Simulations of Viscous Detonations with Detailed Kinetics Using Manifold and Wavelet Techniques

by

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Outline

- Motivation
- Goals
- Description of ILDM technique
- Summary of wavelet technique
- Detailed results for $H_2 - O_2$ detonation
- Strategy for HMX combustion and preliminary results
- Summary

Motivation

- Detailed finite rate kinetics critical in reactive fluid mechanics:
  - Candle flames,
  - Atmospheric chemistry,
  - Internal combustion engines,
  - Gas phase reactions in energetic solid combustion.
- Common detailed kinetic models are computationally expensive.
  - 150 *hr* supercomputer time for calculation of steady, laminar, axisymmetric, methane-air diffusion flame (Smooke)
  - 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^{-14} s to 10^{2} s.
- Reduced kinetics necessary given current computational resources.
- Adaptive discretization necessary for fine spatial structures.
- Inclusion of *physical* diffusion necessary for *numerical* convergence.

Why Diffusion?

- Diffusion traditionally not modelled in detonation studies,
- Argued that very thin shock structures, thickness = $O(\mu m)$, will have minimal influence on reaction events,
- However, inviscid solutions to two-dimensional reactive Euler equations in mildly unstable regimes do not appear to converge, while viscous counterparts do (Singh, Powers, Paolucci, AIAA-99-0966, 1999),
- Hypothesis: inherent numerical diffusion is selecting structures in "inviscid" calculations; these evolve unphysically with grid size,
- When physical diffusion zones are resolved numerically, grid-independent physical diffusion dominates over numerical diffusion.
- Prohibitively expensive to compute simultaneous viscous and reaction zone structures with common numerical techniques and actual physical parametric values.
- SPP modelled systems with reaction length/diffusion length ~ 10 to achieve resolved results; much larger ratios necessary to model real systems.

Goals

- Implement robust new reduced kinetic method of
  - Maas, U., and Pope, S. B., 1992, "Simplifying Chemical Kinetics: Intrinsic Low-Dimensional Manifolds in Composition Space," *Combust. Flame*, 88: 239-264.
  - Lam, S. H., 1993, "Using CSP to Understand Complex Chemical Kinetics," *Combust. Sci. Tech.*, 89: 375-404.
- Extend method to systems with time and space dependency.
- Extend method to systems in which fluid and chemical phenomena evolve over similar time scales.
- Couple method with new wavelet collocation technique (Paolucci & Vasilyev) for spatial discretization.
- Applications:
  - ignition delay in shock tubes; *detailed results*,
  - unstable viscous detonations,
  - Bunsen burner flames,
  - rocket nozzle flows,
  - HMX gas phase reactions; *preliminary manifolds.*

Common Reduced Kinetics Strategies

- Fully frozen limit: no reaction allowed, *uninteresting*
- Fully equilibrated limit: commonly used in some problems
  - has value for events in which fluid time scales are slow with respect to reaction time scales,
  - misses events which happen on chemical time scales.
- Simple one and two step models
  - require significant intuition and curve fitting,
  - can give good first order results,
  - are often not robust.
- Partial equilibrium and steady-state assumptions
  - again require intuition,
  - are not robust.
- Sensitivity analysis
  - can remove need to include unimportant reactions,
  - not guaranteed to remove stiffness.

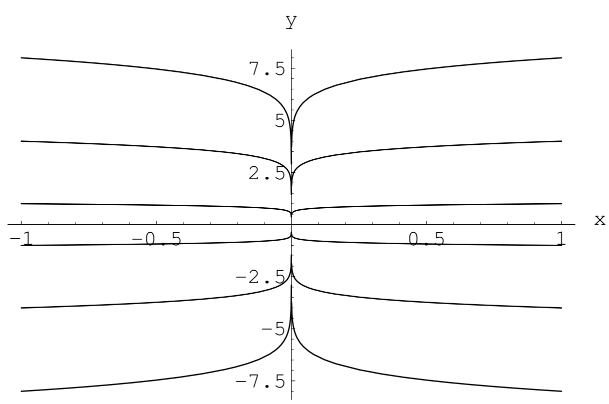
Intrinsic Low-Dimensional Manifold Method (ILDM)

- Uses a 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)

Simplest Example

$$\frac{dx}{dt} = -10x, \qquad x(0) = x_o,$$
$$\frac{dy}{dt} = -y, \qquad y(0) = y_o.$$

- Stable equilibrium at $(x, y) = (0,0)$; stiffness ratio $= 10$.
- ILDM is $x = 0$



- Parameterization of manifold: $x(s) = 0; y(s) = s$.

$$\frac{dy}{dt} = \frac{dy}{ds}\,\frac{ds}{dt}, \qquad \text{chain rule}$$
$$-y(s) = \frac{dy}{ds}\,\frac{ds}{dt}, \qquad \text{substitute from ODE and manifold}$$
$$-s = (1)\frac{ds}{dt}, \qquad \text{no longer stiff!}$$
$$s = s_o e^{-t},$$
$$x(t) = 0; \qquad y(t) = s_o e^{-t}.$$

- Projection onto manifold for s_o, induces small phase error.

Formulation of General Manifolds

- A well stirred chemically reactive system is modeled by a set of non-linear ordinary differential equations:

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

$$\mathbf{x}: \text{ species concentration}; \mathbf{x} \in \Re^n$$

- Equilibrium points defined by

$$\mathbf{x} = \mathbf{x}_{eq} \text{ such that } \mathbf{F}(\mathbf{x}_{eq}) = 0.$$

- Consider a system near equilibrium (the argument can and must be extended for systems away from equilibrium) with $\tilde{\mathbf{x}} = \mathbf{x} - \mathbf{x}_{eq}$.

- Linearization gives

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

where $\mathbf{F_x}$ is a *constant* Jacobian matrix.

- Schur decompose the Jacobian matrix:

$$\mathbf{F_x} = \mathbf{Q} \cdot \mathbf{U} \cdot \mathbf{Q}^T$$

$$\mathbf{Q} = \begin{pmatrix} \vdots & \vdots & & \vdots \\ q_1 & q_2 & \cdots & q_n \\ \vdots & \vdots & & \vdots \end{pmatrix}, \quad \mathbf{U} = \begin{pmatrix} \lambda_1 & u_{12} & \cdots & u_{1n} \\ 0 & \lambda_2 & \cdots & u_{2n} \\ 0 & \cdots & \ddots & \vdots \\ 0 & \cdots & 0 & \lambda_n \end{pmatrix}, \quad \mathbf{Q}^T = \begin{pmatrix} \cdots & q_1^T & \cdots \\ \cdots & q_2^T & \cdots \\ & \vdots & \\ \cdots & q_n^T & \cdots \end{pmatrix}$$

Formulation of General Manifolds (cont.)

- $\mathbf{Q}$ is an orthogonal matrix with real Schur vectors q_i in its columns.
- $\mathbf{U}$ is an upper triangular matrix with eigenvalues of $\mathbf{F_x}$ on its diagonal, sometimes placed in order of decreasing magnitude.
- The Schur vectors q_i form an orthonormal basis which spans the phase space, $\Re^n$.
- We then define m slow time scales, $m \leq n$.
- Next define a non-square matrix $\mathbf{W}$ which has in its rows the Schur vectors associated with the fast time scales:

$$\mathbf{W} = \begin{pmatrix} \cdots & \cdots & q_{m+1}^T & \cdots & \cdots \\ \cdots & \cdots & q_{m+2}^T & \cdots & \cdots \\ & & \vdots & & \\ \cdots & \cdots & q_n^T & \cdots & \cdots \end{pmatrix}.$$

- Letting the fast time scale events equilibrate defines the manifold:

$$\mathbf{W} \cdot \mathbf{F}(\mathbf{x}) = 0.$$

- If $m = 0$, no slow time scales, $\mathbf{W} = \mathbf{Q}^T$, and $\mathbf{W} \cdot \mathbf{F}(\mathbf{x}) = 0$ implies $\mathbf{Q}^T \cdot \mathbf{F}(\mathbf{x}) = 0$, implies $\mathbf{F}(\mathbf{x}) = 0$: the equilibrium point is the low dimensional manifold!

A Simple Example

- Consider

$$\begin{aligned}\frac{dx}{dt} &= -100x + y\sin y, \qquad x(0) = x_o,\\ \frac{dy}{dt} &= x^3 - y, \qquad y(0) = y_o.\end{aligned}$$

- Equilibrium points:

$$\mathbf{F} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} = \begin{pmatrix} -100x + y\sin y \\ x^3 - y \end{pmatrix}, \qquad \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

  Other equilibrium points exist!

- Near the equilibrium point (0,0), linearization gives

$$\begin{pmatrix} \frac{dx}{dt} \\ \frac{dy}{dt} \end{pmatrix} = \begin{pmatrix} -100 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix},$$

  which is obviously stable.

- Schur decomposition is trivial:

$$\mathbf{F_x} = \mathbf{Q} \cdot \mathbf{U} \cdot \mathbf{Q}^T$$

$$\begin{pmatrix} -100 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} -100 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

- Form the manifold:

$$\begin{aligned}\mathbf{W} &= \begin{pmatrix} 1 & 0 \end{pmatrix},\\ \mathbf{W} \cdot \mathbf{F}(\mathbf{x}) &= \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} -100x + y\sin y \\ x^3 - y \end{pmatrix} = 0,\end{aligned}$$

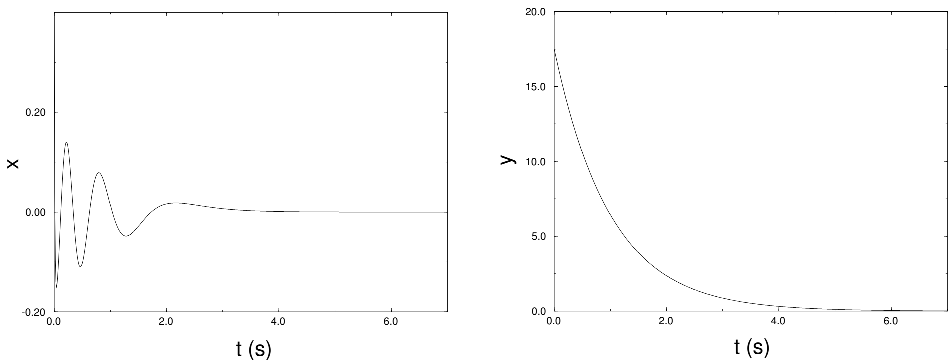
$$-100x + y\sin y = 0 \qquad \text{The ILDM!}$$

A Simple Example

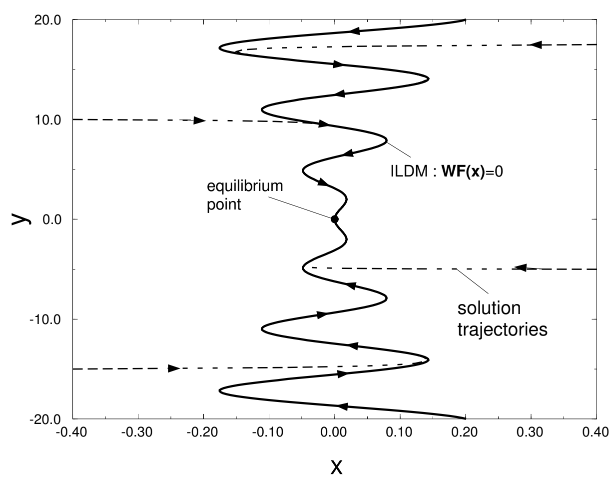
$$\frac{dx}{dt} = -100x + y\sin(y) \qquad x(0) = x_O$$

$$\frac{dy}{dt} = x^3 - y \qquad y(0) = y_O$$

Time Variation of X and Y



Phase Plot



Simple Example: Parameterization and Stiffness Reduction

$$\frac{dx}{dt} = -100x + y \sin y,$$
$$\frac{dy}{dt} = x^3 - y.$$

- Time scales near origin: $\tau_1 = 1.0$, $\tau_2 = 0.01$. Stiff.
- First approximation to manifold is $x = \frac{1}{100} y \sin y$.
- Parameterize manifold as

$$x = \frac{1}{100} s \sin s,$$
$$y = s.$$

- Chain rule gives

$$\frac{dy}{dt} = \frac{dy}{ds}\frac{ds}{dt}.$$

- Substitute from ODEs and parameterization:

$$x^3(s) - y(s) = \frac{dy(s)}{ds}\frac{ds}{dt},$$
$$\frac{1}{10^6} s^3 \sin^3 s - s = (1)\frac{ds}{dt},$$
$$\frac{ds}{dt} = \frac{1}{10^6} s^3 \sin^3 s - s$$

- Linearize near equilibrium at origin:

$$\frac{ds}{dt} = -s.$$

  Time scale: $\tau = 1.0$ No longer stiff!

