A Wavelet/ILDM Method for Computational Combustion

by

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Outline

- Motivation
- Intrinsic Low Dimensional Manifold (ILDM) technique
- Wavelet Adaptive Multilevel Representation (WAMR) technique
- Results for one-dimensional viscous $H_2 - O_2$ detonation with detailed chemical kinetics
- Conclusions

Motivation

- Detailed finite rate kinetics critical in reactive fluid mechanics:
  - Candle flames,
  - Internal combustion engines,
  - Atmospheric chemistry,
- Common detailed kinetic models are computationally expensive.
- Expense increases with
  - number of species and reactions modeled (linear effect),
  - *stiffness*–ratio of slow to fast time scales, (geometric effect).
- Fluid mechanics time scales: 10^{-5} s to 10^{1} s.
- Reaction time scales: 10^{-11} s to 10^{-5} s.
- Reduced kinetics necessary given current computational resources.
- Adaptive discretization necessary for fine spatial structures.

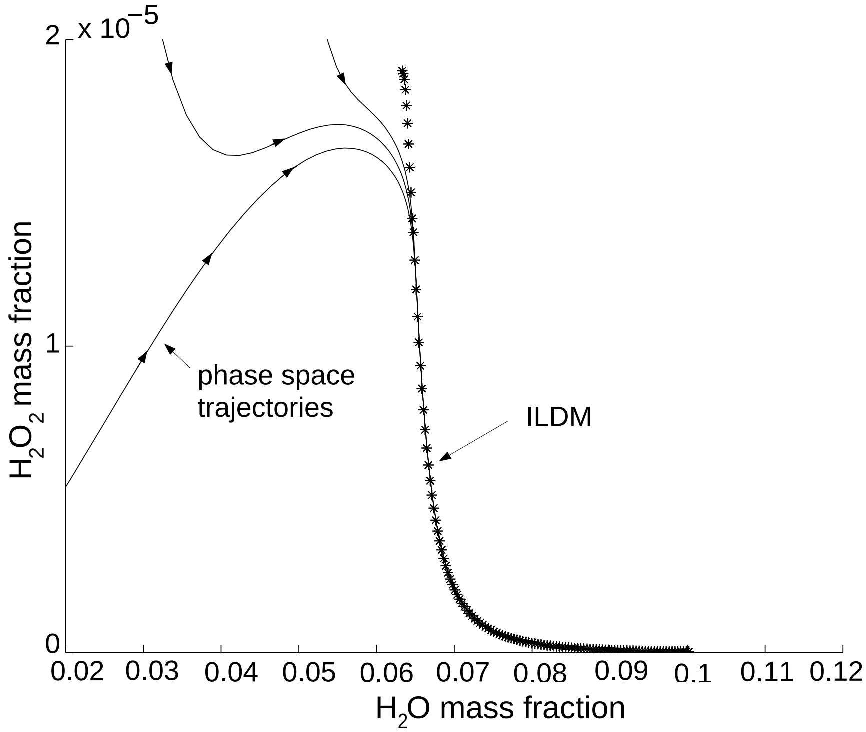
Goals

- Implement robust new reduced kinetic method (Intrinsic Low Dimensional Manifold-ILDM) of Maas and Pope (1992)
- Extend ILDM method to systems with time and space dependency, correctly accounting for convection and diffusion
- Extend WAMR technique (Paolucci & Vasilyev) to combustion systems,
- Couple WAMR and ILDM techniques.

Intrinsic Low-Dimensional Manifold Method (ILDM)

- Uses a formal dynamical systems approach,
- Does not require imposition of *ad hoc* partial equilibrium or steady state assumptions,
- Fast time scale phenomena are systematically equilibrated,
- Slow time scale phenomena are resolved in time,
- n-species gives rise to a n-dimensional phase space (same as composition space) for isochoric, isothermal combustion in well stirred reactors,
- Identifies m-dimensional subspaces (manifolds), $m < n$, embedded within the n-dimensional phase space on which slow time scale events evolve,
  - Fast time scale events rapidly move to the manifold,
  - Slow time scale events move on the manifold.
- Computation time reduced by factor of ~ 10 for non-trivial combustion problems; manifold gives much better roadmap to find solution relative to general implicit solution techniques (Norris, 1998)

