Diffusion correction to slow invariant manifolds in a short length scale limit

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Third International Workshop on
Model Reduction in Reacting Flows

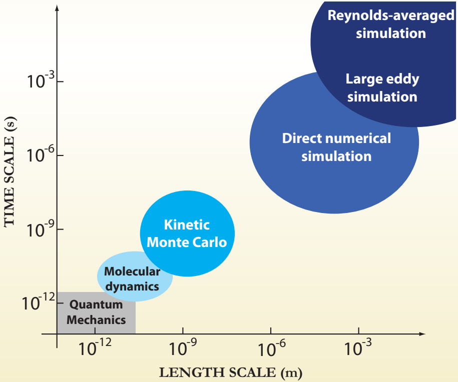
Corfu, Greece

27 April 2011

Outline

Motivation and Background

- Reactive systems induce a wide range of spatial and temporal scales, and subsequently severe stiffness
- DNS resolves all ranges of continuum physical scales present
- Under-resolved simulations account for missed physical phenomena with modeling
- Fully resolved simulations are expensive to compute

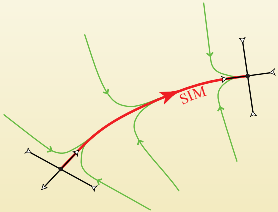


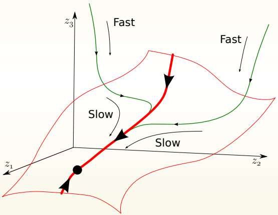
"Research needs for future internal combustion engines," *Physics Today*, Nov. 2008, pp 47-52.

Motivation and Background

- Manifold methods provide potential savings
- Most methods are for spatially homogeneous systems
- We employ the SIM model of Al-Khateeb, et al.

(2009, *Journal of Chemical Physics*)





- We adjust for the dynamics of diffusion in the presence of weak spatial heterogeneity
- This is valid when diffusion is fast relative to reaction, i.e. thin regions of flames

Evolution Equations

Reduce the reactive Navier-Stokes equations

- Negligible advection
- Isothermal, isochoric
- Arrhenius reaction kinetics
- Fick's law of mass diffusion with single constant diffusivity
- Ideal mixture of ideal gases
- Homogeneous Neumann boundary conditions
- Element conservation

- Evolution of species

$$\frac{\partial z_i}{\partial t} = \frac{\dot{\omega}(z_n)}{\rho} + \mathcal{D}\frac{\partial^2 z_i}{\partial x^2}$$

- Boundary conditions

$$\left.\frac{\partial z_i}{\partial x}\right|_{x=0} = \left.\frac{\partial z_i}{\partial x}\right|_{x=\ell} = 0$$

Galerkin Reduction to ODEs

- Assume a spectral decomposition of the reduced variables

$$z_i(x,t) = \sum_{m=0}^{\infty} z_{i,m}(t)\phi_m(x)$$

- Basis functions, $\phi_m(x)$, chosen as orthogonal eigenfunctions of diffusive operator that match boundary conditions

$$\phi_m(x) = \cos\left(\frac{m\pi x}{\ell}\right)$$

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

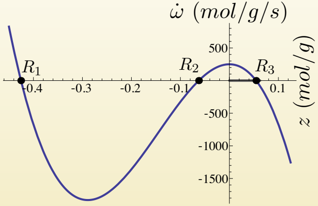
$$\frac{dz_{i,m}}{dt} = \frac{\langle \phi_m, \dot{\omega}_i\left(\sum_{m=0}^{\infty} z_{i,n}\phi_n\right)\rangle}{\langle \phi_m, \phi_m\rangle} - \frac{\pi^2 m^2 \mathcal{D}}{\ell^2} z_{i,m}$$

Oxygen Dissociation

$$O + O + M \;\leftrightharpoons\; O_2 + M$$

- $N = 2$ species
- $J = 1$ reactions
- $L = 1$ constraints
- $N - L = 1$ reduced variables
  $z = z_O$

