Slow Invariant Manifolds for Reaction-Diffusion Systems

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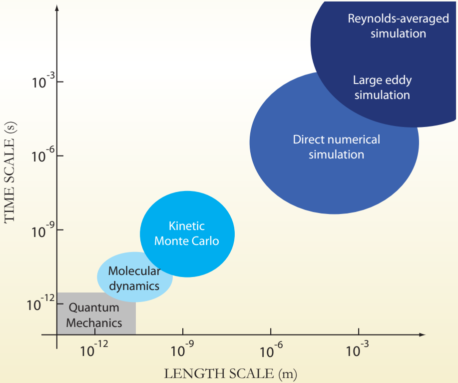
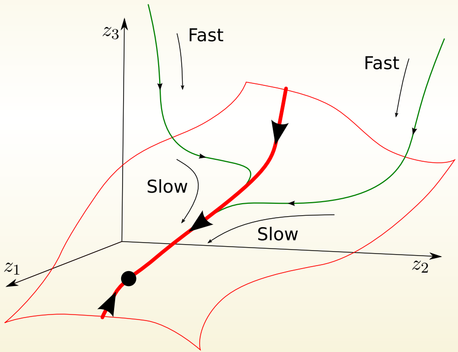
Motivation and Background

- Disparity in scales, "stiffness," creates problems
- Simulations must be verified and validated to ensure accurate results
- All scales must be resolved or accurately modeled
- Fully resolved simulations are expensive to compute

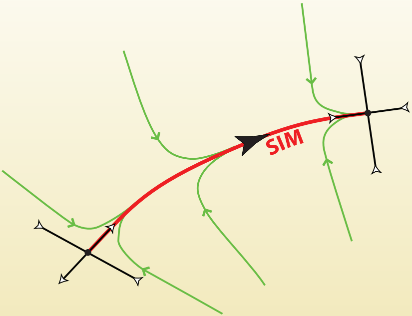


"Research needs for future internal combustion engines," Physics Today, Nov. 2008, pp. 47–52.

Slow Invariant Manifold: (SIM)



- Slow Manifolds provide a roadmap to system's dynamics
- Invariant: trajectory in phase space



- Other trajectories collapse onto SIM at fast time-scale
- Integrate from saddle equilibrium to sink equilibrium

Time-Scale Coupling

$$\frac{\partial z_i}{\partial t} = \dot{\omega}_i(z) + \mathcal{D}\frac{\partial^2 z_i}{\partial x^2},\ i \in [1, N-L]$$

- Stoichiometric constraints removed algebraically

Reaction

$$\tau_{\mathcal{R}} \propto \frac{1}{\lambda_{\mathcal{R}_i}},\ i \in [1, N-L]$$

Diffusion

$$\tau_{\mathcal{D}} \propto \frac{\ell^2}{m^2\ \mathcal{D}},\ m \in [1, \infty)$$

- Interaction between reaction and diffusion time-scales

Fourier Decompostion

- Represent spatial inhomogeneity as a Fourier cosine series

$$z(x,t) = \sum_{m=0}^{M} z_m(t) \cos\left(\frac{m\pi x}{\ell}\right)$$

- Galerkin projection changes the PDE in $z(x,t)$ into a series of M ODEs in $z_m(t)$
- Truncate at sufficiently large M
- High frequency mode, z_M – diffusion
- Low frequency mode, z_1 – reaction and diffusion
- Spatially-homogeneous mode, z_0 – reaction

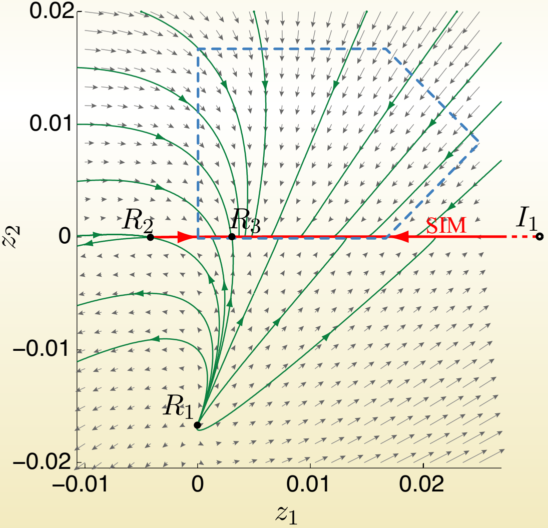
Zel'dovich Mechanism

$$N + NO \rightleftharpoons N_2 + O$$
$$N + O_2 \rightleftharpoons NO + O$$

- 5 species, 2 reactions
- Stoichiometric constraints, 2 reduced variables
  $z_1 = z_{NO}, \; z_2 = z_N$
- Isothermal, Isobaric, Isochoric
  $T = 4000 \; K$
  $V = 1 \times 10^{-3} \; cm^3$
  $P = 1.64 \; atm$

Phase Space

- Spatially homogeneous system – two dimensional phase space
- Find and classify system's equilibria
  - R_1 – Source
  - R_2 – Saddle
  - R_3 – Sink
- SIM branch from R_2 to R_3