Formulation of ILDM's



- A well-stirred reactive system of form:

$$\frac{d\mathbf{x}}{dt} = \mathbf{F}(\mathbf{x}), \qquad \mathbf{x}(0) = \mathbf{x}_o,$$

- Local linearization gives

$$\frac{d\tilde{\mathbf{x}}}{dt} = \mathbf{F_x} \cdot \tilde{\mathbf{x}},$$

- Use local Schur decomposition of the Jacobian matrix $\mathbf{F_x}$ to identify reaction time scales and fast and slow subspaces.

- ILDM defined algebraically by $\mathbf{W} \cdot \mathbf{F}(\mathbf{x}) = 0$, where $\mathbf{W}$ is the fast subspace.

Wavelet Adaptive Multilevel Representation (WAMR) Technique

- See e.g. Vasilyev and Paolucci, "A Fast Adaptive Wavelet Collocation Algorithm for Multidimensional PDEs," *J. Comp. Phys.*, 1997,
- Basis functions have compact support,
- Well-suited for problems with widely disparate spatial scales,
- Good spatial and spectral localization, and fast (spectral) convergence,
- Easy adaptable to steep gradients via adding collocation points,
- Spatial adaptation is automatic and dynamic to achieve prescribed error tolerance.

Algorithm Description

- Approximate initial function using wavelet basis,

$$\mathbf{P}^J u(x) = \sum_k u_{0,k}\phi_{0,k}(x) + \sum_{j=1}^{J}\sum_k d_{j,k}\psi_{j,k}(x)$$

- Discard non-essential wavelets if amplitude below threshold value (here we look only at P, T, u, and ρ, species could be included),

$$\mathbf{P}^J u(x) = u^J_{\geq}(x) + u^J_{<}(x)$$

$$u^J_{\geq}(x) = \sum_k u_{0,k}\phi_{0,k}(x) + \sum_{j=1}^{J}\sum_k d_{j,k}\psi_{j,k}(x), |d_{j,k}| \geq \epsilon$$

$$u^J_{<}(x) = \sum_{j=1}^{J}\sum_k d_{j,k}\psi_{j,k}(x), |d_{j,k}| < \epsilon$$

- Assign a collocation point to every essential wavelet,
- Establish a neighboring region of potentially essential wavelets,
- Discretize the spatial derivatives; five points used here (related to order of wavelet family),
- Integrate in time; linearized trapezoidal method (implicit) used here,
- Repeat

Ignition Delay in Premixed H_2-O_2

- Consider standard problem of Fedkiw, Merriman, and Osher, *J. Comp. Phys.*, 1996,
- Shock tube with premixed H_2, O_2, and Ar in 2/1/7 molar ratio,
- Initial inert shock propagating in tube,
- Reaction commences shortly after reflection off end wall,
- Detonation soon develops,
- Model assumptions
  - One-dimensional,
  - Mass, momentum, and energy diffusion,
  - Nine species, thirty-seven reactions,
  - Ideal gases with variable specific heats.

Compressible Reactive Navier-Stokes Equations for H_2-O_2 Problem

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

$$\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}\left(\rho u^2 + P - \tau\right) = 0, \qquad \text{momentum}$$

$$\frac{\partial}{\partial t}\left(\rho\left(e + \frac{u^2}{2}\right)\right) + \frac{\partial}{\partial x}\left(\rho u\left(e + \frac{u^2}{2}\right) + u(P - \tau) + q\right) = 0, \qquad \text{energy}$$

$$\frac{\partial}{\partial t}(\rho Y_i) + \frac{\partial}{\partial x}(\rho u Y_i + j_i) = \sum_{j=1}^{M} a_j T^{\alpha_j} \exp\left(\frac{-E_j}{\Re T}\right) \nu_{ij} M_i \prod_{k=1}^{N}\left(\frac{\rho Y_k}{M_k}\right)^{\nu_{kj}}, \qquad \text{species}$$

