

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

by

Joseph M. Powers

Associate Professor

Department of Aerospace and Mechanical Engineering

University of Notre Dame

presented at

Los Alamos National Laboratory

15 July 1999

Report Documentation Page

Form Approved
OMB No. 0704-0188

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1. REPORT DATE 15 JUL 1999		2. REPORT TYPE		3. DATES COVERED 00-00-1999 to 00-00-1999	
4. TITLE AND SUBTITLE Simulations of Viscous Detonations with Detailed Kinetics Using Manifold and Wavelet Techniques				5a. CONTRACT NUMBER	
				5b. GRANT NUMBER	
				5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S)				5d. PROJECT NUMBER	
				5e. TASK NUMBER	
				5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) University of Notre Dame, Department of Aerospace and Mechanical Engineering, Notre Dame, IN, 46556				8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)				10. SPONSOR/MONITOR'S ACRONYM(S)	
				11. SPONSOR/MONITOR'S REPORT NUMBER(S)	
12. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release; distribution unlimited					
13. SUPPLEMENTARY NOTES					
14. ABSTRACT					
15. SUBJECT TERMS					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT unclassified	b. ABSTRACT unclassified	c. THIS PAGE unclassified			

Support

National Science Foundation
Chemical and Transport Systems, CTS-9705150,
Air Force Office of Scientific Research,
Directorate of Mathematics and Geosciences
AFOSR Grant No. F49620-98-1-0206,
and
Los Alamos National Laboratory

Acknowledgments

Prof. Samuel Paolucci, ND-AME
Dr. Christopher Bowman, Post-Doc, ND-AME,
Mr. Sandeep Singh, Ph.D. Candidate, ND-AME
Mr. Yevgenii Rastigejev, Ph.D. Candidate, ND-AME

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.

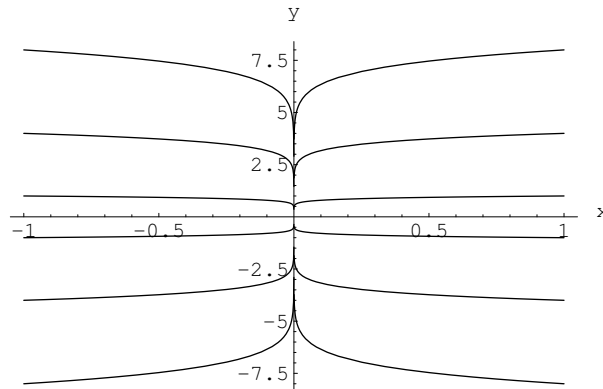
Intrinsic Low-Dimensional Manifold Method (ILDm)

- 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

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

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



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

$$\frac{dy}{dt} = \frac{dy}{ds} \frac{ds}{dt}, \quad \text{chain rule}$$

$$-y(s) = \frac{dy}{ds} \frac{ds}{dt}, \quad \text{substitute from ODE and manifold}$$

$$-s = (1) \frac{ds}{dt}, \quad \text{no longer stiff!}$$

$$s = s_o e^{-t},$$

$$x(t) = 0; \quad y(t) = s_o e^{-t}.$$

- 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:

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

\mathbf{x} : species concentration; $\mathbf{x} \in \mathfrak{R}^n$

- 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

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

where $\mathbf{F}_{\mathbf{x}}$ is a *constant* Jacobian matrix.

- Schur decompose the Jacobian matrix:

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

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 $\mathbf{F}_{\mathbf{x}}$ on its diagonal, sometimes placed in order of decreasing magnitude.
- The Schur vectors q_i form an orthonormal basis which spans the phase space, \mathfrak{R}^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

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

- Equilibrium points:

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

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:

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

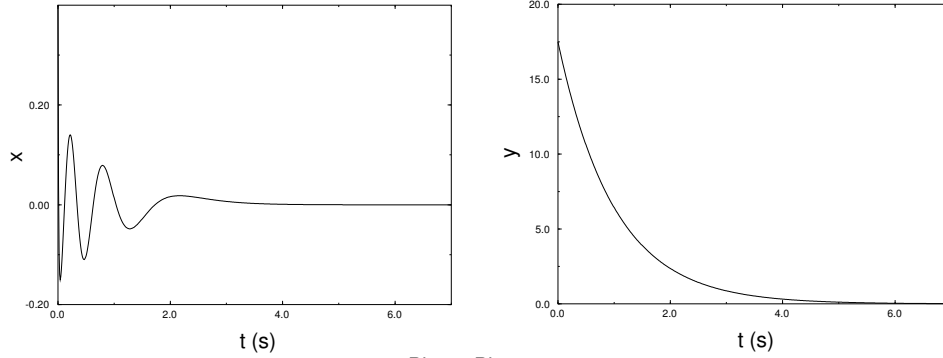
$$-100x + y \sin y = 0 \quad \text{The ILDM!}$$