- Solve ODE for $s(t)$, substitute to get $x(s(t))$, $y(s(t))$:

$$x \sim \frac{1}{100} s_o e^{-t} \sin\left(s_o e^{-t}\right), \qquad y \sim s_o e^{-t}.$$

Example: Zeldovich Mechanism of NO Formation

- Mechanism (two elements, five species, two reactions):

  1. $O + N_2 \rightarrow NO + N$, $\quad k_1 = 1.8 \times 10^{14} \frac{cm^3}{mol\ s} \exp\left(\frac{-38370\ K}{T}\right)$,
  2. $NO + N \rightarrow O + N_2$, $\quad k_2 = 3.8 \times 10^{13} \frac{cm^3}{mol\ s} \exp\left(\frac{-425\ K}{T}\right)$,
  3. $N + O_2 \rightarrow NO + O$, $\quad k_3 = 1.8 \times 10^{10} \frac{cm^3}{mol\ s\ K} T \exp\left(\frac{-4680\ K}{T}\right)$,
  4. $NO + O \rightarrow N + O_2$, $\quad k_4 = 3.8 \times 10^{9} \frac{cm^3}{mol\ s\ K} T \exp\left(\frac{-20820\ K}{T}\right)$,

- Take $T = 1400\ K$, then

  1. $k_1 = 2.252 \times 10^2 \frac{cm^3}{mol\ s}$
  2. $k_2 = 2.805 \times 10^{13} \frac{cm^3}{mol\ s}$
  3. $k_3 = 8.905 \times 10^{11} \frac{cm^3}{mol\ s}$
  4. $k_4 = 1.851 \times 10^{6} \frac{cm^3}{mol\ s}$

- Law of mass action for $[N_2]$, for example, gives

$$\frac{d[N_2]}{dt} = -k_1[N_2][O] + k_2[NO][N].$$

- For all species, law of mass action yields five non-linear ODEs:

$$\frac{d}{dt}\begin{pmatrix}[N]\\ [NO]\\ [N_2]\\ [O]\\ [O_2]\end{pmatrix} = \begin{pmatrix}1 & -1 & -1 & 1\\ 1 & -1 & 1 & -1\\ -1 & 1 & 0 & 0\\ -1 & 1 & 1 & -1\\ 0 & 0 & -1 & 1\end{pmatrix}\begin{pmatrix}k_1[N_2][O]\\ k_2[N][NO]\\ k_3[N][O_2]\\ k_4[NO][O]\end{pmatrix}$$

Example: Zeldovich Mechanism of NO Formation, cont.

- To elucidate naturally conserved variables, use elementary row operations to cast system in non-unique row echelon form:

$$\frac{d}{dt}\begin{pmatrix} [N] \\ [NO]-[N] \\ 2[N_2]+[NO]+[N] \\ [O]+[N] \\ 2[O_2]+[NO]-[N] \end{pmatrix} = \begin{pmatrix} 1 & -1 & -1 & 1 \\ 0 & 0 & 2 & -2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} k_1[N_2][O] \\ k_2[N][NO] \\ k_3[N][O_2] \\ k_4[NO][O] \end{pmatrix}$$

- We are left with
  - two ODEs
  - three algebraic constraints: conservation of N atoms, O atoms, and number of molecules
  - easily reduced to two ODEs in two unknowns: $[N], [NO]$.
- We will reduce the two ODEs to one ODE by imposing the manifold equation $\mathbf{W} \cdot \mathbf{F}(\mathbf{x}) = 0$, effectively equilibrating the fast time scale.

Example: Zeldovich Mechanism of NO Formation, cont.

- Consider first the intrinsic algebraic constraints:

$$\frac{d}{dt}\begin{pmatrix} 2[N_2]+[NO]+[N] \\ [O]+[N] \\ 2[O_2]+[NO]-[N] \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}.$$

- Integrate these equations:

$$\begin{aligned} 2[N_2]+[NO]+[N] &= C_1, \\ [O]+[N] &= C_2, \\ 2[O_2]+[NO]-[N] &= C_3. \end{aligned}$$

The constants C_1, C_2, C_3 come from initial conditions.

- Solve equations for secondary variables in terms of $[N], [NO]$:

$$\begin{aligned} [N_2] &= \frac{1}{2}\left(C_1 - [NO] - [N]\right) \\ [O] &= C_2 - [N] \\ [O_2] &= \frac{1}{2}\left(C_3 - [NO] + [N]\right) \end{aligned}$$

- Note that rearrangement of the algebraic constraints demonstrates element and molecule conservation:

$$\begin{aligned} 2[N_2]+[N]+[NO] &= C_1, \\ 2[O_2]+[NO]+[O] &= C_2 + C_3, \\ [N]+[NO]+[N_2]+[O]+[O_2] &= \frac{C_1+C_3}{2} + C_2. \end{aligned}$$

Example: Zeldovich Mechanism of NO Formation, cont.

- Substitution of algebraic constraints into ODEs for $[N]$ and $[NO]$ gives two autonomous ODEs well-suited for dynamic systems analysis:

$$\begin{aligned}
\frac{d[N]}{dt} &= \frac{k_1}{2}\left(C_2 - [N]\right)\left(C_1 - [N] - [NO]\right) \\
&\quad -k_2[N][NO] \\
&\quad -\frac{k_3}{2}[N]\left(C_3 + [N] - [NO]\right) \\
&\quad +k_4[NO]\left(C_2 - [N]\right) \\
\frac{d[NO]}{dt} &= \frac{k_1}{2}\left(C_2 - [N]\right)\left(C_1 - [N] - [NO]\right) \\
&\quad -k_2[N][NO] \\
&\quad +\frac{k_3}{2}[N]\left(C_3 + [N] - [NO]\right) \\
&\quad -k_4[NO]\left(C_2 - [N]\right)
\end{aligned}$$

- Take as initial conditions

$$[N] = [NO] = [N_2] = [O] = [O_2] = 0.001\ \frac{mole}{cm^3}.$$

- Equilibrium when right hand side zero
- Three roots-one physical, two unphysical:

$$\begin{pmatrix} [N] \\ [NO] \end{pmatrix} = \begin{pmatrix} 1.16 \times 10^{-11}\ \frac{mole}{cm^3} \\ 2.78 \times 10^{-6}\ \frac{mole}{cm^3} \end{pmatrix}, \begin{pmatrix} -1.15 \times 10^{-11}\ \frac{mole}{cm^3} \\ -2.78 \times 10^{-6}\ \frac{mole}{cm^3} \end{pmatrix}, \begin{pmatrix} -2.00 \times 10^{-3}\ \frac{mole}{cm^3} \\ 0.00 \times 10^{0}\ \frac{mole}{cm^3} \end{pmatrix},$$

Example: Zeldovich Mechanism of NO Formation, cont.

- Linearization of equations near physical equilibrium gives

$$\frac{d}{dt}\begin{pmatrix}[N]-1.16\times10^{-11}\\ [NO]-2.78\times10^{-6}\end{pmatrix} = \underbrace{\begin{pmatrix}-9.67\times10^{8} & 3.38\times10^{3}\\ 8.11\times10^{8} & -4.03\times10^{3}\end{pmatrix}}_{\mathbf{F_x}}\begin{pmatrix}[N]-1.16\times10^{-11}\\ [NO]-2.78\times10^{-6}\end{pmatrix}$$

$$\frac{d}{dt}\begin{pmatrix}[N]-1.16\times10^{-11}\\ [NO]-2.78\times10^{-6}\end{pmatrix} = \underbrace{\begin{pmatrix}-0.766 & -0.643\\ 0.643 & -0.766\end{pmatrix}}_{\mathbf{Q}}\underbrace{\begin{pmatrix}-9.67\times10^{8} & 3.38\times10^{3}\\ 0 & -1.19\times10^{3}\end{pmatrix}}_{\mathbf{U}}\underbrace{\begin{pmatrix}-0.766 & 0.643\\ -0.643 & -0.766\end{pmatrix}}_{\mathbf{Q}^T}\begin{pmatrix}[N]-1.16\times10^{-11}\\ [NO]-2.78\times10^{-6}\end{pmatrix}$$

- Condition number (stiffness ratio) $= \left|\frac{-9.67\times10^{8}}{-1.19\times10^{3}}\right| = 8.1\times10^{5}$.

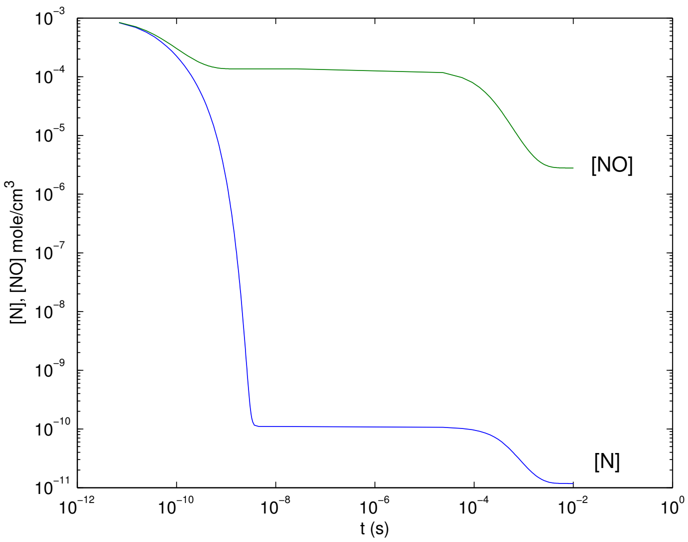
- Locally the ILDM is defined by

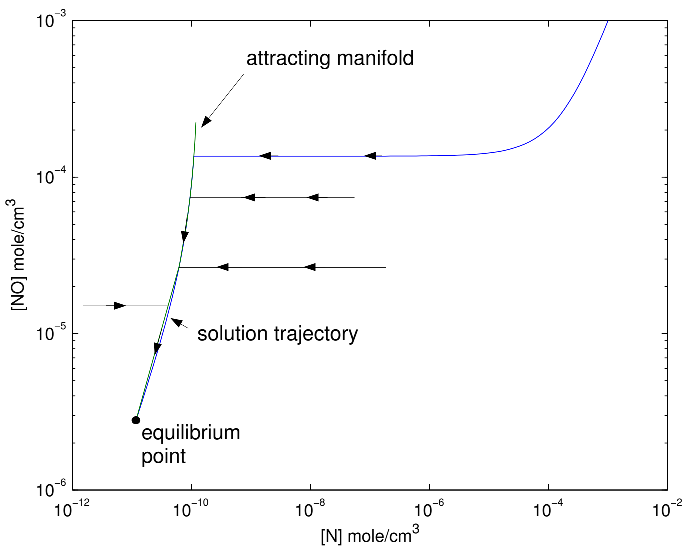
$$\begin{aligned}\mathbf{W}\cdot\mathbf{F}(\mathbf{x}) &= 0,\\ \begin{pmatrix}-0.766 & 0.643\end{pmatrix}\begin{pmatrix}F_1([N],[NO])\\ F_2([N],[NO])\end{pmatrix} &= 0.\end{aligned}$$

- Use arc length continuation methods to define complete ILDM

- The physical equilibrium has negative eigenvalues: stable.