$$P = \rho \Re T \sum_{i=1}^{N} \frac{Y_i}{M_i}, \qquad \text{thermal equation of state}$$

$$e = \sum_{i=1}^{N} Y_i \left(h_i^o + \int_{T_o}^{T} c_{pi}(\hat{T}) d\hat{T}\right) - \frac{P}{\rho}, \qquad \text{caloric equation of state}$$

$$\tau = \frac{4}{3}\mu \frac{\partial u}{\partial x}, \qquad \text{Newtonian gas with Stokes' assumption}$$

$$j_i = -\rho \sum_{j=1}^{N} \mathcal{D}_{ij} \frac{\partial Y_j}{\partial x}, \qquad \text{Fick's law}$$

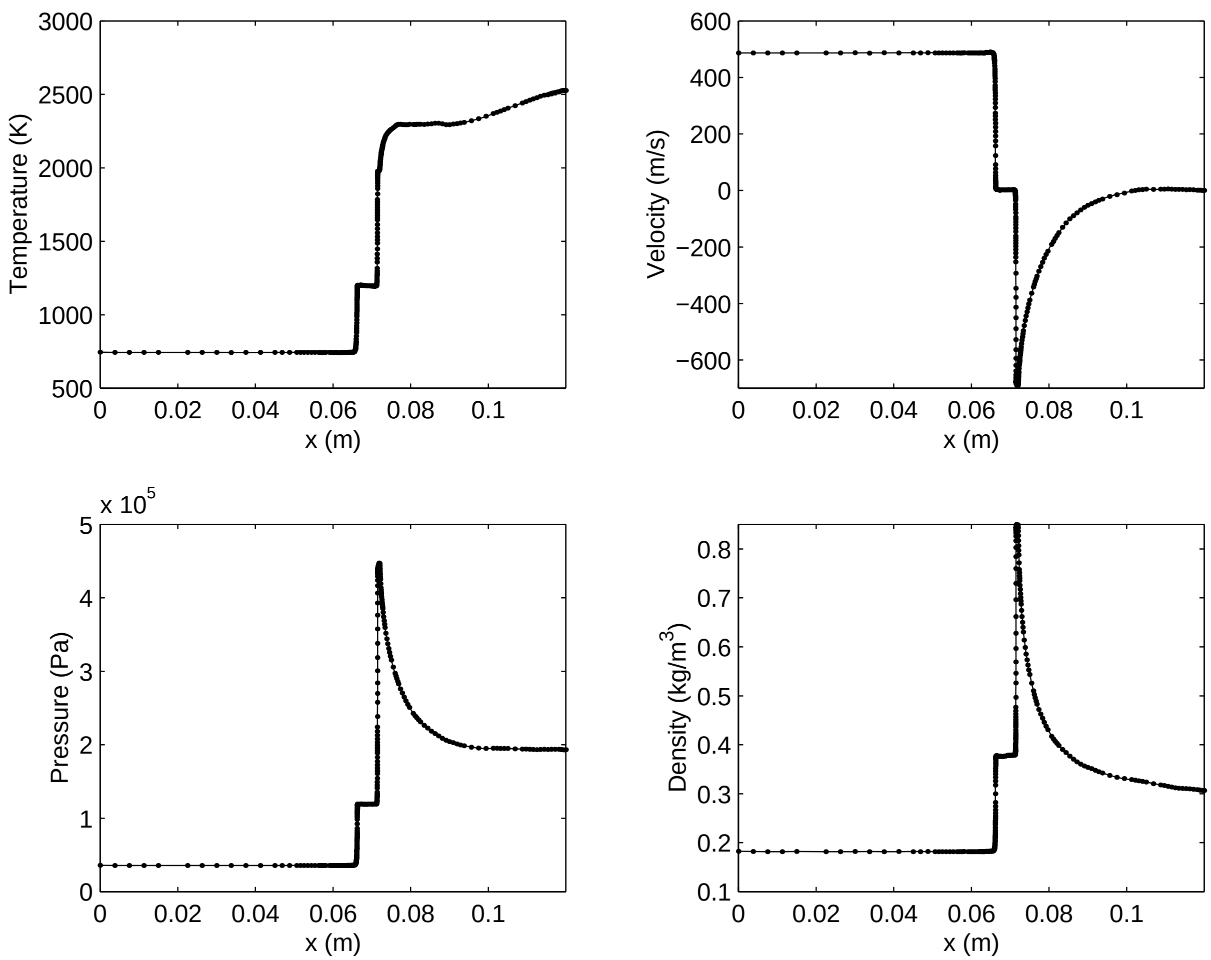
$$q = -k\frac{\partial T}{\partial x} + \sum_{i=1}^{N} j_i \left(h_i^o + \int_{T_o}^{T} c_{pi}(\hat{T}) d\hat{T}\right) \qquad \text{augmented Fourier's law.}$$