- Isochoric,
  $\rho = 1.6 \times 10^{-4}\ g/cm^3$
- Isothermal, $T = 5000\ K$



Spatially homogeneous evolution equation

$$\frac{dz}{dt} = 249.84130 - 74734.78\ z^2 - 172406.48\ z^3$$

Galerkin Projection

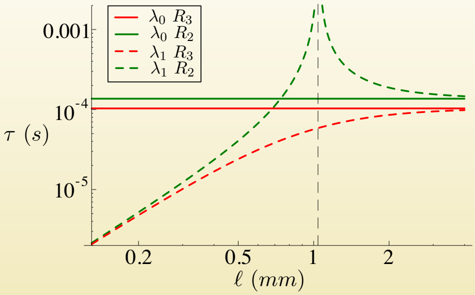
- One spatial mode ($M = 1$) evolution equation

$$\frac{dz_0}{dt} = 249.84130 - 74734.78 \left(z_0^2 + \frac{z_1^2}{2}\right) - 172406.48 \left(z_0^3 + \frac{3z_0 z_1^2}{2}\right)$$

$$\frac{dz_1}{dt} = -74734.78 \,(2z_0 z_1) - 172406.48 \left(3z_0^2 z_1 + \frac{3z_1^3}{4}\right) - \frac{\pi^2 \mathcal{D}}{\ell^2} z_1$$

- Spatially homogeneous evolution when $z_1 = 0$
- Equilibria from spatially homogeneous retained
- Eigenvalues about these equilibria are modified

$$\lambda_1 = \lambda_0 - \frac{\pi^2 \mathcal{D}}{\ell^2}$$



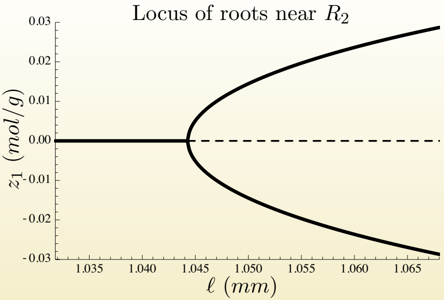
Bifurcation

- Change in sign of modified eigenvalue, $\lambda_1 = \lambda_0 - \frac{\pi^2 \mathcal{D}}{\ell^2}$, identifies a critical length where SIM start point changes character

- Bifurcation occurs at R_2 equilibrium

$$\frac{\pi^2 \mathcal{D}}{\ell^2} = \lambda_0 = 7321.5 \ s^{-1}$$
$$\ell = 1.04 \ mm$$

- Diffusion corrected SIM start point shifts to bifurcated branches



- Bold branches are saddles, dashed branch is source

Poincaré Sphere

- Map variables into a space where infinity is on the unit circle

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

- Graphically displays dynamics of entire system

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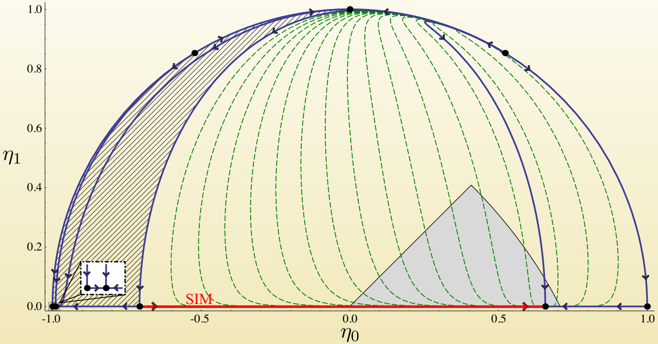
$\ell = 0.334\ mm$



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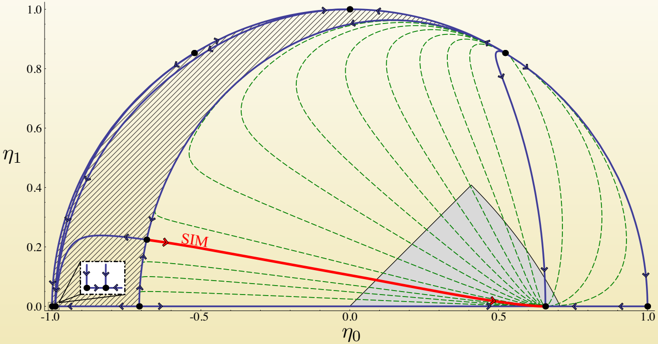
$\ell = 1.05\ mm$



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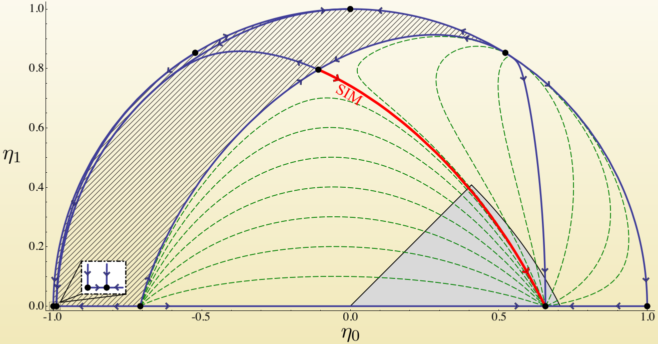
$\ell = 3.34\ mm$