- The non-physical equilibria have positive eigenvalues: unstable.


[NO]
[N]
[N], [NO] mole/cm3
t (s)
10−3
10−4
10−5
10−6
10−7
10−8
10−9
10−10
10−11
10−12
10−10
10−8
10−6
10−4
10−2
100


attracting manifold
solution trajectory
equilibrium point
[NO] mole/cm3
[N] mole/cm3
10−3
10−4
10−5
10−6
10−12
10−10
10−8
10−6
10−4
10−2

Adaptive Multilevel Wavelet Collocation Technique

- Summary of standard spatial discretization techniques
  - Finite difference-good spatial localization, poor spectral localization, and slow convergence,
  - Finite element- good spatial localization, poor spectral localization, and slow convergence,
  - Spectral–good spectral localization, poor spatial localization, but fast convergence.
- Wavelet 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,
  - Good spatial localization, good spectral localization, and fast convergence,
  - Easily formulated to adapt spatially to capture steep gradients via adding collocation points,
  - Spatial adaptation is automatically and dynamically adaptive to achieve prescribed error tolerance.

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,
  - No diffusion (one case); mass, momentum, and energy diffusion (another case),
  - 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

Operator Splitting Technique

- Equations are of form

$$\frac{\partial}{\partial t}\mathbf{q}(x,t) + \frac{\partial}{\partial x}\mathbf{f}(\mathbf{q}(x,t)) = \mathbf{g}(\mathbf{q}(x,t)).$$

  where

$$\mathbf{q} = \left(\rho, \rho u, \rho\left(e + \frac{u^2}{2}\right), \rho Y_i\right)^T$$

- $\mathbf{f}$ models convection and diffusion
- $\mathbf{g}$ models reaction source terms
- Splitting

  1. Inert convection diffusion step:

$$\frac{\partial}{\partial t}\mathbf{q}(x,t) + \frac{\partial}{\partial x}\mathbf{f}(\mathbf{q}(x,t)) = 0,$$
$$\frac{d}{dt}\mathbf{q}_i(t) = -\Delta_x \mathbf{f}(\mathbf{q}_i(t)).$$

     Δ_x is either Godunov *or* wavelet discretization operator.

  2. Reaction source term step:

$$\frac{\partial}{\partial t}\mathbf{q}(x,t) = \mathbf{g}(\mathbf{q}(x,t)),$$
$$\frac{d}{dt}\mathbf{q}_i(t) = \mathbf{g}(\mathbf{q}_i(t)).$$

- Operator splitting with implicit stiff source solution can induce non-physical wave speeds! (LeVeque and Yee, *JCP* 1990)

ILDM Implementation in Operator Splitting

- Form of equations in source term step:

$$\frac{d}{dt}\begin{pmatrix} \rho \\ \rho u \\ \rho\left(e+\frac{u^2}{2}\right) \\ \rho Y_i \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \omega \end{pmatrix}.$$

- Equations reduce to

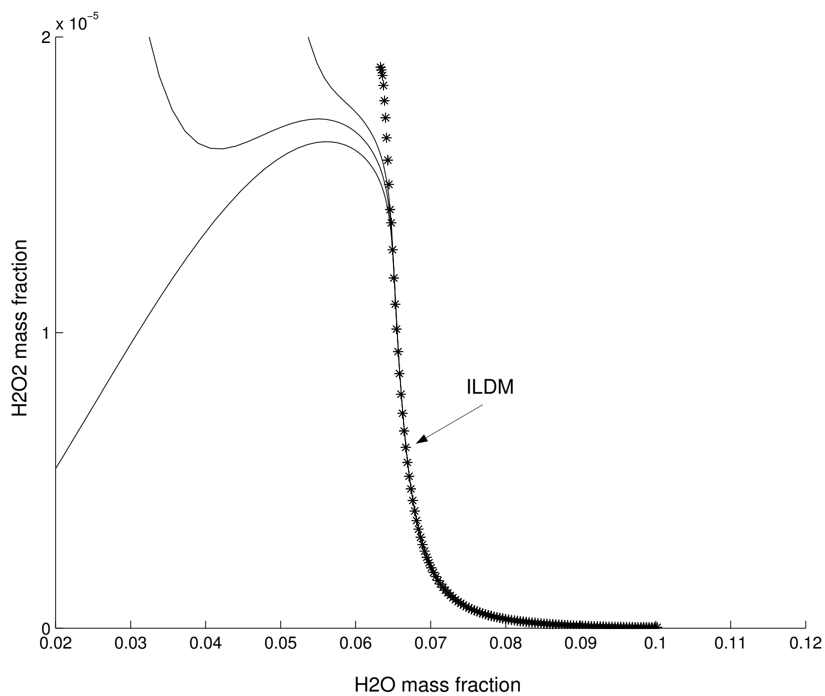
$$\rho = \rho_o, \qquad u = u_o, \qquad e = e_o,$$

$$\frac{dY_i}{dt} = \frac{\omega}{\rho_o}.$$

- ω has dependency on ρ, e, and Y_i
- ODEs for Y_i can be attacked with manifold methods when manifold with ρ, e, H and O parameterization is available.
- In premixed problem, H and O element concentrations are remarkably constant, reducing the dimension by two!
- Full equations integrated until sufficiently close to manifold
- Once on manifold, simple projection used to return to manifold following convection-diffusion step

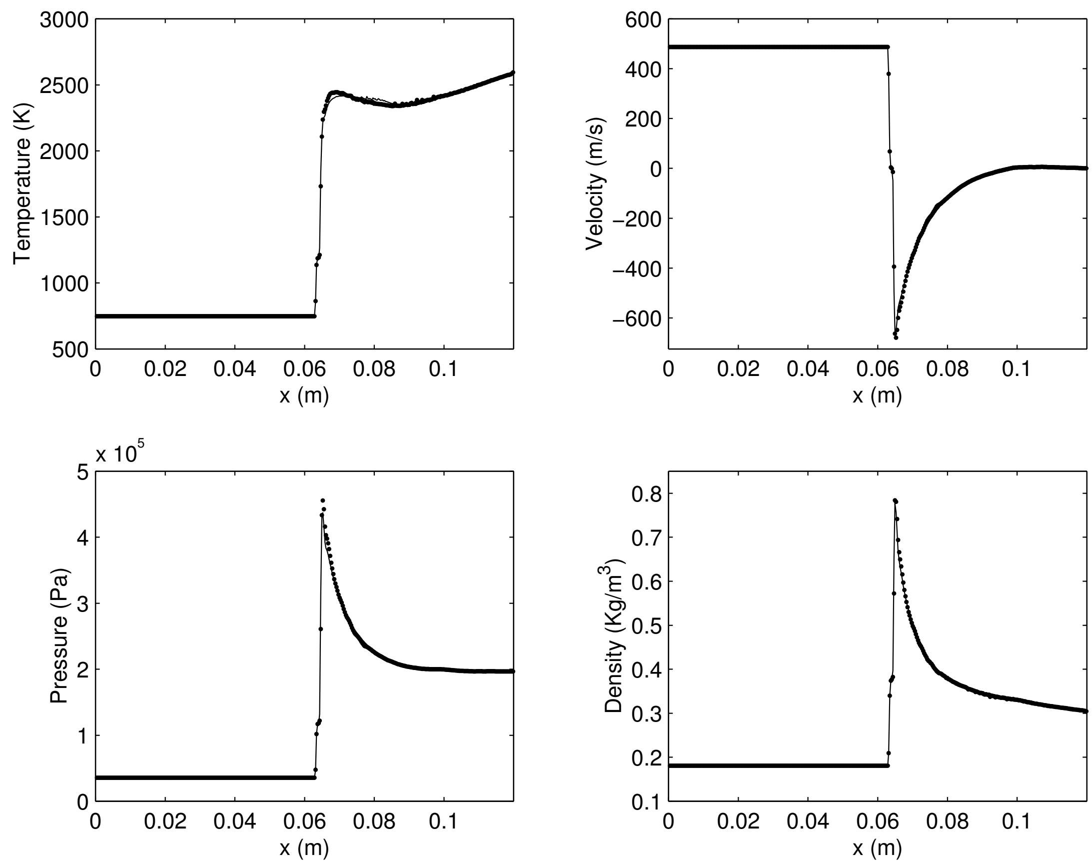
Sample ILDM for $H_2 - O_2$

- Projection of ILDM in H_2O, H_2O_2 plane,
- Adiabatic ($e = 525\, kJ/kg$), isochoric ($\rho = 0.25\, kg/m^3$), element concentrations of H and O constant,
- Complete manifold tabulated in three dimensions: ρ, e, Y_{H_2O},
- So we have e.g. $P\left(\rho, e, Y_{H_2O}\right), T\left(\rho, e, Y_{H_2O}\right), Y_H\left(\rho, e, Y_{H_2O}\right), \ldots$
- Linear interpolation used for points not in table,
- Captures $\sim 0.1\ \mu s$ reaction events.

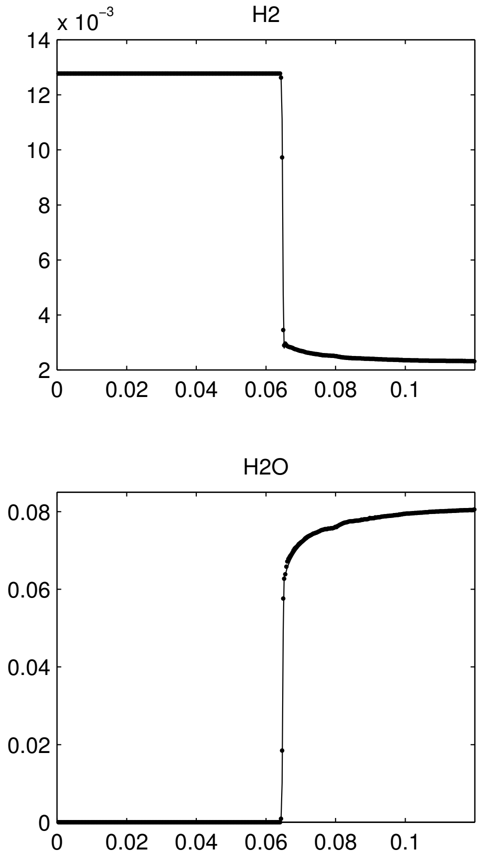


Inviscid $H_2 - O_2$ Ignition Delay with and without ILDM

- No diffusion,
- Godunov spatial discretization, 400 uniform finite difference cells,
- Implicit (trapezoidal) convection step; Implicit (dlsode) *or* ILDM reaction step,
- Correction of Fedkiw adopted to suppress artificial entropy layer after shock reflection (see Menikoff, 1994).

