Spatial and Temporal Scales Coupling in Reactive Flows

Ashraf N. Al-Khateeb

REACTIVE FLOW MODELING LABORATORY

KING ABDULLAH UNIVERSITY OF SCIENCE & TECHNOLOGY, SAUDI ARABIA

Joseph M. Powers *and* *Samuel Paolucci*

AEROSPACE & MECHANICAL ENGINEERING DEPARTMENT

UNIVERSITY OF NOTRE DAME, NOTRE DAME, INDIANA, USA

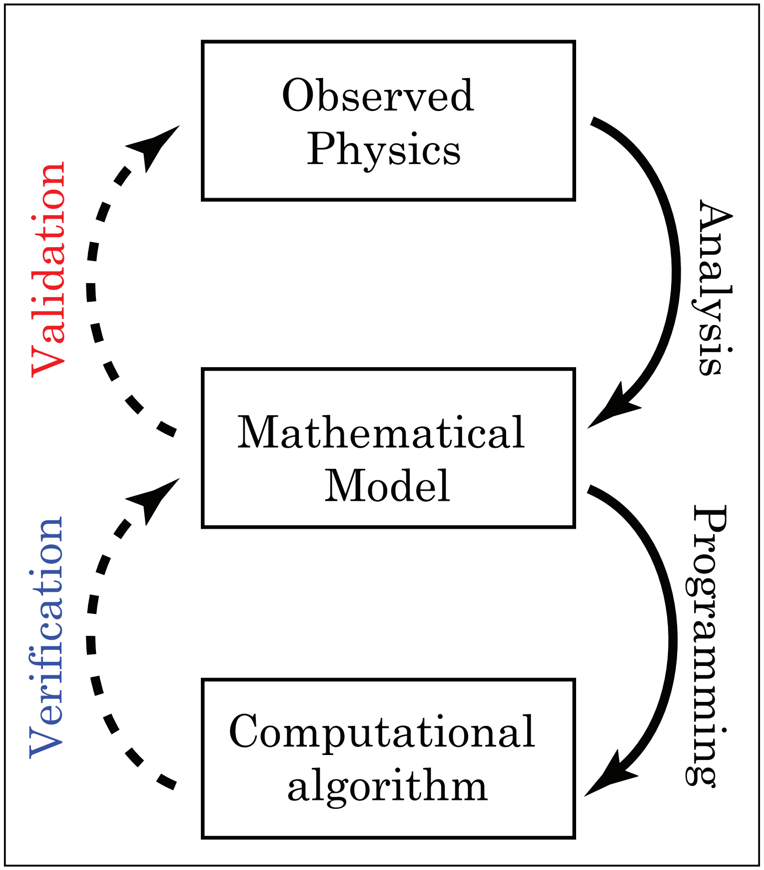
The 3^{rd} International Workshop on Model Reduction in Reacting Flows

Corfu, Greece

27 April 2011

Motivation and Background

- Severe stiffness, temporal and spatial, arises in detailed kinetics modeling.
- Typical reactive flow systems admit multi-scale character.
- To achieve DNS, the interplay between chemistry and transport needs to be captured.
- The interplay between reaction and diffusion length and time scales is well summarized by the classical formula $\ell \sim \sqrt{D\,\tau}$.
- Segregation of chemical dynamics from transport dynamics is a prevalent notion in reduced kinetics combustion modeling. Is this valid?
- Spectral analysis is a tool to understand the coupling between chemistry's and transport's reaction and diffusion scales.



- Computations should have fidelity with the underlying mathematics: verification.
- The mathematical model needs to represent observed physics: validation.
- In computational studies, it is a necessity to address these two issues.
- Proper numerical resolution of all scales is critical to draw correct conclusions.
- All relevant scales have to be brought into simultaneous focus for DNS.

Objectives

- To identify all the physical scales inherent in reacting systems with detailed kinetics and diffusive transport.
- To illustrate the coupling of time and length scales in reactive flows.
- To identify the scales associated with each Fourier mode of varying wavelength for unsteady spatially inhomogenous reactive flow problems.

