Diffusion Effects on Slow Invariant Manifolds

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Outline

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, $\ell_{\mathcal{D}} = \sqrt{\mathcal{D}\tau_R}$.
- 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.

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, diffusion is fast relative to reaction and the short wavelength limit is more appropriate.
- This analysis considers the short wavelength limit by the use of a Galerkin projection.

Mathematical model

- Spatially homogeneous system,

$$\frac{d\mathbf{z}}{dt} = \mathbf{f}(\mathbf{z}).$$

- Simple mass diffusion,

$$\frac{\partial \mathbf{z}}{\partial t} = \mathbf{f}(\mathbf{z}) + \mathcal{D}\frac{\partial^2 \mathbf{z}}{\partial x^2}.$$

- Boundary conditions,

$$\left.\frac{\partial \mathbf{z}}{\partial x}\right|_{x=0} = \left.\frac{\partial \mathbf{z}}{\partial x}\right|_{x=L} = 0.$$

Galerkin projection

- Assume infinite series solution,

$$\mathbf{z} = z_i = \sum_{m=0}^{\infty} z_{i,m}(t)\phi_m(x), \quad i = 1, \dots, R.$$

- Complete set of basis functions, with eigenvalues $\mu_n = -(n\,\pi/L)^2$,

$$\phi_n = \cos\left(\frac{n\pi}{L}x\right), \quad n = 0, \dots, \mathcal{N}, \dots, \infty.$$

- Inner product of governing PDE with basis functions,

$$\frac{dz_{i,n}}{dt} = \frac{\langle \phi_n, f_i(\sum_{m=0}^{\infty} z_{i,m}\phi_m)\rangle}{\langle \phi_n, \phi_n\rangle} + \mu_n \mathcal{D} z_{i,n}.$$

- Truncate series at sufficiently large $\mathcal{N}$.

Example problem

Zel'dovich mechanism

$$N + NO \leftrightharpoons N_2 + O$$

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- Isothermal and isochoric, $T = 3500\ K$.
- Bimolecular, isobaric, $P = 1.455\ bar$.
- 5 species, 3 constraints,
- Reduces to 2 free variables, $z_1 = z_{NO},\ z_2 = z_N$.

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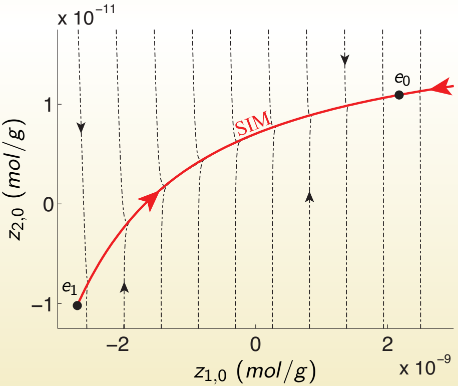
Spatially homogeneous ($\mathcal{N} = 0$)



Results similar to Al-Khateeb et al., J. Chem. Phys., 2009.

Jacobian and time scales

- Jacobian matrix,

$$\mathbf{J} = \frac{\partial \mathbf{f}}{\partial \mathbf{z}}.$$

- Eigenvalues of Jacobian at equilibrium, λ.
- Classification of equilibria:
  - e_0 – Sink (Physical),
  - e_1 – Saddle $(+,-)$.
- Timescales,

$$\tau = 1/\lambda.$$

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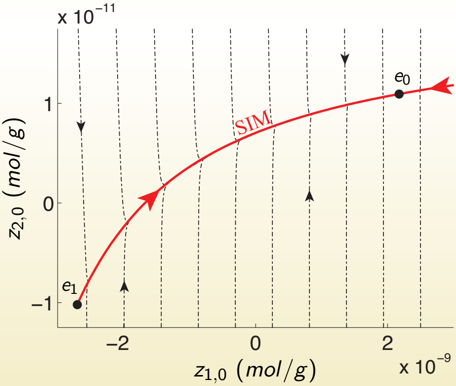


Short wavelength limit

- Short, finite length scale, $\mathcal{N} = 1$,

$$\begin{aligned} \frac{dz_{i,0}}{dt} &= f_i(z_{j,0}), \\ \frac{dz_{i,1}}{dt} &= f_{i,1}(z_{j,0}, z_{j,1}) - \frac{\pi^2 \mathcal{D}}{L^2} z_{i,1}. \end{aligned}$$

- Analysis for longer lengths with larger $\mathcal{N}$ is consistent with $\mathcal{N} = 1$.
- Spatially homogeneous phase space is $z_{i,0}$ subspace.
- The Jacobian of spatially homogenous equilibria retain original eigenvalues and gain additional diffusion-modified eigenvalues.