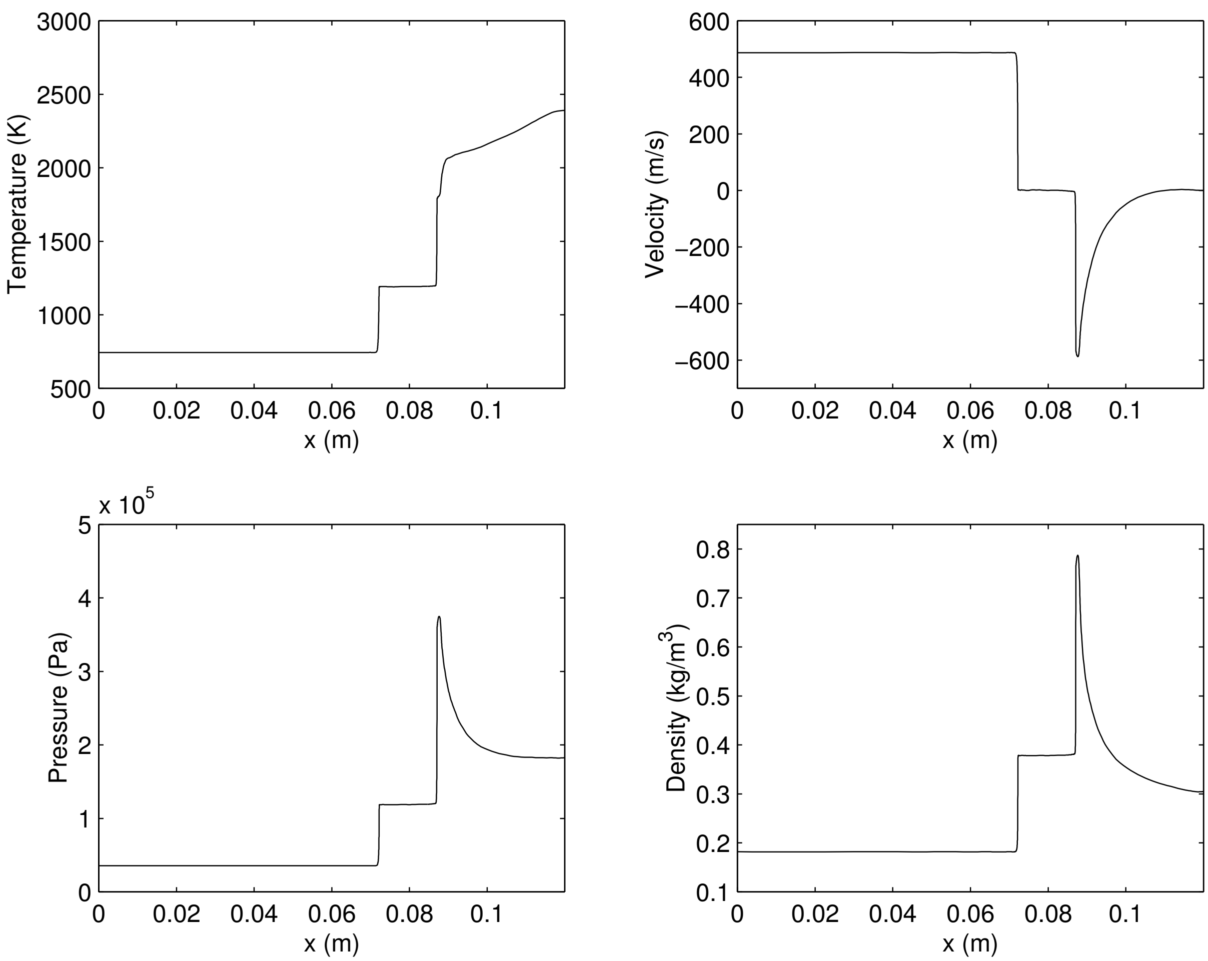


Inviscid $H_2 - O_2$ Ignition Delay with and without ILDM



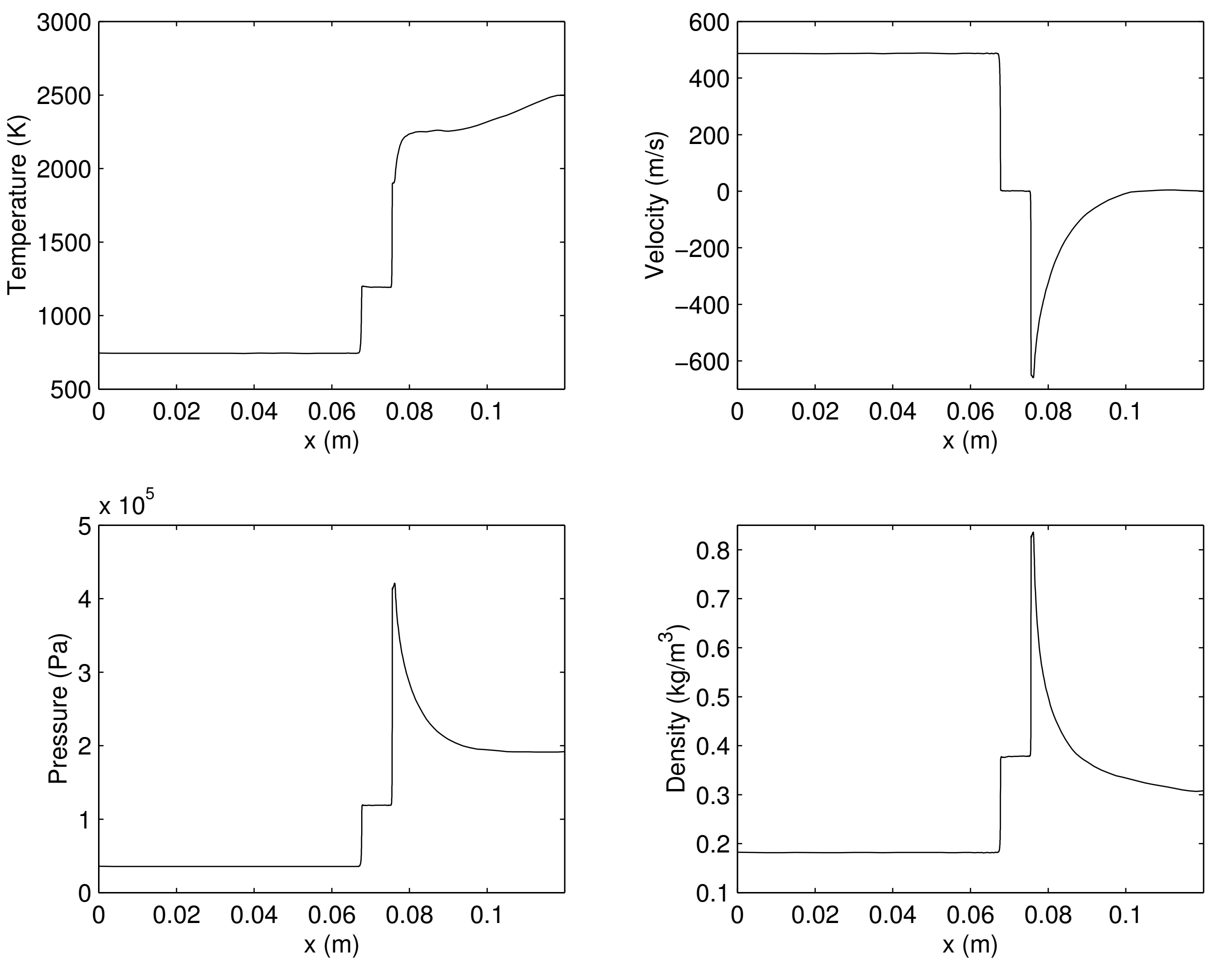
Viscous $H_2 - O_2$ Ignition Delay with Wavelets

- Mass, momentum, and energy diffusion modelled,
- Wavelet spatial discretization, explicit convection-diffusion time stepping, implicit reaction time stepping,
- 300 collocation points, 15 wavelet levels,
- *Viscous shocks, induction zones, and entropy layers spatially resolved!*
- $t = 180\ \mu s$.



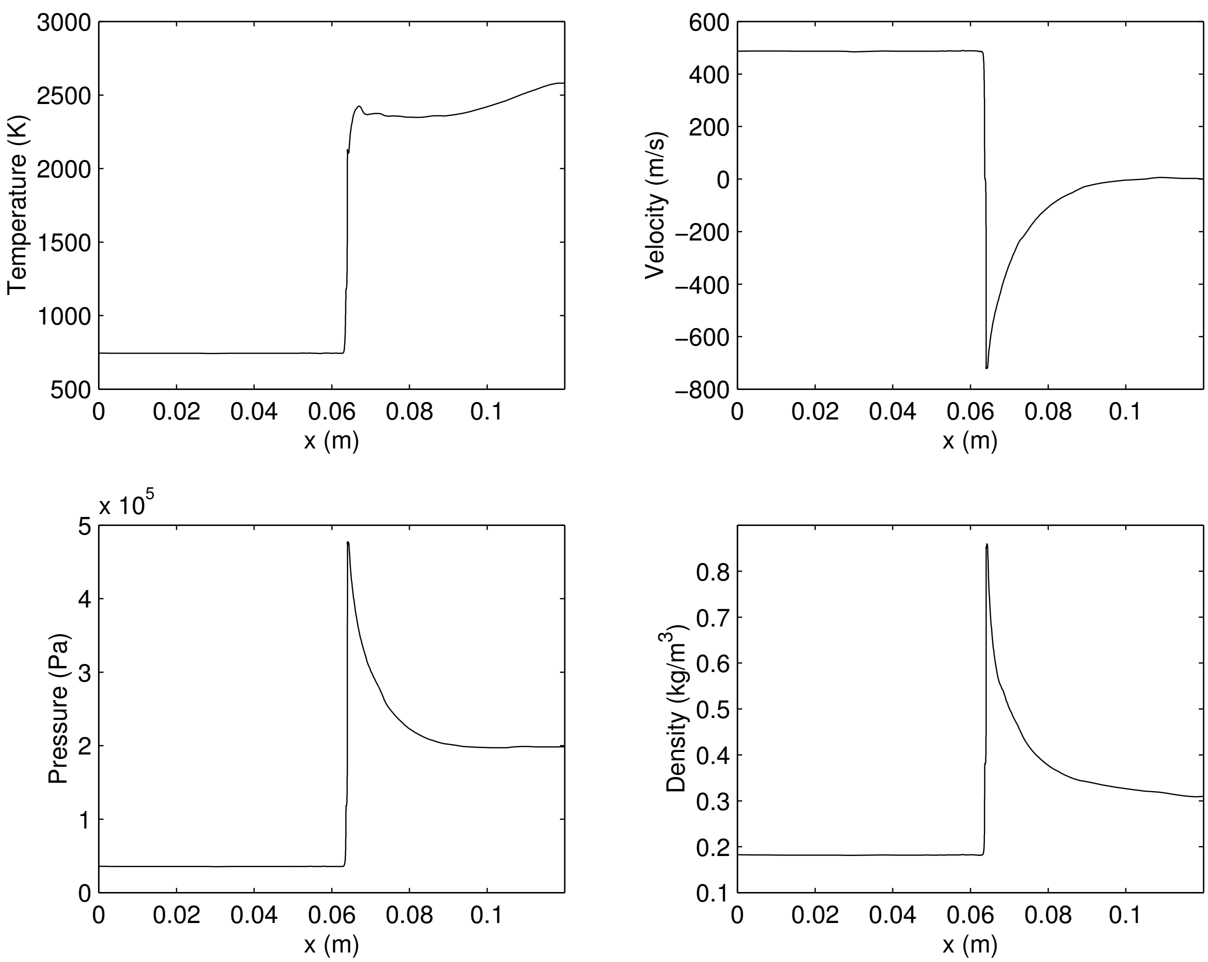
Viscous $H_2 - O_2$ Ignition Delay with Wavelets