Illustrative Model Problem

A linear one species model for reaction, advection, and diffusion:

$$\frac{\partial \psi(x,t)}{\partial t} + u\frac{\partial \psi(x,t)}{\partial x} = D\frac{\partial^2 \psi(x,t)}{\partial x^2} - a\psi(x,t),$$

$$\psi(0,t) = \psi_u, \quad \left.\frac{\partial \psi}{\partial x}\right|_{x \to \mathtt{L}} = 0, \qquad \psi(x,0) = \psi_u.$$

Time scale spectrum

For the spatially homogenous version: $\psi_h(t) = \psi_u \exp\left(-at\right),$

reaction time constant: $\tau = \dfrac{1}{a} \implies \Delta t \ll \tau.$

Length Scale Spectrum

- The steady structure:

$$\psi_s(x) = \psi_u \left(\frac{\exp(\mu_1 x) - \exp(\mu_2 x)}{1 - \frac{\mu_1}{\mu_2} \exp(\mathtt{L}(\mu_1 - \mu_2))} + \exp(\mu_2 x) \right),$$

$$\mu_1 = \frac{u}{2D} \left(1 + \sqrt{1 + \frac{4aD}{u^2}} \right), \qquad \mu_2 = \frac{u}{2D} \left(1 - \sqrt{1 + \frac{4aD}{u^2}} \right),$$

$$\ell_i = \left| \frac{1}{\mu_i} \right|.$$

- For fast reaction ($a \gg u^2/D$):

$$\ell_1 = \ell_2 = \sqrt{\frac{D}{a}} = \sqrt{D\tau} \implies \Delta x \ll \sqrt{D\tau}.$$

Spatio-Temporal Spectrum

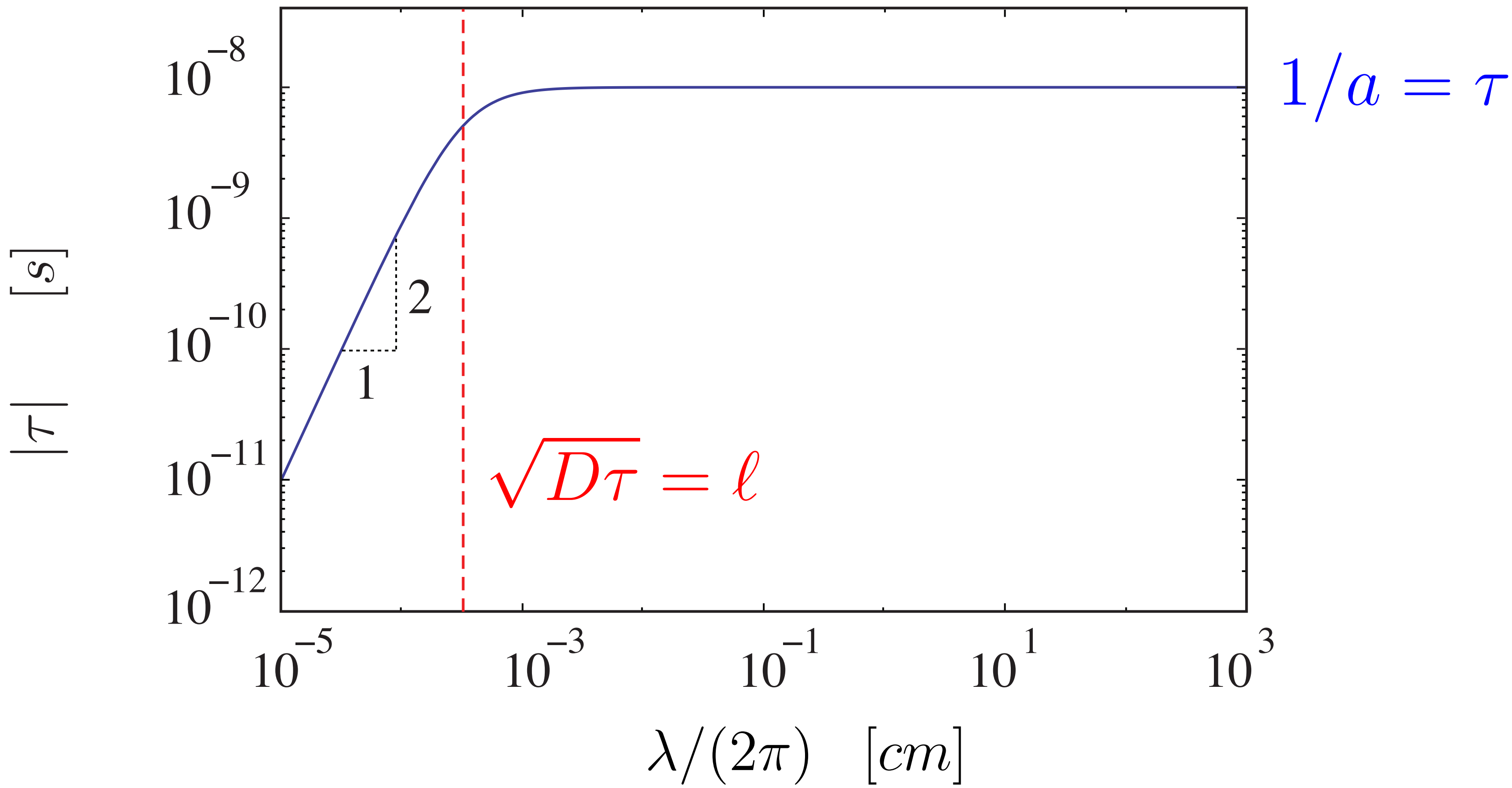
$$\psi(x,t) = \Psi(t)e^{\mathbf{i}kx} \quad \Rightarrow \quad \Psi(t) = C\exp\left(-a\left(1+\frac{\mathbf{i}ku}{a}+\frac{Dk^2}{a}\right)t\right).$$