Diffusion-modified eigenvalues

- Eigenvalues of $\mathcal{N} = 1$ system,

$$\begin{aligned} \lambda_{i,0} &= \lambda_i, \\ \lambda_{i,1} &= \lambda_i - \frac{\pi^2 \mathcal{D}}{L^2}. \end{aligned}$$

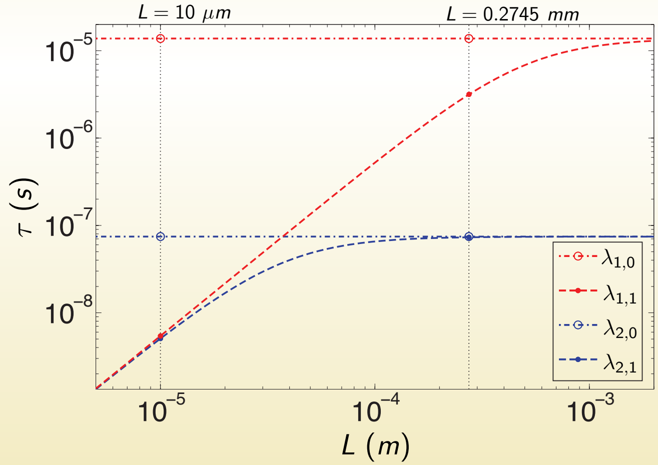
- Character of e_0 remains a sink.
- Character of e_1 saddle changes $(+,-,-,-)$ / $(+,+,-,-)$.
- This change is indicative of a bifurcation in the system.

Additional equilibria bifurcation

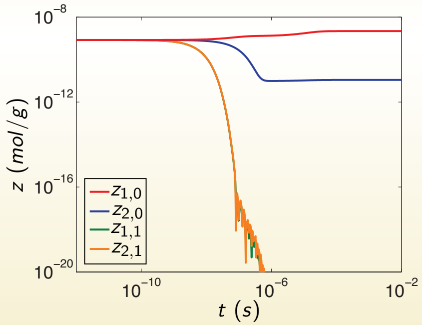
- When L is increased, e_1 changes from 1 to 2 positive eigenvalues.
- Where this change occurs, 2 additional equilibria converge from the complex domain through e_1 and emerge in real space.
- These 2 additional equilibria have heteroclinic orbits that connect to e_0 and are $(+,-,-,-)$.
- For this system with the given parameters this occurs at $L = 0.2745\ mm$.

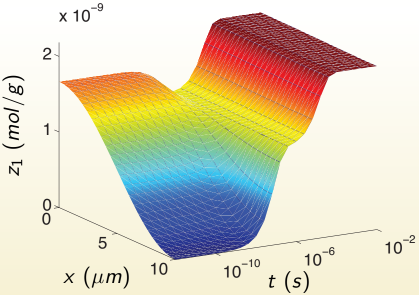
Time scales as a function of length

At equilibrium e_0



Evolution at $L = 10\ \mu m$





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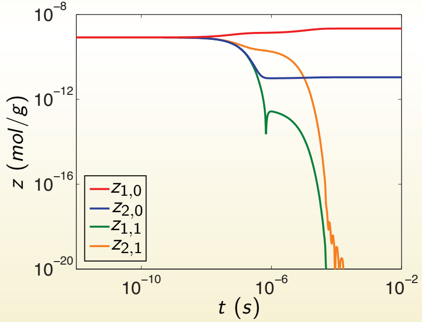
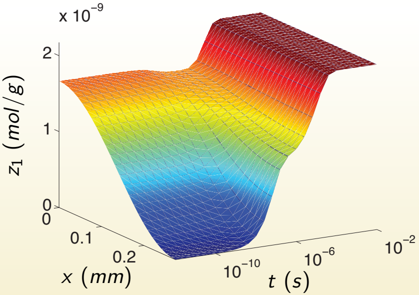
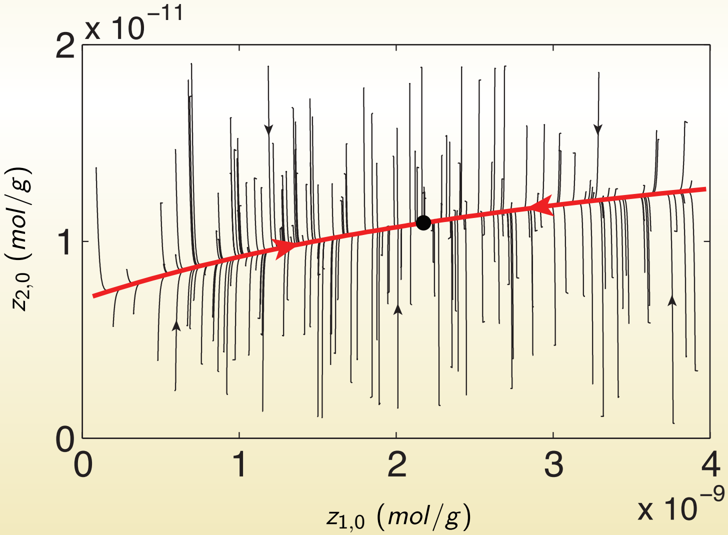