- $t = 190\ \mu s$



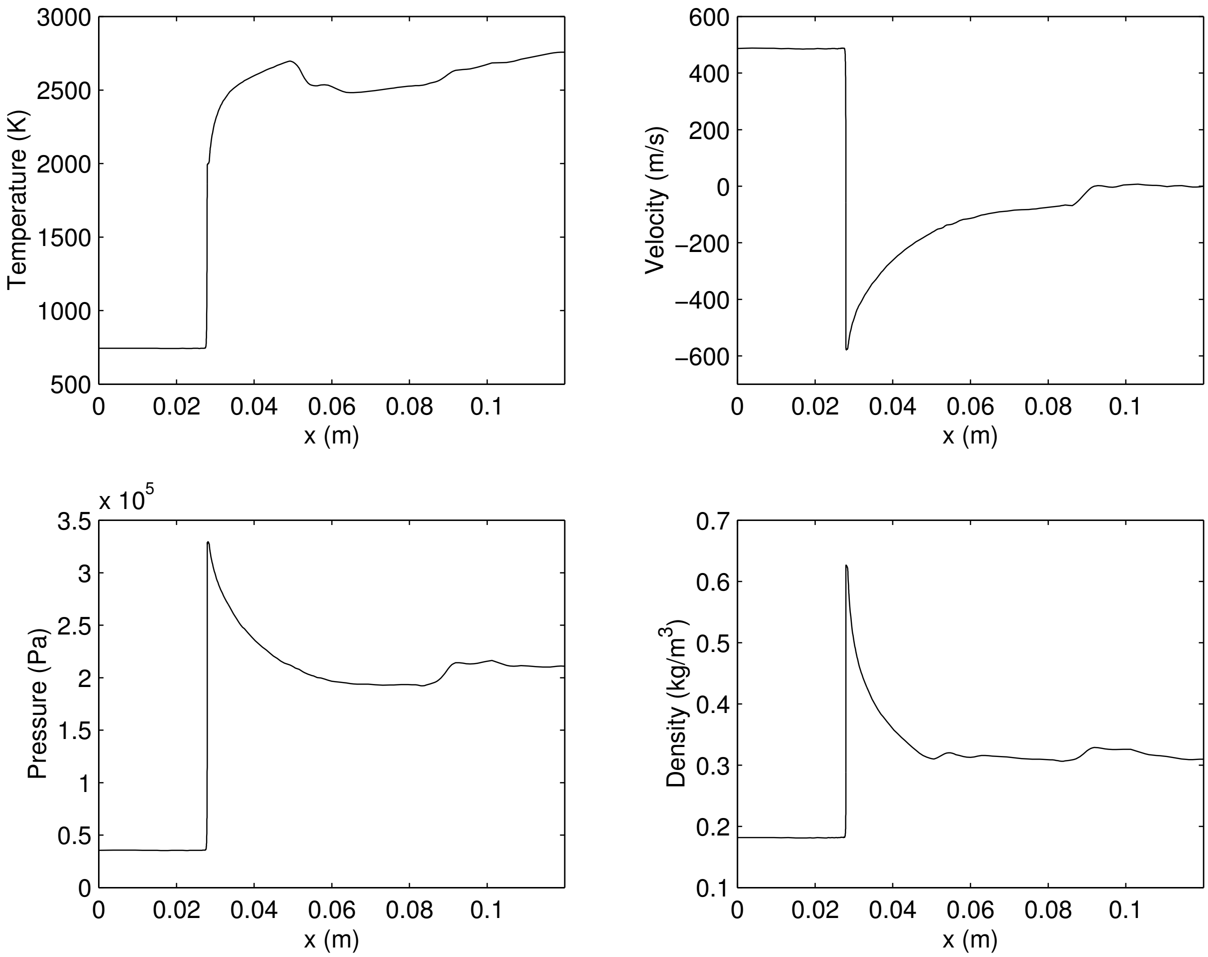
Viscous $H_2 - O_2$ Ignition Delay with Wavelets

- $t = 200\ \mu s$



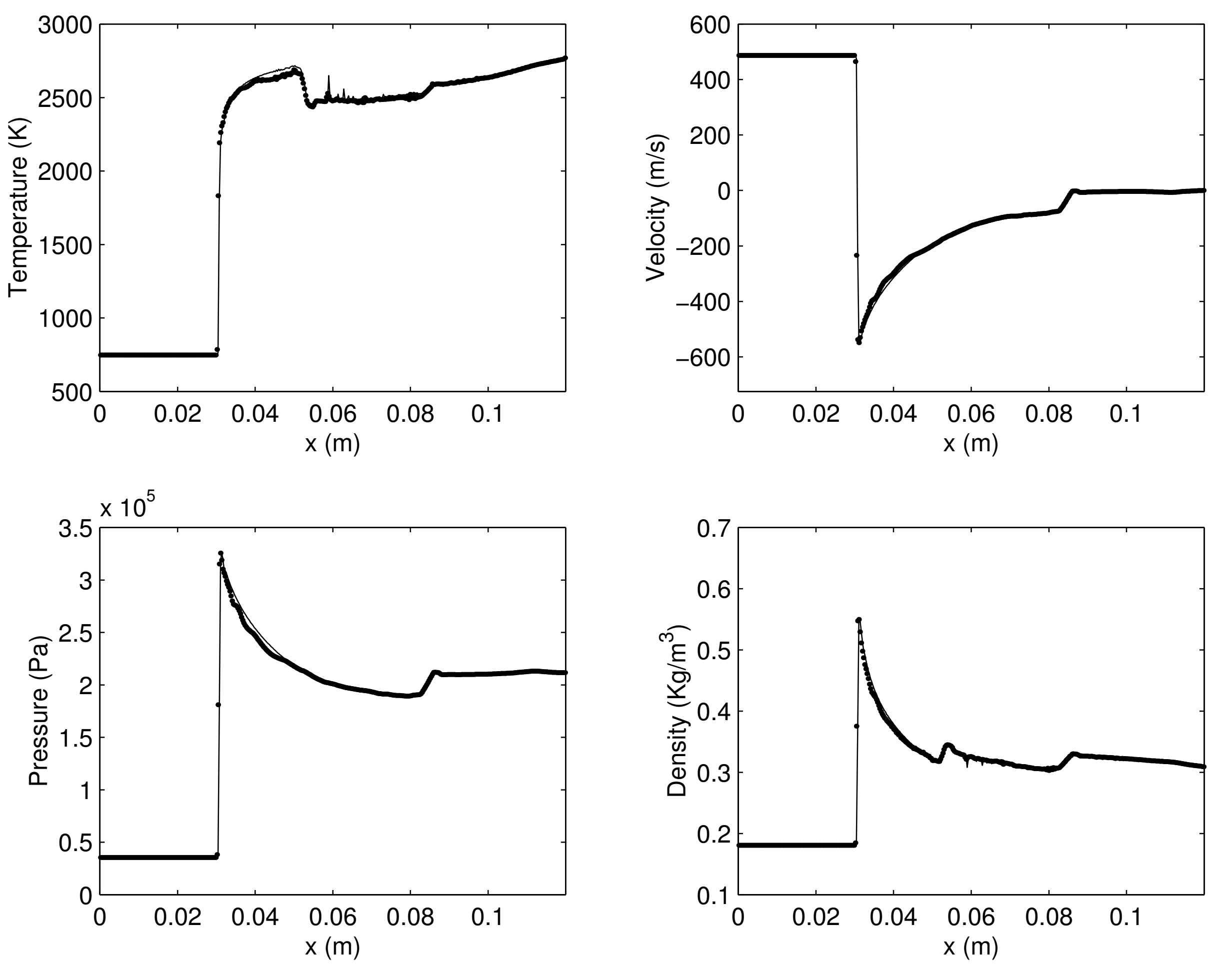
Viscous $H_2 - O_2$ Ignition Delay with Wavelets

- $t = 230\ \mu s$



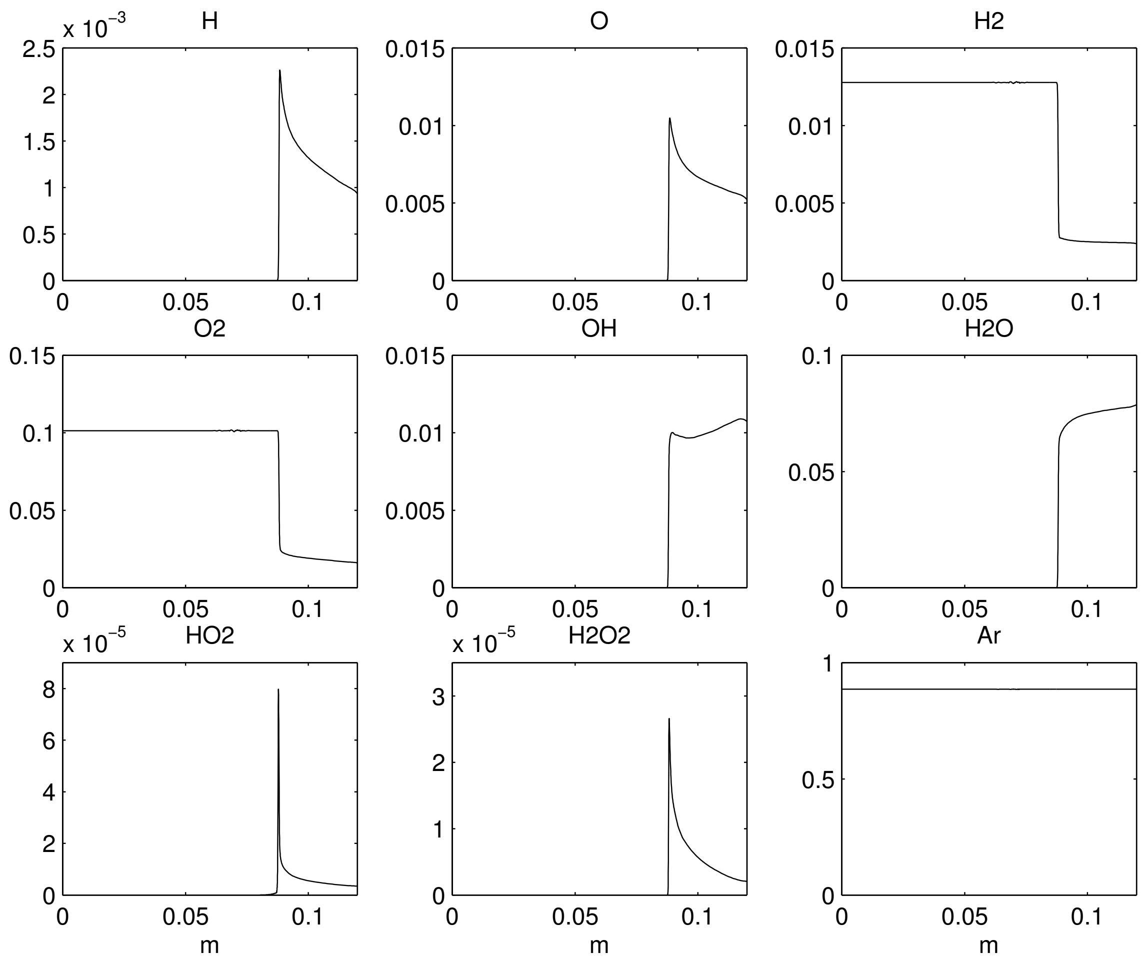
Comparison with Inviscid/ILDM Result at Same Time