- For fast reaction: $\lim_{k\to 0}\tau = \lim_{\lambda\to\infty}\tau = \frac{1}{a},$
- For slow reaction: $\lim_{k\to\infty}\tau = \lim_{\lambda\to 0}\tau = \frac{\lambda^2}{4\pi^2}\frac{1}{D},$

$$\left.\right\} \quad \mathcal{S}_t = \left(\frac{2\pi}{\lambda}\sqrt{\frac{D}{a}}\right)^2.$$

- Balance between reaction and diffusion at $k \equiv \frac{2\pi}{\lambda} = \sqrt{\frac{a}{D}} = 1/\ell,$
- Using Taylor expansion:

$$|\tau| = \frac{1}{a}\left(1 - \frac{D}{a\left(\frac{\lambda}{2\pi}\right)^2} - \frac{u^2}{2a^2\left(\frac{\lambda}{2\pi}\right)^2}\right) + \mathcal{O}\left(\frac{1}{\lambda^4}\right).$$



- Similar to $H_2 - air$: $\tau = 1/a = 10^{-8}\ s$, $D = 10\ cm^2/s$,
- $\ell = \sqrt{\frac{D}{a}} = \sqrt{D\tau} = 3.2 \times 10^{-4}\ cm$.

Laminar Premixed Flames

Adopted Assumptions:

- One-dimensional,
- Low Mach number,
- Neglect thermal diffusion effects and body forces.

Governing Equations:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) = 0,$$

$$\rho \frac{\partial h}{\partial t} + \rho u \frac{\partial h}{\partial x} + \frac{\partial \mathrm{J}^q}{\partial x} = 0,$$

$$\rho \frac{\partial y_l}{\partial t} + \rho u \frac{\partial y_l}{\partial x} + \frac{\partial \mathrm{j}_l^m}{\partial x} = 0, \quad l = 1, \ldots, L-1,$$

$$\rho \frac{\partial Y_i}{\partial t} + \rho u \frac{\partial Y_i}{\partial x} + \frac{\partial \mathrm{J}_i^m}{\partial x} = \dot{\omega}_i \bar{m}_i, \quad i = 1, \ldots, N-L.$$

- Unsteady spatially homogeneous reactive system:

$$\frac{d\mathbf{z}(t)}{dt} = \mathbf{f}\left(\mathbf{z}(t)\right), \qquad \mathbf{z}(t) \in \mathbb{R}^N, \quad \mathbf{f} : \mathbb{R}^N \rightarrow \mathbb{R}^N.$$

$$0 = (\mathbf{J} - \lambda \mathbf{I}) \cdot \boldsymbol{v}.$$

$$\mathcal{S}_t = \frac{\tau_{slowest}}{\tau_{fastest}}, \quad \tau_i = \frac{1}{|Re(\lambda_i)|}, \qquad i = 1, \ldots, R \leq N - L.$$