Zel'dovich Mechanism

$$\begin{aligned} N + NO &\leftrightharpoons N_2 + O \\ N + O_2 &\leftrightharpoons NO + O \end{aligned}$$

- $N = 5$ species
- $J = 2$ reactions
- $L = 3$ constraints
- $N - L = 2$ reduced variables

  $z_1 = z_{NO},\ z_2 = z_N$

- Isochoric, $\rho = 1.2002\ g/cm^3$
- Isothermal, $T = 4000\ K$
- Bimolecular, isobaric, $P = 1.6629 \times 10^6\ dyne/cm^2 = 1.64\ atm$

Spatially homogeneous evolution equations – second order polynomials.

$$\begin{aligned} \frac{dz_1}{dt} &= 250 - 9.97{\times}10^4 z_1 + 1.16{\times}10^7 z_2 - 3.22{\times}10^9 z_1 z_2 + 6.99{\times}10^8 z_2^2 \\ \frac{dz_2}{dt} &= 250 + 8.47{\times}10^4 z_1 - 1.17{\times}10^7 z_2 - 1.84{\times}10^9 z_1 z_2 - 6.98{\times}10^8 z_2^2 \end{aligned}$$

Spatially Homogeneous Isothermal Phase Space

- Identify equilibria
- Characterize equilibria by eigenvalues of their Jacobian matrix
- Classify time scales as fast and slow
- Identify SIM as a heteroclinic orbit from saddle to sink

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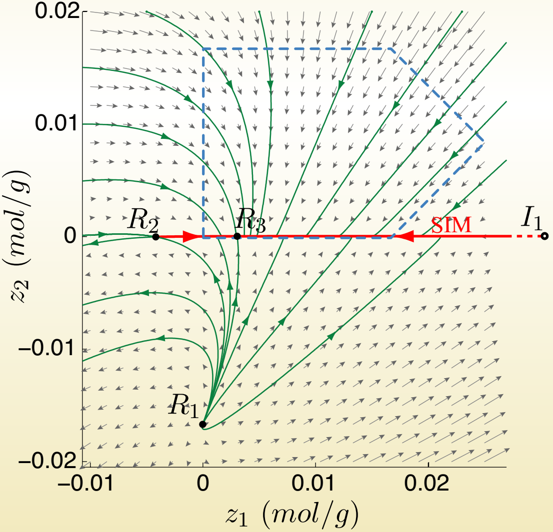

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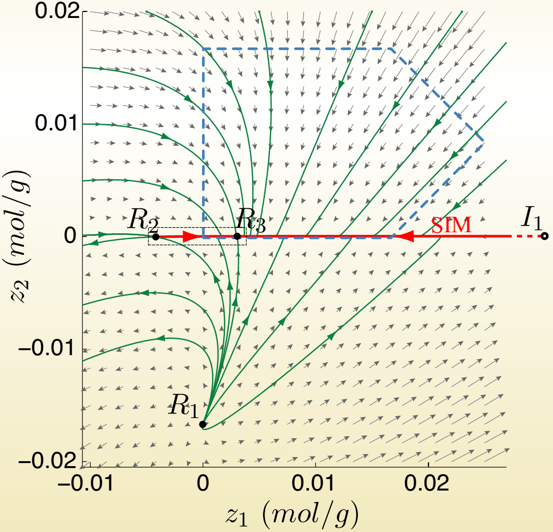