- $t = 230\ \mu s$



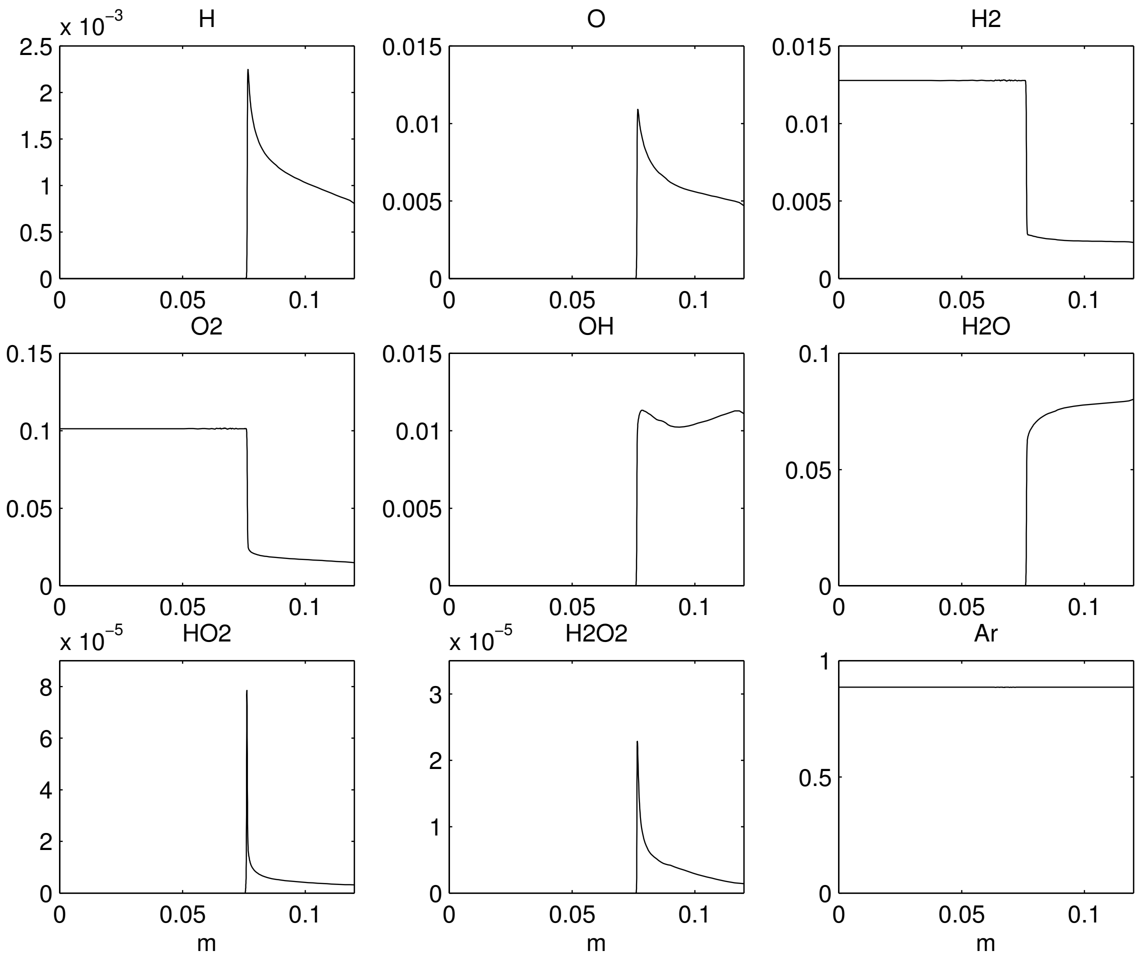
Viscous $H_2 - O_2$ Ignition Delay with Wavelets

- $t = 180\ \mu s$
- species mass fractions plotted vs. distance



Viscous $H_2 - O_2$ Ignition Delay with Wavelets

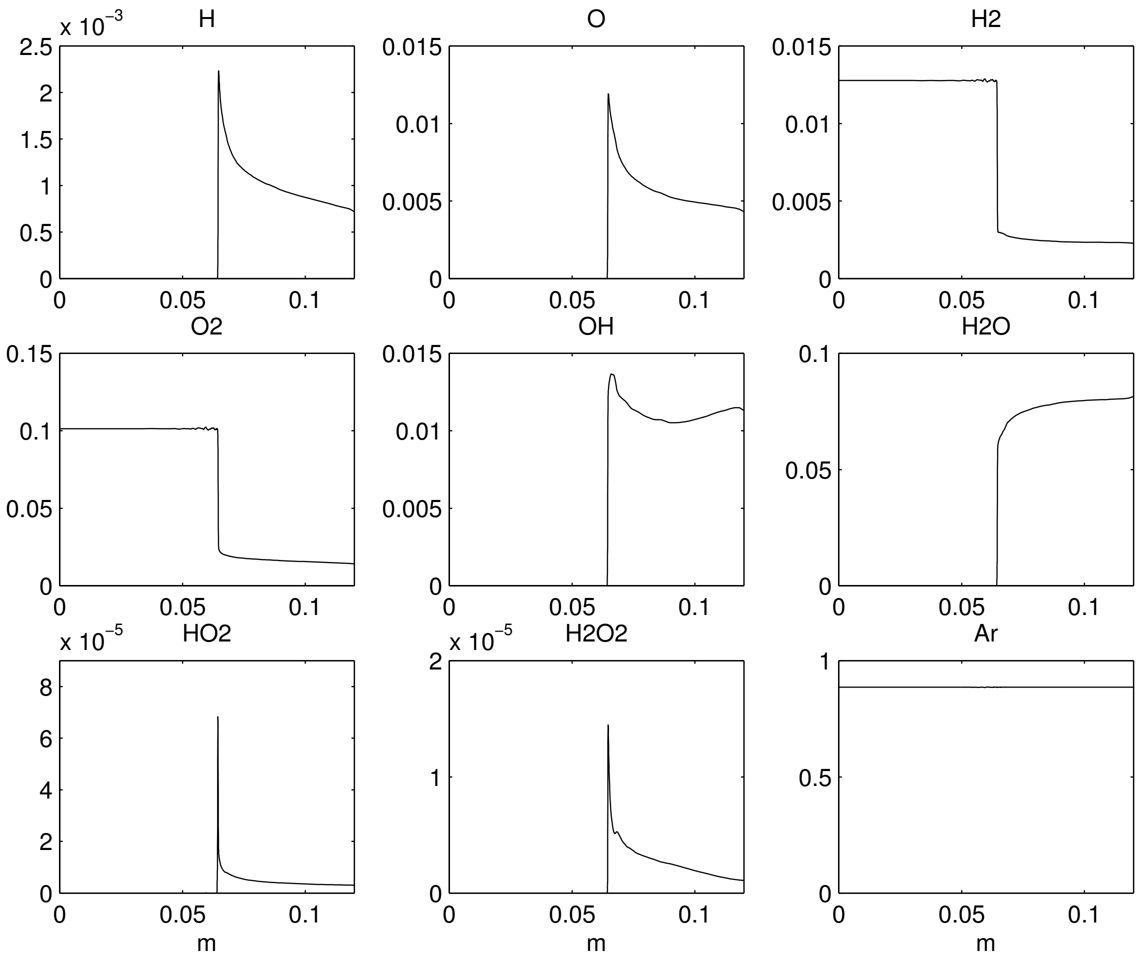
- $t = 190\ \mu s$
- species mass fractions plotted vs. distance