- Steady spatially inhomogeneous reactive system:

$$\tilde{\mathbf{B}}\left(\tilde{\mathbf{z}}(x)\right) \cdot \frac{d\tilde{\mathbf{z}}(x)}{dx} = \tilde{\mathbf{f}}\left(\tilde{\mathbf{z}}(x)\right), \qquad \tilde{\mathbf{z}}(x) \in \mathbb{R}^{2N+2}, \quad \tilde{\mathbf{f}} : \mathbb{R}^{2N+2} \rightarrow \mathbb{R}^{2N+2}.$$

$$\tilde{\lambda}\tilde{\mathbf{B}} \cdot \tilde{\boldsymbol{v}} = \left(\tilde{\mathbf{J}} - \tilde{\boldsymbol{\Psi}} \cdot \frac{d\tilde{\mathbf{z}}}{dx}\right) \cdot \tilde{\boldsymbol{v}}.$$

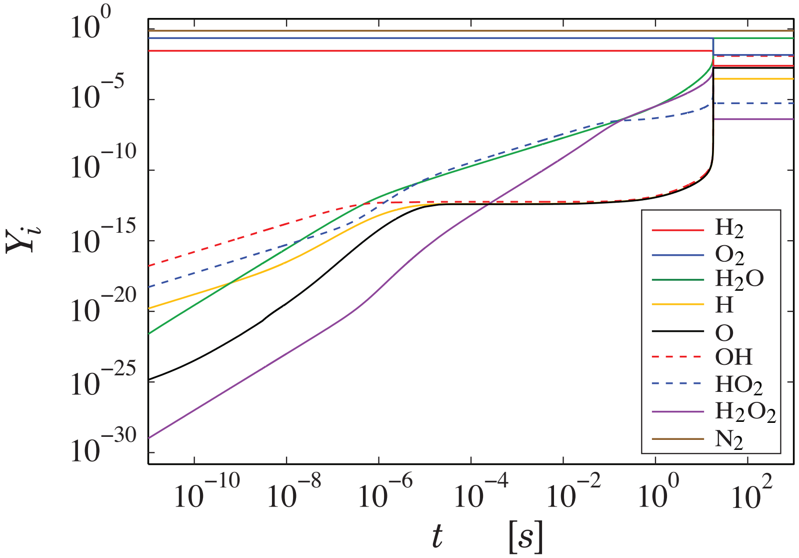
$$\mathcal{S}_x = \frac{\ell_{coarsest}}{\ell_{finest}}, \quad \ell_i = \frac{1}{|Re(\tilde{\lambda}_i)|}, \qquad i = 1, \ldots, 2N - L.$$