$N = 9$ species: H_2, O_2, H, O, OH, H_2O_2, H_2O, HO_2, Ar

$M = 37$ reactions

Viscous $H_2 - O_2$ Ignition Delay with Wavelets and ILDM

- $t = 195\ \mu s$, 300 collocation points, 15 wavelet levels
- ILDM gives nearly identical results as full chemistry
- Wavelet spatial discretization, explicit convection-diffusion time stepping, implicit reaction time stepping (Strang splitting)
- *Viscous shocks, induction zones, and entropy layers spatially resolved!*



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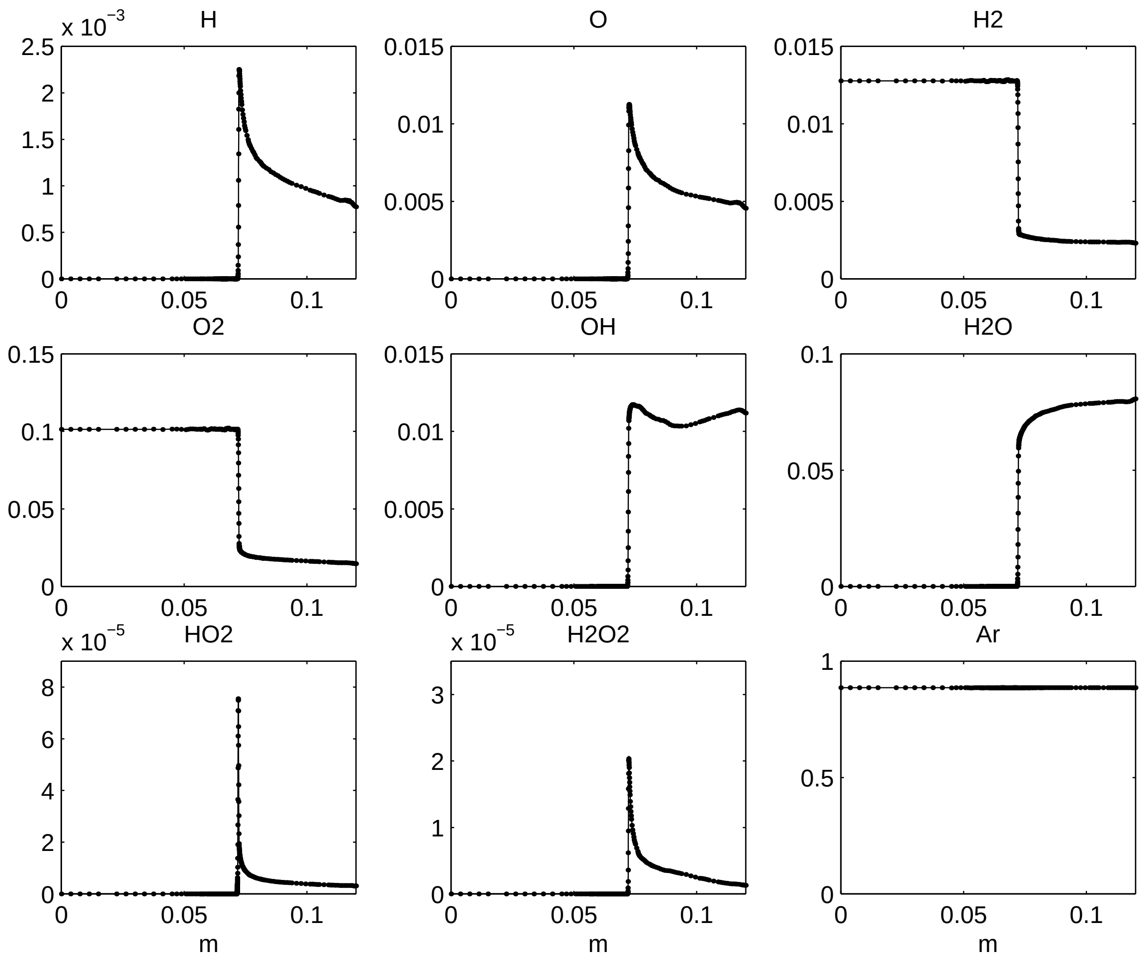
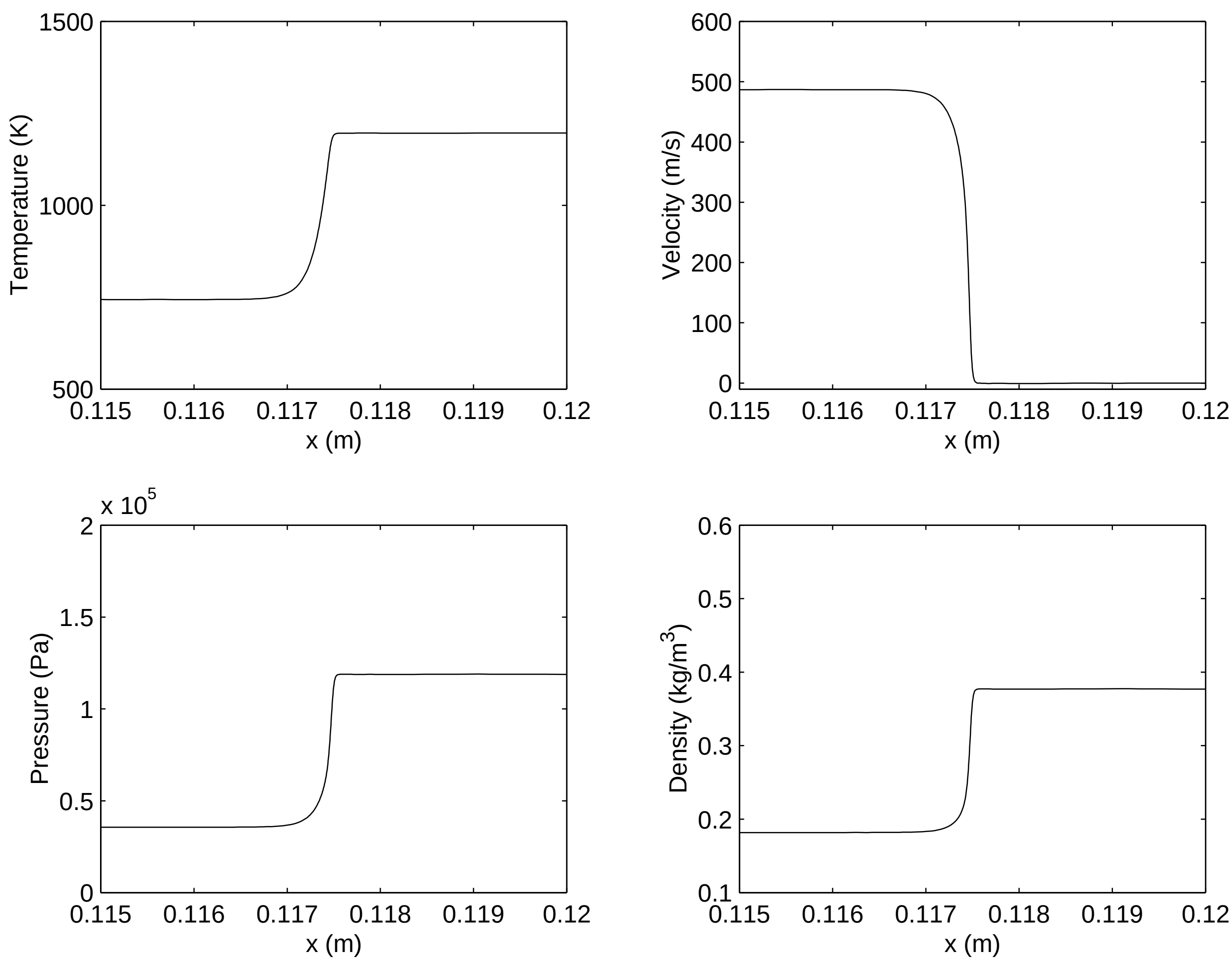