Viscous $H_2 - O_2$ Ignition Delay with Wavelets

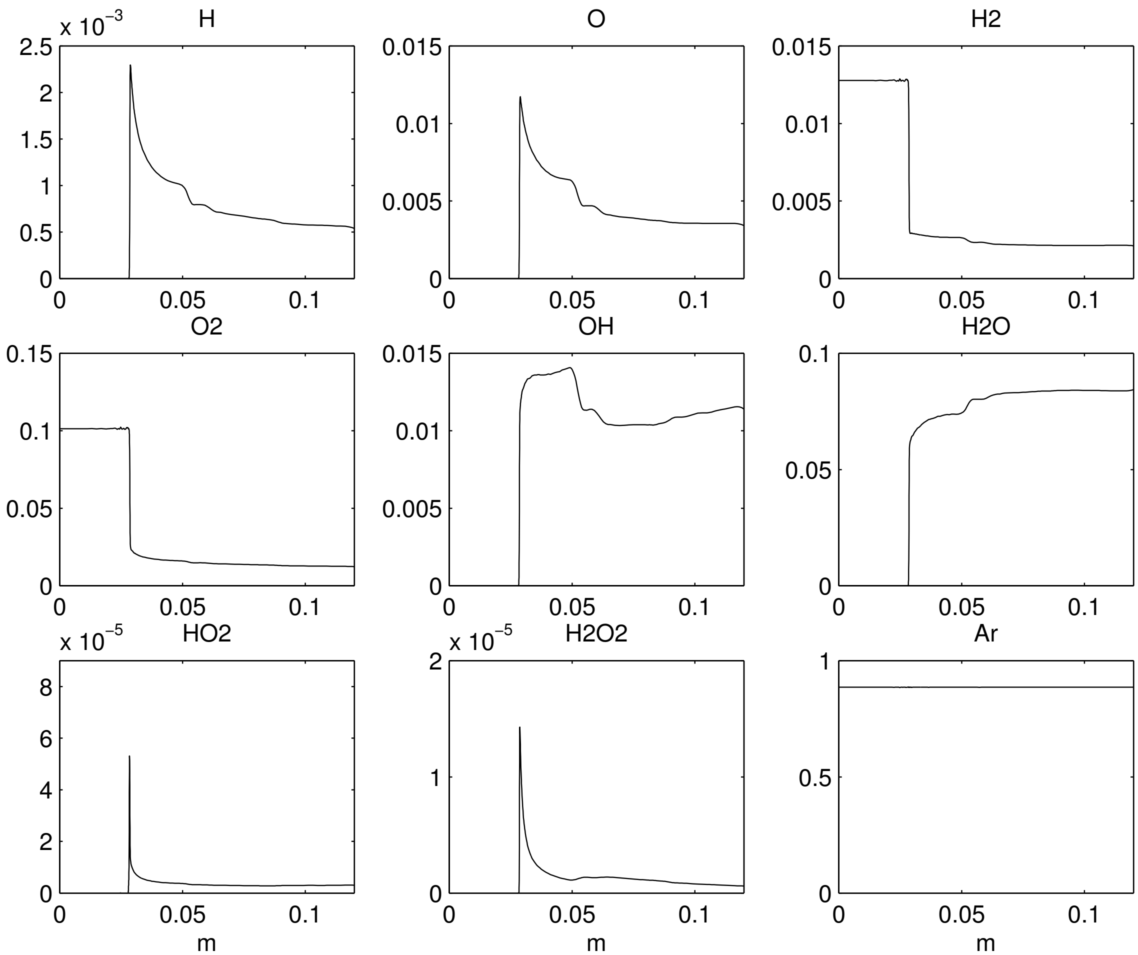
- $t = 200\ \mu s$

- species mass fractions plotted vs. distance



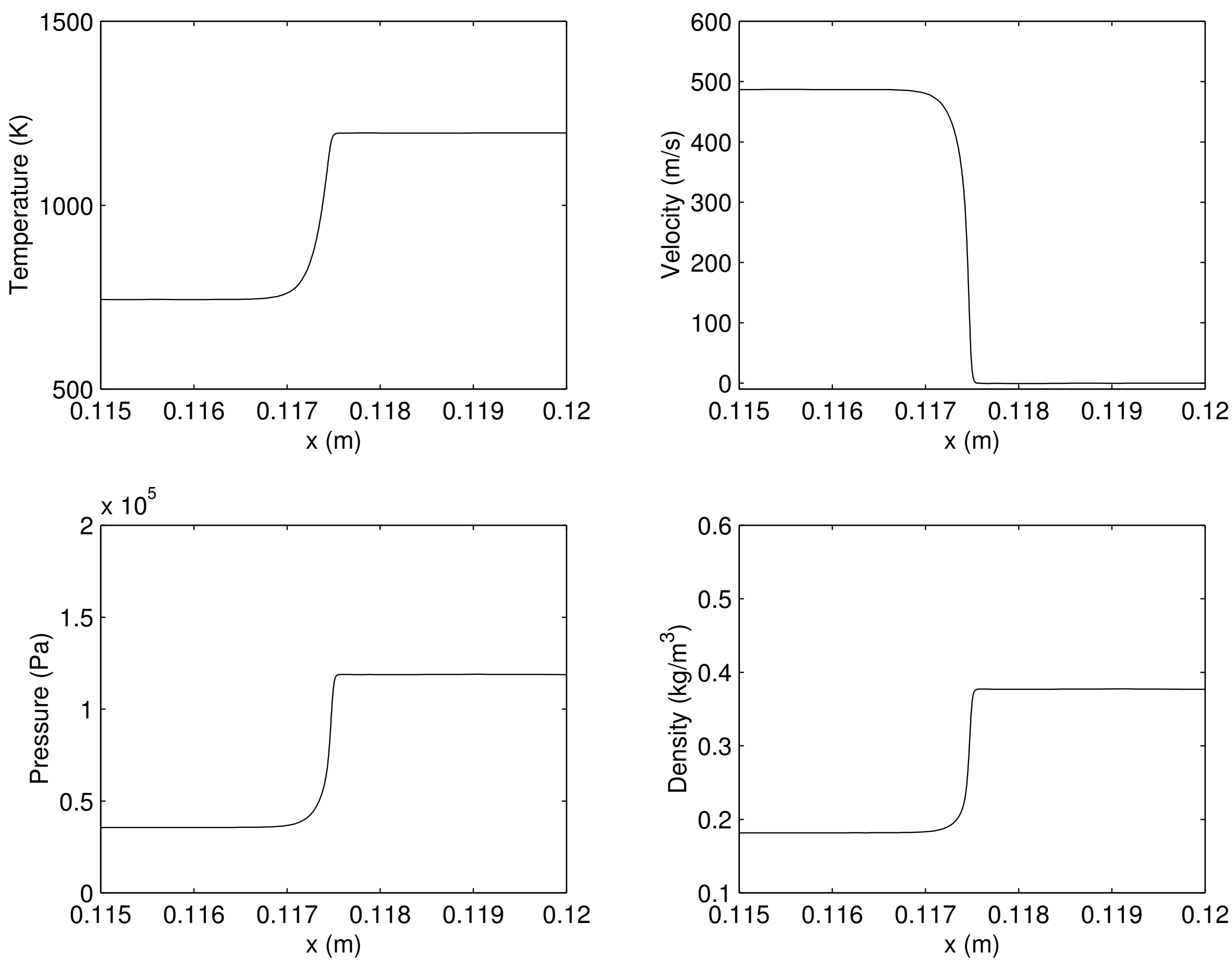
Viscous $H_2 - O_2$ Ignition Delay with Wavelets

- $t = 230\ \mu s$
- species mass fractions plotted vs. distance



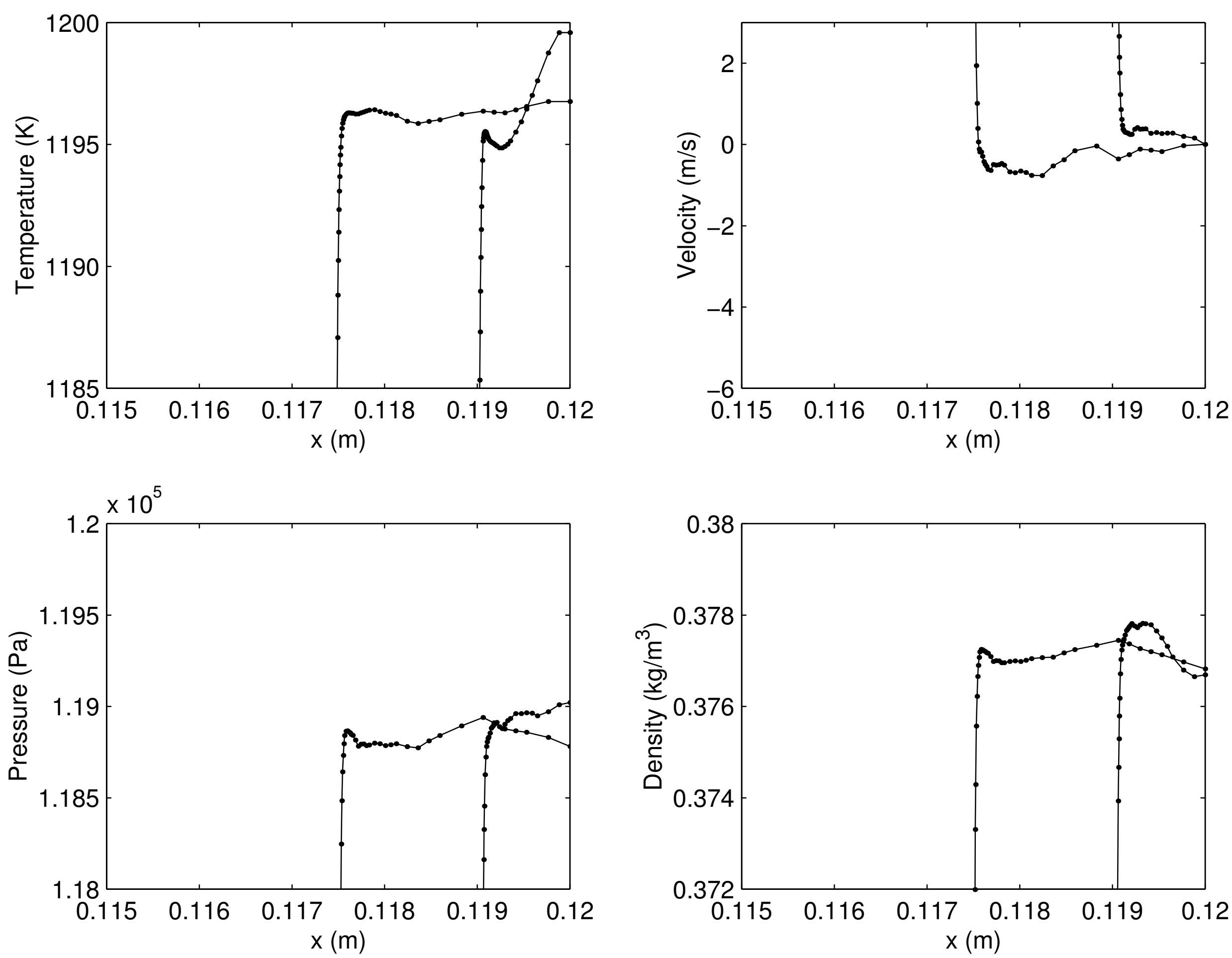
Post Reflection Entropy Layer?: Viscous Wavelet Results

- 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

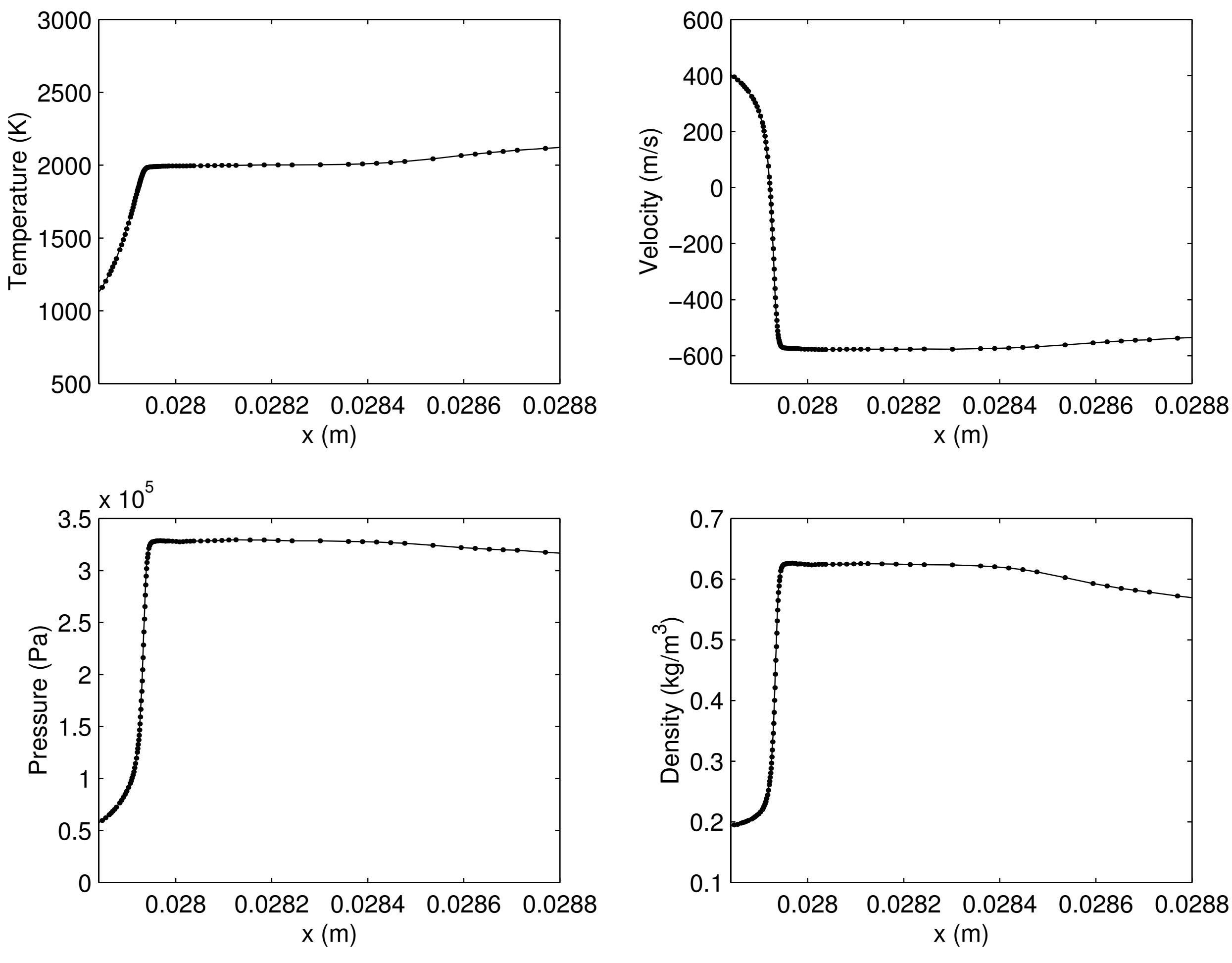
- small entropy layer evident on finer scale,
- temperature rise $\sim 5\ K$; dissipates quickly,
- inviscid calculations before adjustment give persistent temperature rise of $\sim 20\ K$; reaction acceleration small.