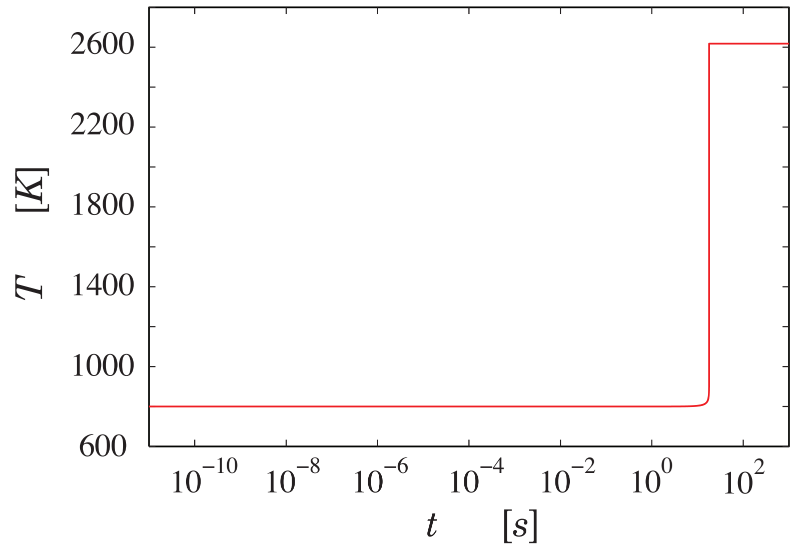
Laminar Premixed Hydrogen–Air Flame

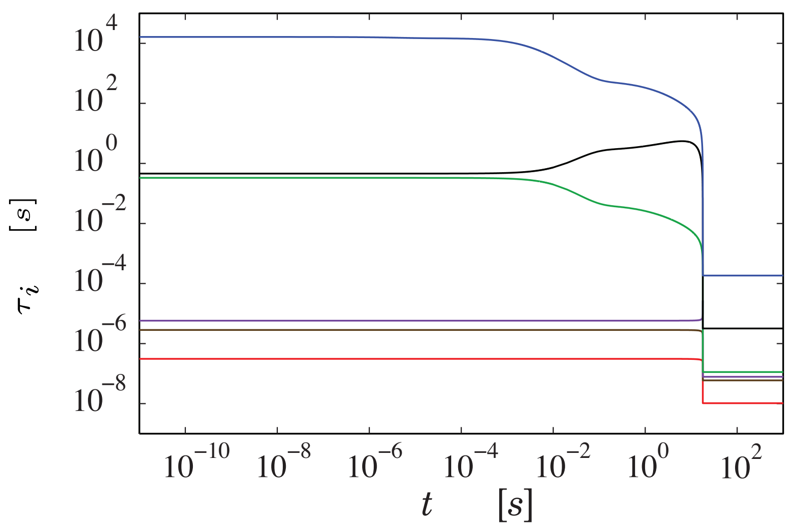
- Standard detailed mechanism[a]; $N = 9$ species, $L = 3$ atomic elements, and $J = 19$ reversible reactions,
- stoichiometric hydrogen-air: $2H_2 + (O_2 + 3.76N_2)$,
- adiabatic and isobaric: $T_u = 800\ K,\ p = 1\ atm$,
- calorically imperfect ideal gases mixture,
- neglect Soret effect, Dufour effect, and body forces,
- CHEMKIN and IMSL are employed.

[a] J. A. Miller, R. E. Mitchell, M. D. Smooke, and R. J. Kee, *Proc. Combust. Ins.* **19**, p. 181, 1982.

- Unsteady spatially homogeneous reactive system:





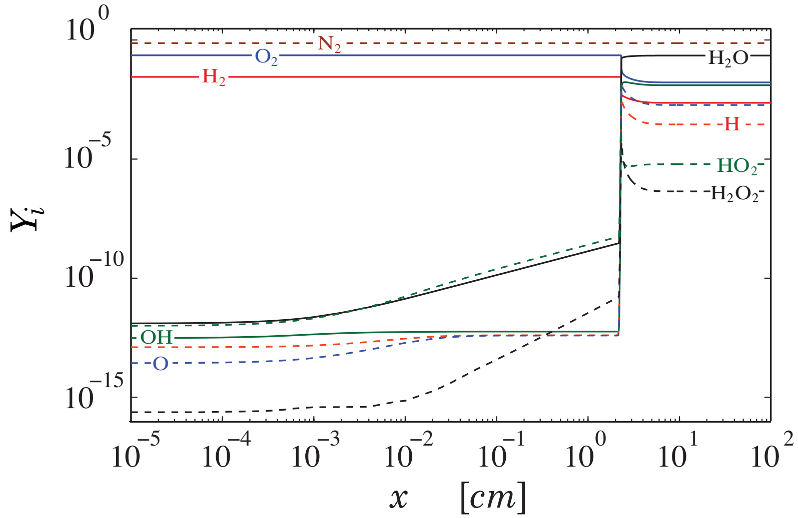


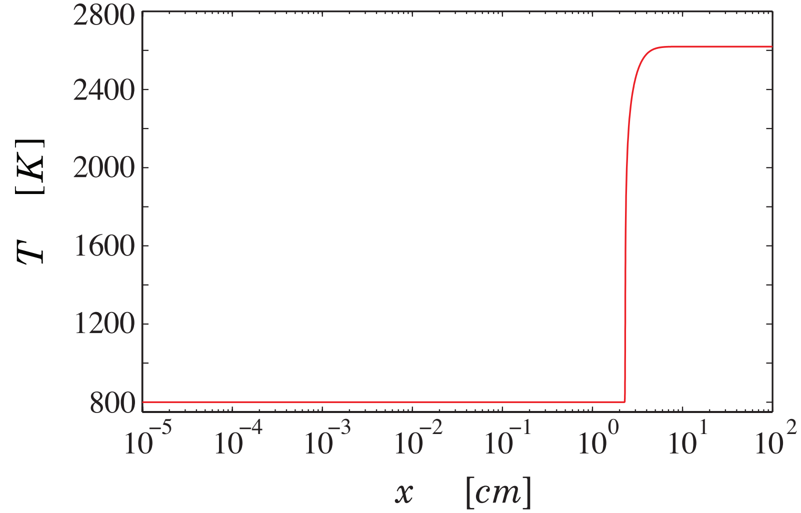
$$\tau_{slowest} = 1.8\times10^{-2}\ s$$