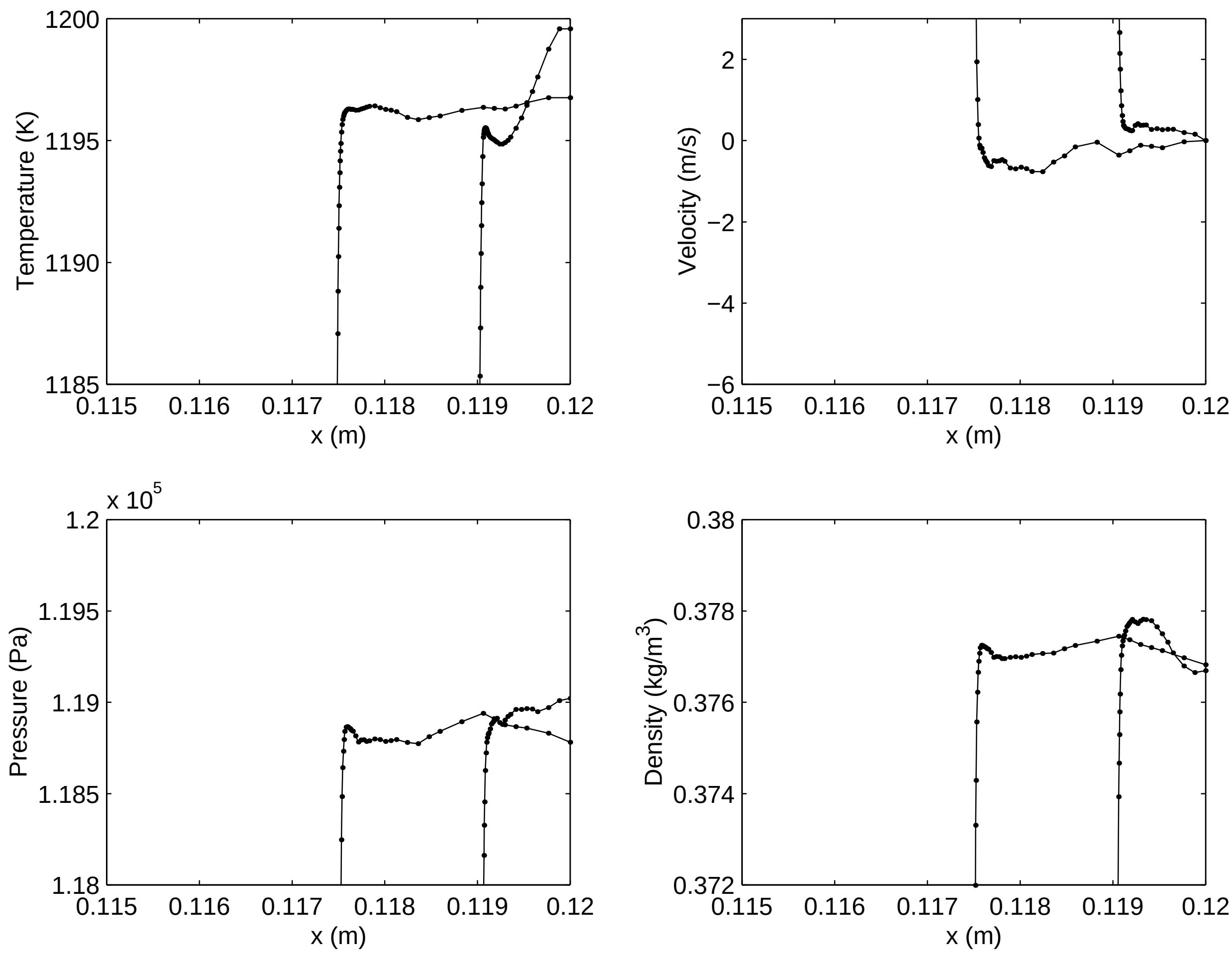
Post Reflection Entropy Layer?: Viscous Wavelet Results

