$
 - $\tau_D = \frac{\ell^2}{\pi^2 \mathcal{D}} \sim 10^{-5} \text{ s}$
- Slow dynamics change from reaction to diffusion at ℓ_c



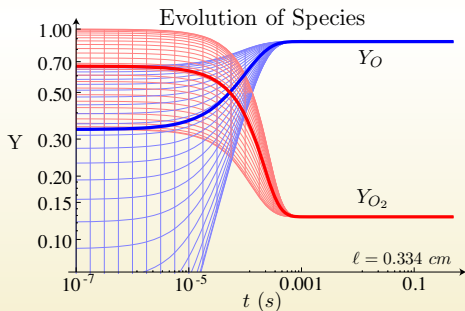
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- The SIM isolates the slowest dynamics, making it ideal for a reduction technique.
- For sufficiently short length scales, diffusion time scales are faster than reaction time scales, and the system dynamics are dominated by reaction.
- When lengths are near or above a critical length where the diffusion time scale is on the same order as reaction time scales, diffusion will play a more important role.
- In the limit of large length scales, a truncation at $M = 1$ is insufficient, and more terms are required to fully resolve the dynamics.

Acknowledgments



Partial support provided by NSF Grant No. CBET-0650843 and
Notre Dame ACMS Department Fellowship