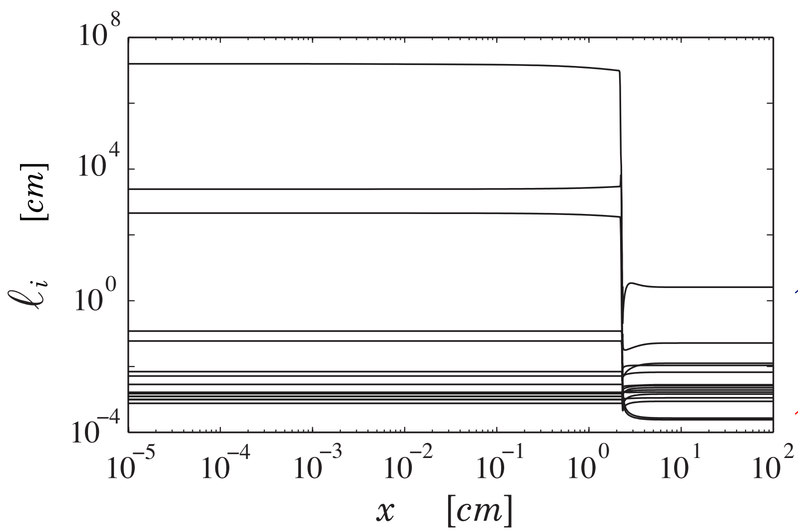
$$\tau_{fastest} = 1.0\times10^{-8}\ s$$

$$\mathcal{S}_t \sim \mathcal{O}\left(10^4\right).$$

- Steady spatially inhomogeneous reactive system:[a]







$\ell_{coarsest} = 2.6 \times 10^{0}\ cm$

$\ell_{finest} = 2.4 \times 10^{-4}\ cm$

$$\mathcal{S}_x \sim \mathcal{O}\left(10^4\right).$$

[a] A. N. Al-Khateeb, J. M. Powers, and S. Paolucci, *Comm. Comp. Phys.* 8(2): 304, 2010.

Spatio-Temporal Spectrum

- PDEs $\longrightarrow \quad 2N+2$ PDAEs,

$$\mathbf{A}(\mathbf{z})\cdot\frac{\partial\mathbf{z}}{\partial t}+\mathbf{B}(\mathbf{z})\cdot\frac{\partial\mathbf{z}}{\partial x}=\mathbf{f}(\mathbf{z}).$$

- Spatially homogeneous system at chemical equilibrium subjected to a spatially inhomogeneous perturbation, $\mathbf{z}'=\mathbf{z}-\mathbf{z}^e$,

$$\mathbf{A}^e\cdot\frac{\partial\mathbf{z}'}{\partial t}+\mathbf{B}^e\cdot\frac{\partial\mathbf{z}'}{\partial x}=\mathbf{J}^e\cdot\mathbf{z}'.$$