- No significant entropy layer evident on macroscale after shock reflection when resolved viscous terms considered,
- Inviscid codes with coarse gridding introduce a larger entropy layer due to numerical diffusion,
- Unless suppressed, unphysically accelerates reaction rate.



Post Reflection Entropy Layer: Viscous Wavelet Results

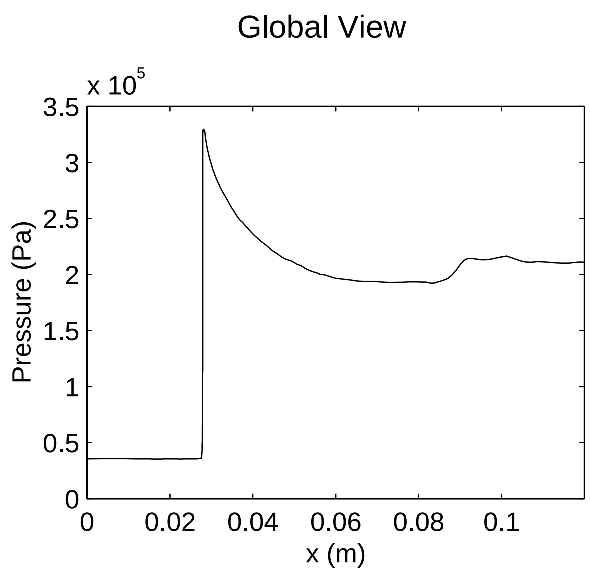
- small entropy layer evident on finer scale,
- temperature rise $\sim 5\ K$; dissipates quickly,
- inviscid calculations before adjustment give persistent temperature rise of $\sim 20\ K$