Phase space diagrams

$L = 10\ \mu m$



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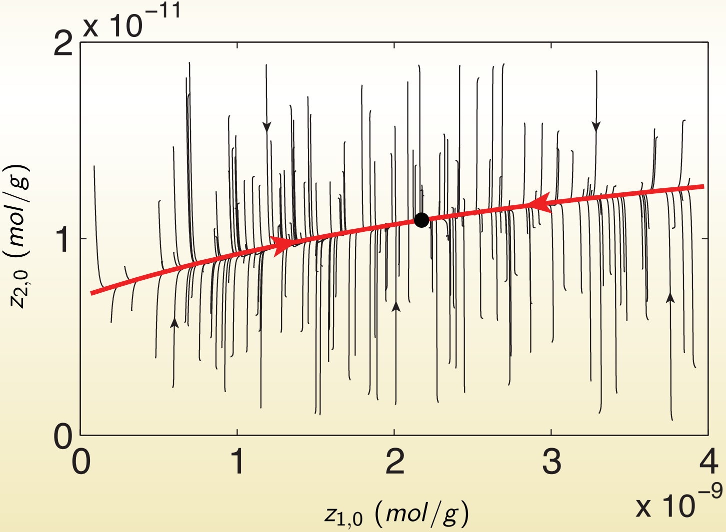

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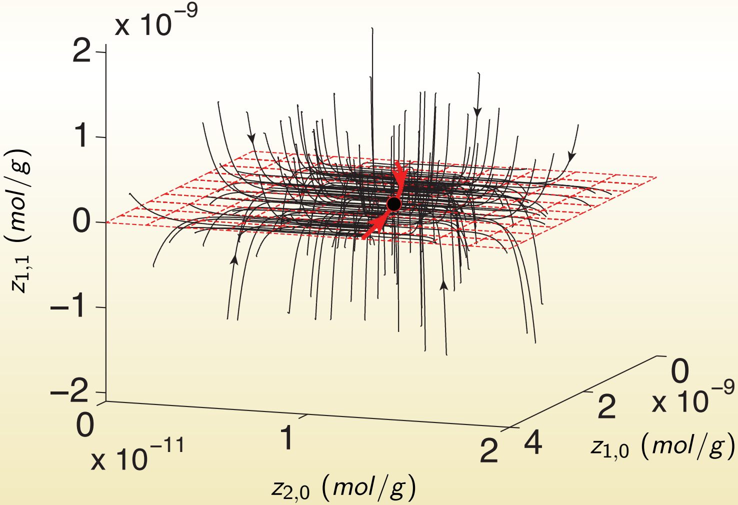

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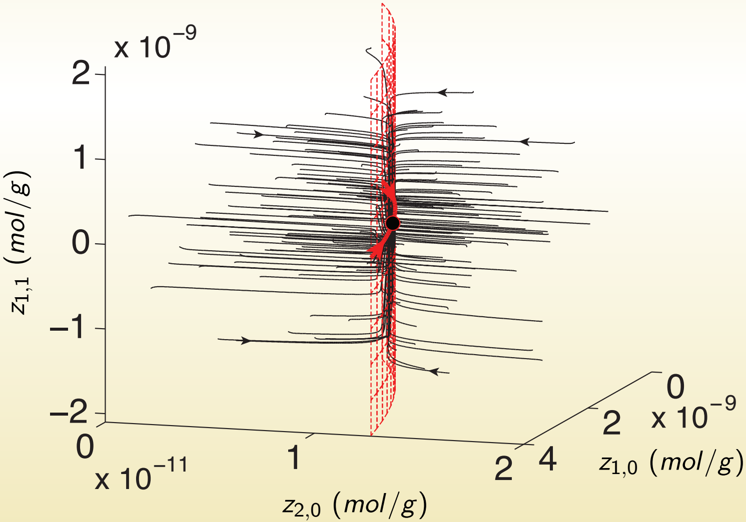

Conclusions

- For long wavelengths, reaction governs the time scales.
- For short wavelengths, diffusion dictates the fast time scales; however, slower reaction time scales are still present.
- The boundary between short and long wavelengths is identified by this method.
- This method isolates the slowest dynamics making it ideal for reduction technique.
- It is easily extended to larger $\mathcal{N}$ to evaluate systems with longer domain lengths.
- This technique provides a framework for further evaluation of the coupling of spatial and temporal scales.

Acknowledgements

Questions?

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