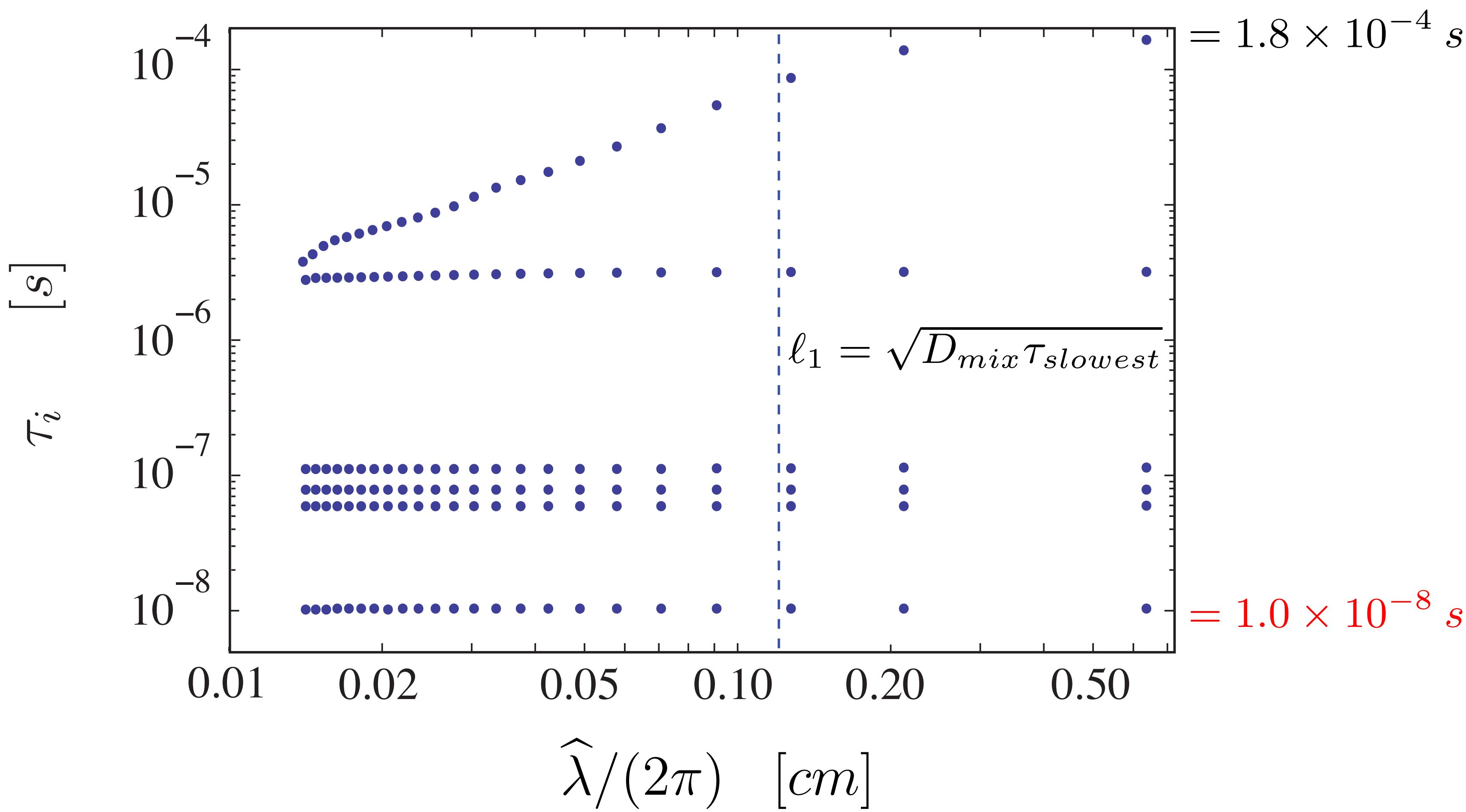
- Spatially discretized spectrum,

$$\boldsymbol{\mathcal{A}}^e\cdot\frac{d\boldsymbol{\mathcal{Z}}}{dt}=\left(\boldsymbol{\mathcal{J}}^e-\boldsymbol{\mathcal{B}}^e\right)\cdot\boldsymbol{\mathcal{Z}},\qquad \boldsymbol{\mathcal{Z}}\in\mathbb{R}^{2\mathcal{N}(N+1)}.$$