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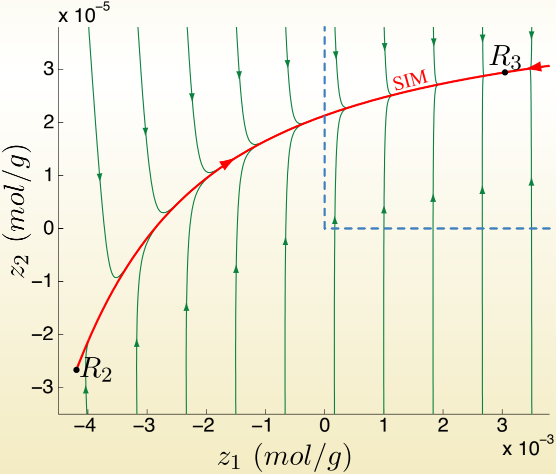
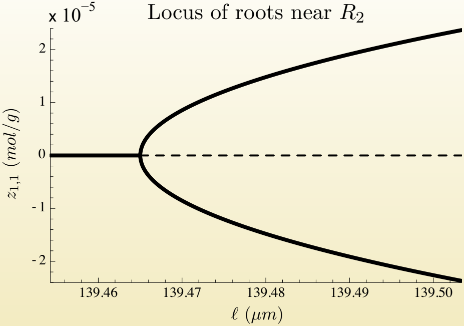
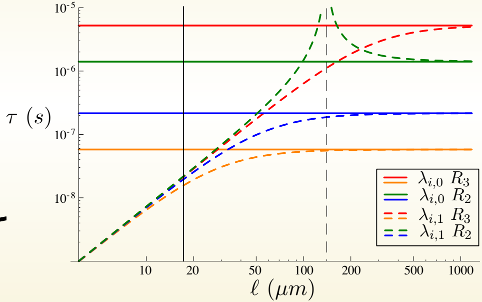


Galerkin Projection

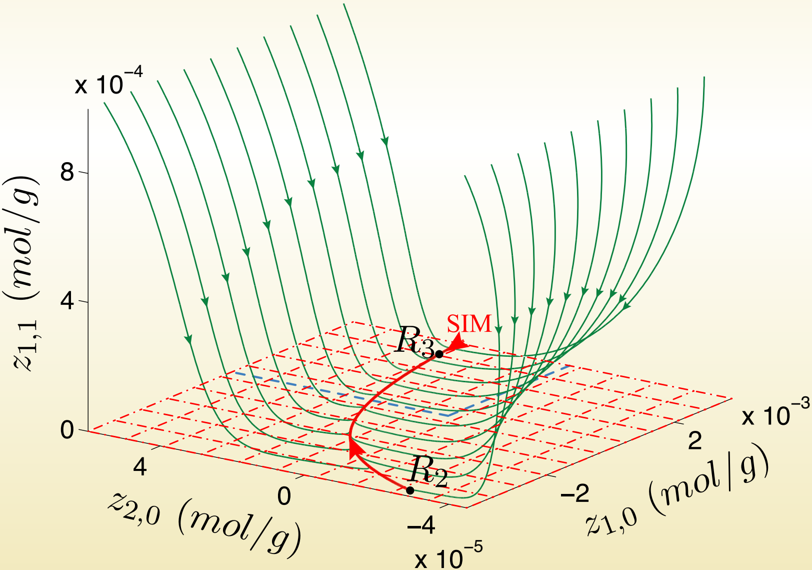
- First diffusion mode adds modified time scale
- Positive eigenvalue identifies critical length scale



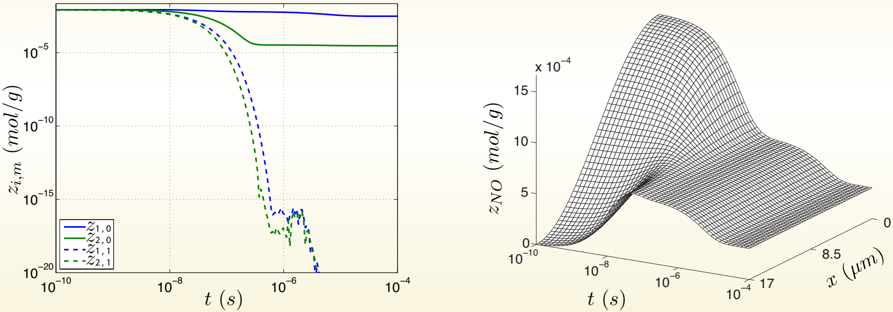


- Bifurcation occurs at this length scale
- Let us examine a length below this critical length scale, $\ell = 17$ μm

Diffusion Correction Isothermal Phase Space



Diffusion Correction Isothermal Evolution



- Two additional fast time scales from diffusion
- Spatially inhomogeneous amplitudes decay earlier than either reaction time scale

Conclusions

- The SIM isolates the slowest dynamics, making it ideal for a reduction technique
- A critical length scale has been identified where a bifurcation occurs that affects the slow dynamics of the system
- 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 the critical length, diffusion will play a more important role

Acknowledgments

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