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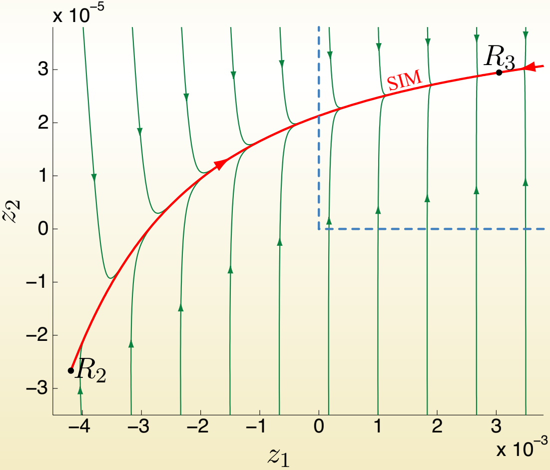
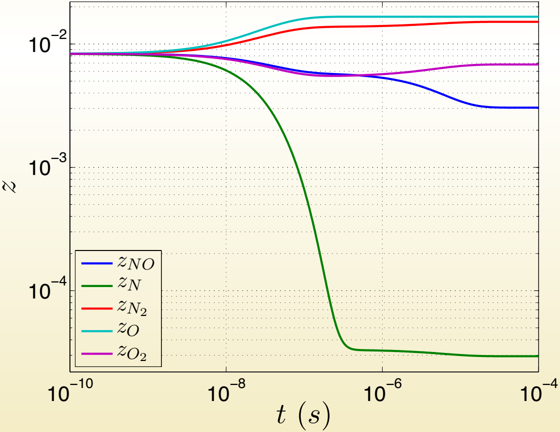


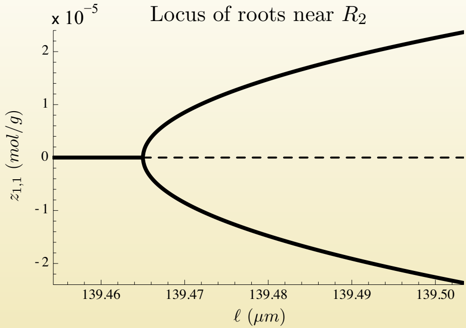
Evolution

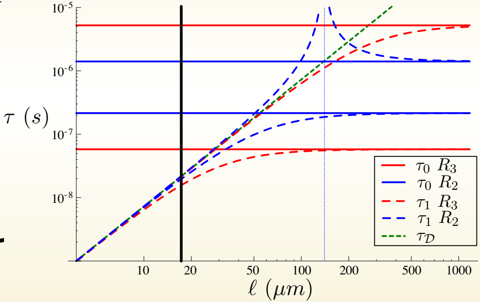
- Fast and slow time-scales apparent
- Fast time-scale: $(10^{-7}s)$
  - Evolution toward SIM
  - Projection onto manifold
- Slow time-scale: $(10^{-5}s)$
  - Evolution along SIM toward equilibrium
  - Manifold look-up table



Local Time-Scales

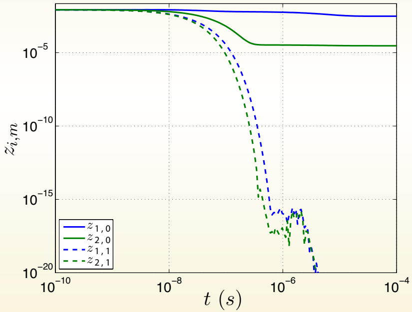
- Examine time scales for $M = 1$ truncation
- $m = 0$ – reaction only
- $m = 1$ – reaction-diffusion

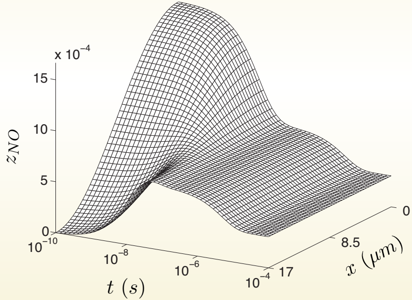




- Bifurcation occurs when time scales are equal, $\ell_c = 140\ \mu m$
- Examine short wavelength, $\ell = 17\ \mu m$

Fourier Amplitude Evolution

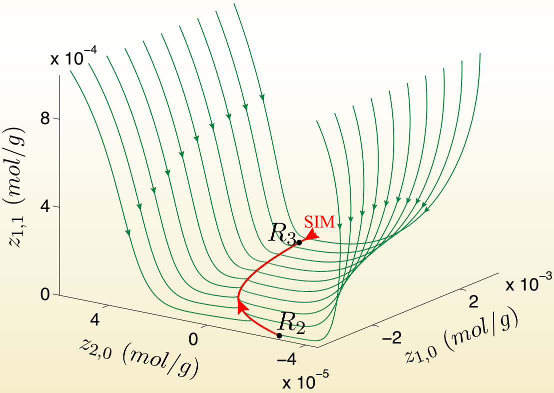




- Short wavelength: diffusion drives additional fast time-scales
- Fast diffusion time-scale allows use of spatially homogeneous manifold method

Galerkin Projection Phase Space

- Galerkin $M = 1$ projection – four dimensional phase space
- Spatially homogeneous SIM branch from R_2 to R_3
- Diffusion mode decays rapidly
- Spatially homogeneous dynamics in long time



Conclusions

- Reaction and diffusion couple the spatial and temporal scales, and hence the stiffness
- For short wavelength modes, diffusion is faster than reaction
- Spatially resolution is necessary to use a manifold method
- Framework for examining the coupling of reaction and diffusion processes

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