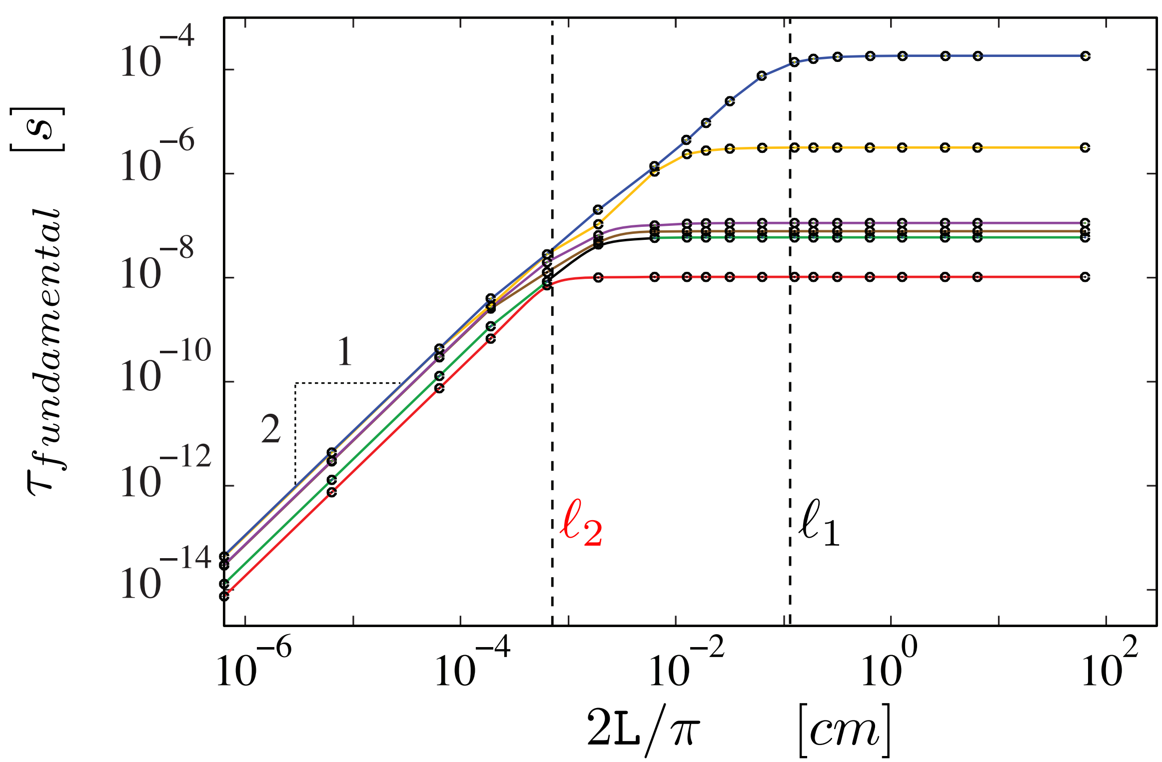
- The time scales of the generalized eigenvalue problem,

$$\tau_i=\frac{1}{\left|Re\left(\lambda_i\right)\right|},\quad i=1,\ldots,(\mathcal{N}-1)(N-1).$$

- $\mathtt{L} = 1\ cm$ and $D_{mix} = 64\ cm^2/s$,
- modified wavelength: $\widehat{\lambda} = 4\mathtt{L}/(2\mathfrak{n} - 1)$,
- associated length scale: $\ell = \widehat{\lambda}/(2\pi) \;\Rightarrow\; \ell = \frac{2\mathtt{L}}{(2\mathfrak{n}-1)\pi}$,



- $D_{mix} = \frac{1}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} \mathfrak{D}_{ij}$,
- $\ell_1 = \sqrt{D_{mix} \tau_{slowest}} = 1.1 \times 10^{-1}\ cm$,
- $\ell_2 = \sqrt{D_{mix} \tau_{fastest}} = 8.0 \times 10^{-4}\ cm \approx \ell_{finest} = 2.4 \times 10^{-4}\ cm$.



$\tau_{fastest} = 1.8 \times 10^{-4}\ s$

$\tau_{slowest} = 1.0 \times 10^{-8}\ s$

Conclusions

- Time and length scales are coupled.
- Coarse wavelength modes have time scales dominated by reaction.
- Short wavelength modes have time scales dominated by diffusion.
- Fourier modal analysis reveals a cutoff length scale for which time scales are dictated by a balance between transport and chemistry.
- Fine scales, temporal and spatial, are essential to resolve reacting systems; the finest length scale is related to the finest time scale by $\ell \sim \sqrt{D\tau}$.
- For a $p = 1\ atm, H_2 + air$ laminar flame, the length scale where fast reaction balances diffusion is $\sim 2\ \mu m$, the necessary scale for a DNS.