Viscous $H_2 - O_2$ Ignition Delay with Wavelets

Close-up: Viscous Shock Stucture and Induction Zone

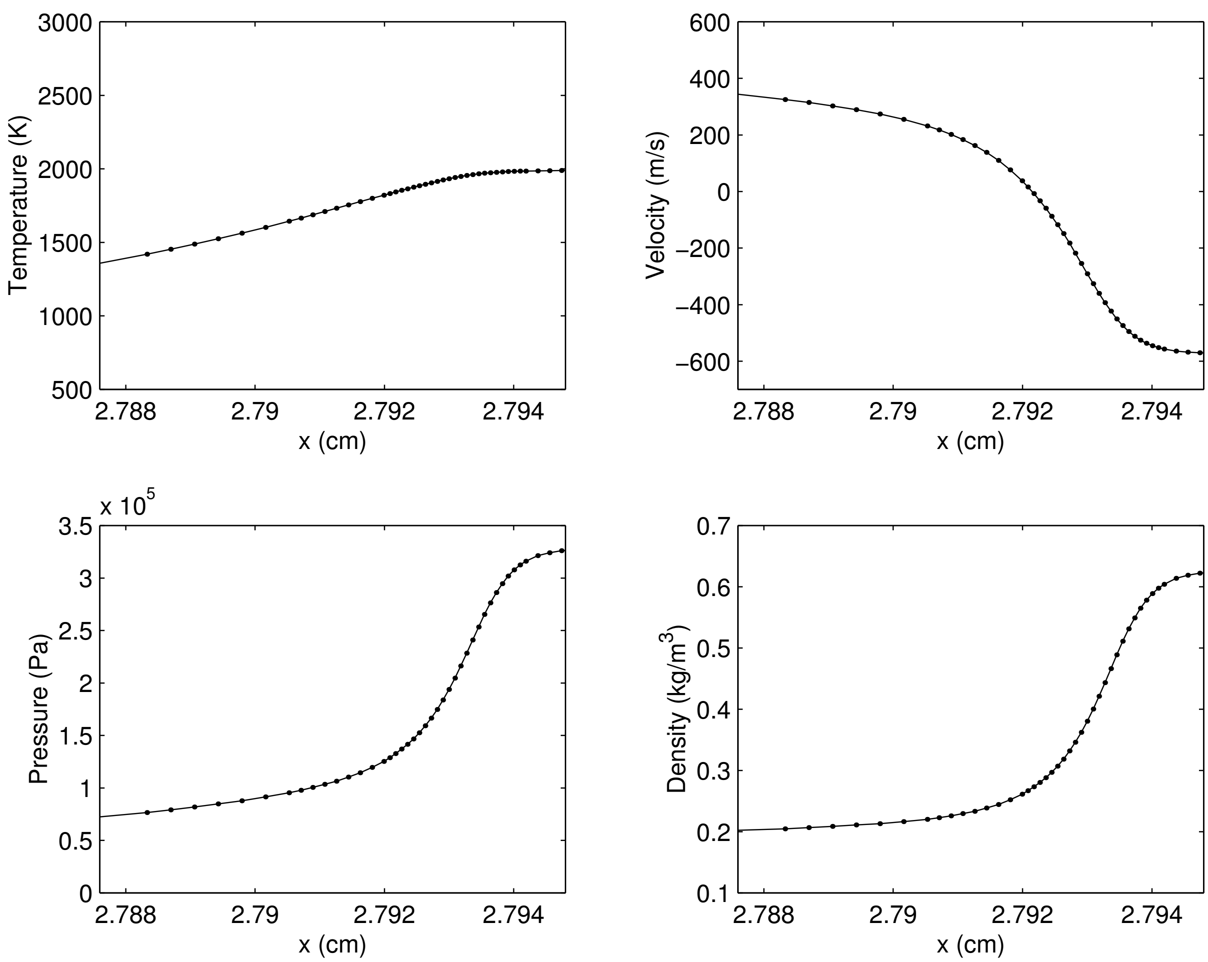
- $t = 230\ \mu s$,
- Induction zone length: $\sim 470\ \mu m$,
- No significant reaction in viscous shock zone.



Viscous $H_2 - O_2$ Ignition Delay with Wavelets

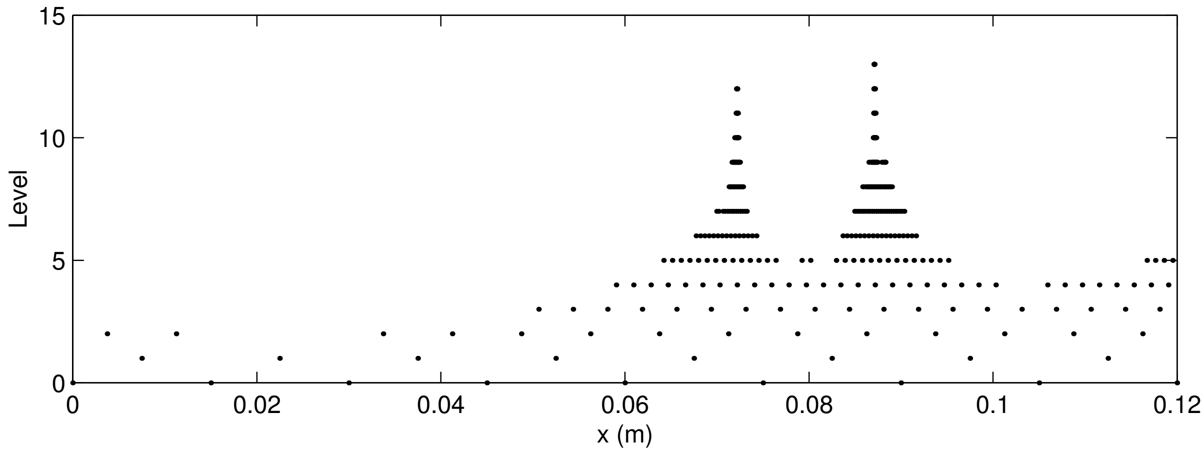
Closer-up: Viscous Shock Stucture Only

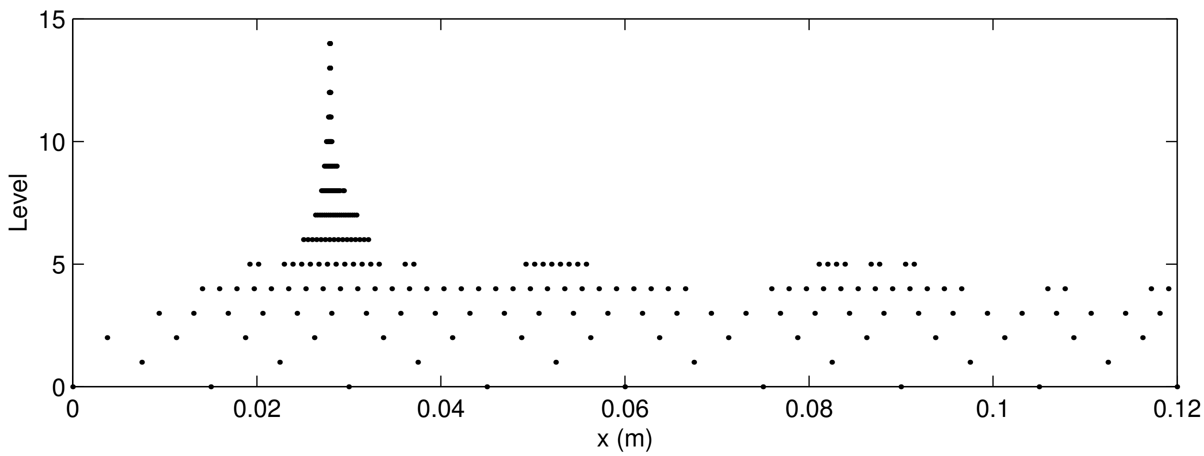
- $t = 230\ \mu s$
- predicted shock thickness: $\sim 50\ \mu m$.



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.





Application to Gas Phase HMX System

- Simulating isobaric HMX combustion computationally intensive,
- Most effort in solving gas phase convection, reaction, diffusion,
- Based on 45 species, 232 step mechanism of Yetter, et al.,
- Fastest time scales predicted 10^{-16} s (non-physical?),
- Stiffness ratio 10^{11} (vs. 10^9 for $H_2 - O_2$),
- Equations for gas phase combustion of HMX are of form

$$\frac{\partial}{\partial t}\mathbf{q}(x,t) + \frac{\partial}{\partial x}\mathbf{f}(\mathbf{q}(x,t)) = \mathbf{g}(\mathbf{q}(x,t)),$$

- Adiabatic, isobaric,
- Operator splitting appropriate,
- For *non-premixed* problem, higher dimension (≥ 8?!) manifolds necessary!
- Will need to parameterize by $(h, \rho, H, O, N, C, Ar, \ \geq$ one free parameter)

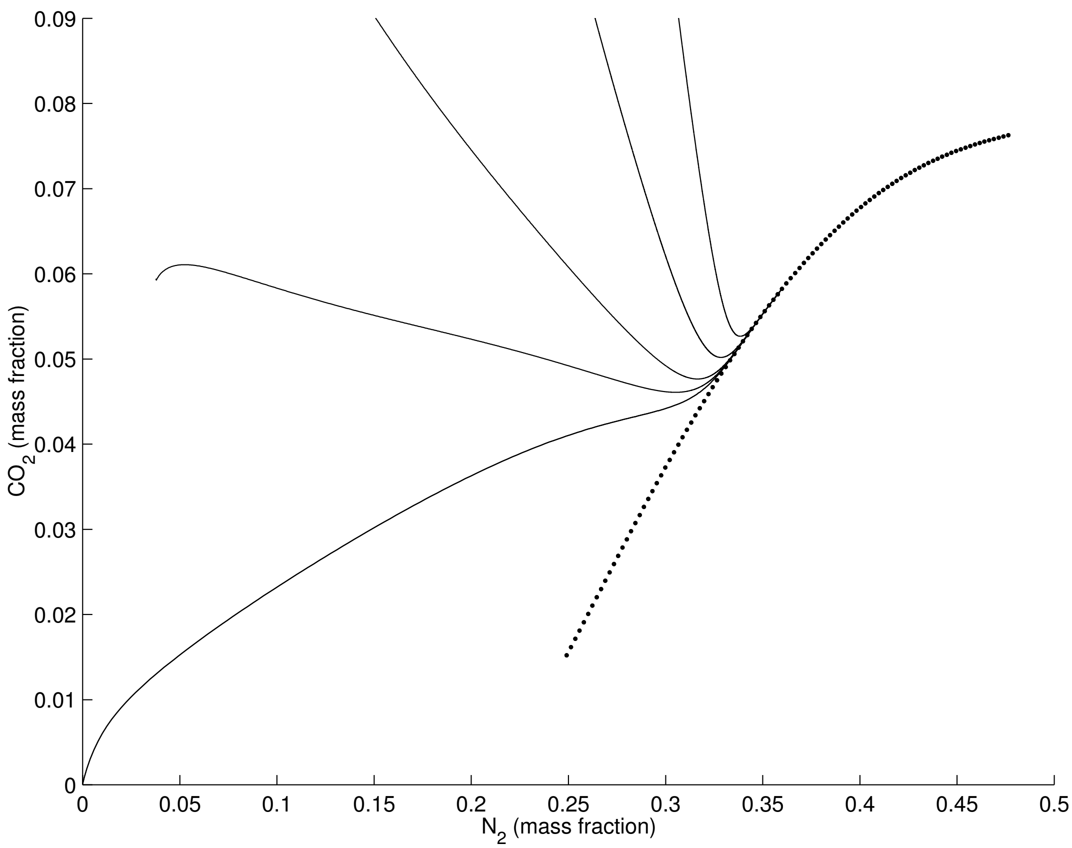
  $10^7 < h < 10^{11}\ erg/g; 10^{-5} < \rho < 10^{-3}\ g/cm^3; 10^{-32} < \chi_{Ar} < 10^{-2};$

  $$0 < \chi_C < 10^1; 0 < \chi_H < 10^1; 0 < \chi_N < 10^1; 0 < \chi_O < 10^1.$$

  (Liau, 1999)
- Three-dimensional manifold for preliminary premixed problem?

ILDM for Gas Phase HMX System

- Based on 45 species, 232 step mechanism of Yetter, et al.,
- Adiabatic ($h = 62 \times 10^9\ erg/g$) , isobaric ($P = 32\ bar$),
- projection in Y_{N_2}, Y_{CO_2} plane.



Summary

- Robust method in place to compute manifolds with arbitrary variables held constant (e.g. P, ρ, h),
- Effort still needed on improving technique of projecting onto manifold initially,
- Fast linear interpolation scheme in place for table lookup,
- Robust method in place to solve less stiff differential equations on or near manifold,
- Operator splitting allows implementation of manifold in solving PDEs,
- Adaptive multilevel wavelet collocation method gives dramatic spatial resolution,
- Full coupling of ILDM and wavelet methods soon forthcoming,
- Detailed studies of efficiency improvement necessary,
- More general manifold techniques need developed to allow strong fluid-chemistry coupling and relaxation of eigenmodes to steady state solutions.