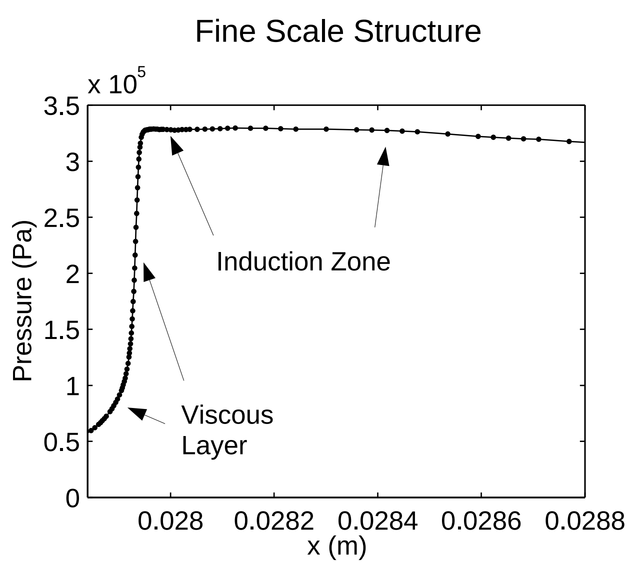


Viscous $H_2 - O_2$ Ignition Delay with Wavelets

Global and Fine Scale Structures

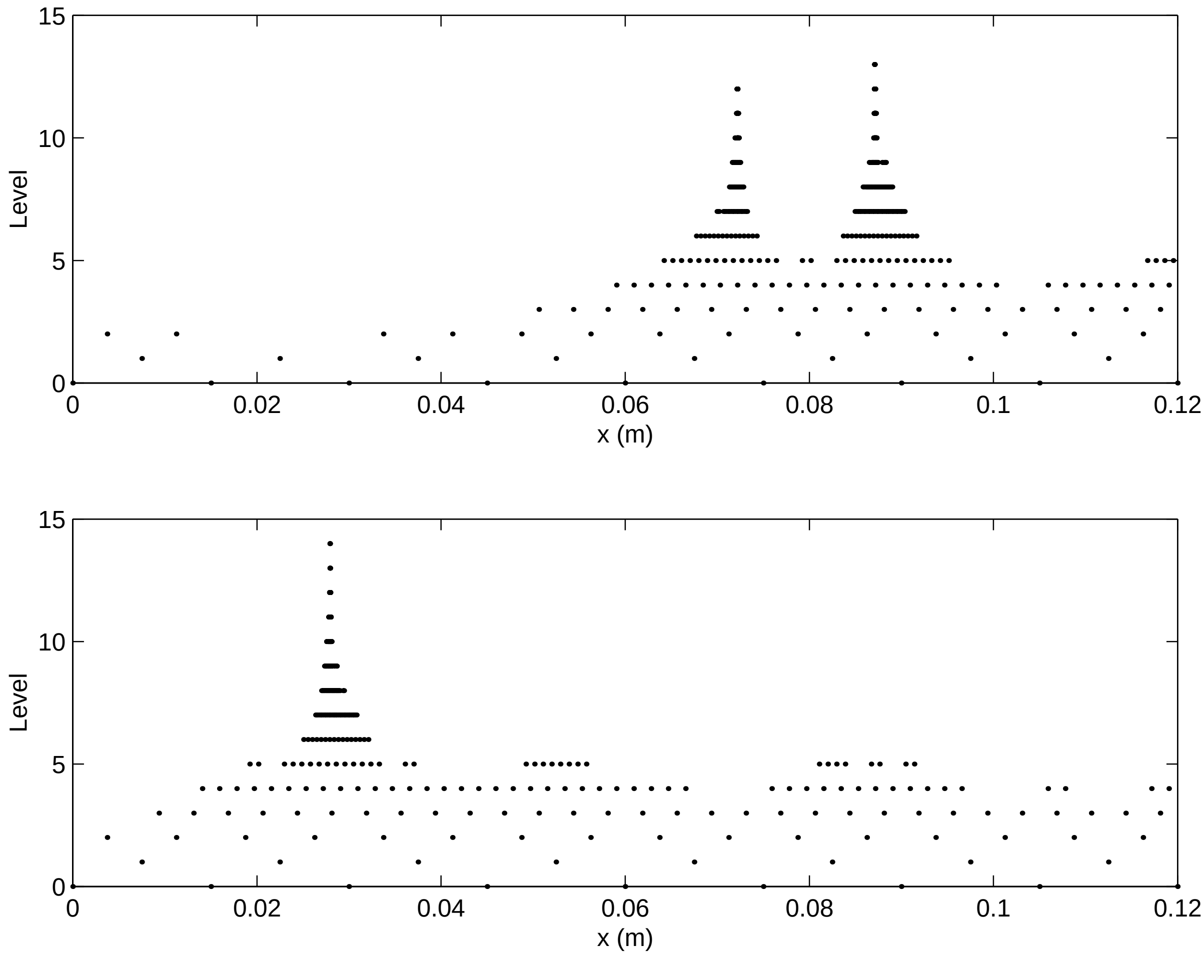
- $t = 230\ \mu s$





Viscous $H_2 - O_2$ Ignition Delay with Wavelets, Instantaneous Distributions of Collocation Points

- $t = 180\ \mu s$, two-shock structure with consequent collocation point distribution,
- $t = 230\ \mu s$, one-shock structure with evolved collocation point distribution.



Conclusions

- Adaptive multilevel wavelet collocation method gives dramatic spatial resolution in viscous one-dimensional H_2/O_2 detonations with detailed kinetics; viscous shocks, entropy layers, and induction zones are resolved,
- Preliminary results on well-stirred systems indicate at least a tenfold increase in computational efficiency with use of intrinsic low dimensional manifolds,
- Operator splitting allows straightforward implementation of ILDM method in solving PDEs, while correctly accounting for convection and diffusion.