A Simple Example

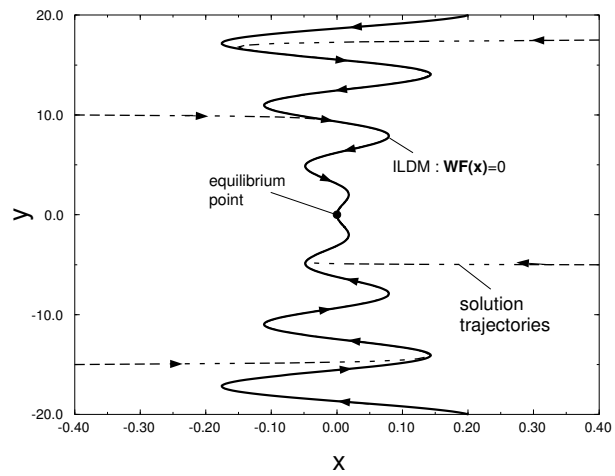
$$\frac{dx}{dt} = -100x + y \sin(y) \quad x(0) = x_0$$

$$\frac{dy}{dt} = x^3 - y \quad y(0) = y_0$$

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:

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

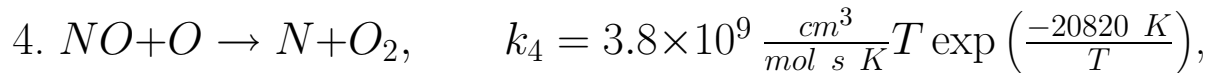
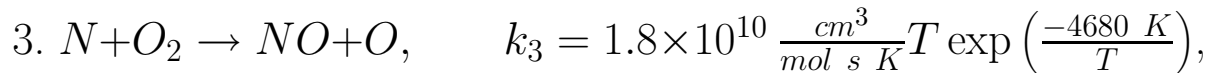
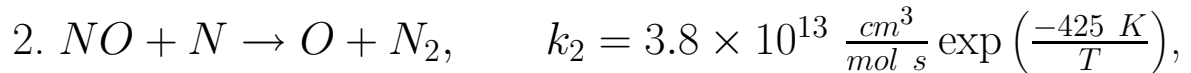
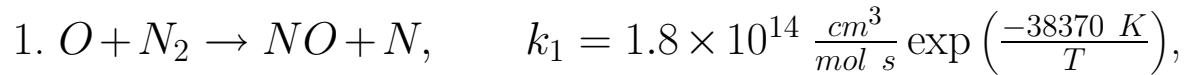
Time scale: $\tau = 1.0$ No longer stiff!

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

$$x \sim \frac{1}{100}s_0 e^{-t} \sin(s_0 e^{-t}), \quad y \sim s_0 e^{-t}.$$

Example: Zeldovich Mechanism of NO Formation

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



- 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:

$$2[N_2] + [NO] + [N] = C_1,$$

$$[O] + [N] = C_2,$$

$$2[O_2] + [NO] - [N] = C_3.$$

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

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

$$[N_2] = \frac{1}{2}(C_1 - [NO] - [N])$$

$$[O] = C_2 - [N]$$

$$[O_2] = \frac{1}{2}(C_3 - [NO] + [N])$$

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

$$2[N_2] + [N] + [NO] = C_1,$$

$$2[O_2] + [NO] + [O] = C_2 + C_3,$$

$$[N] + [NO] + [N_2] + [O] + [O_2] = \frac{C_1 + C_3}{2} + C_2.$$

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:

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

- Take as initial conditions

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

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

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

Example: Zeldovich Mechanism of NO Formation, cont.

- Linearization of equations near physical equilibrium gives

$$\frac{d}{dt} \begin{pmatrix} [N] - 1.16 \times 10^{-11} \\ [NO] - 2.78 \times 10^{-6} \end{pmatrix} = \begin{pmatrix} -9.67 \times 10^8 & 3.38 \times 10^3 \\ 8.11 \times 10^8 & -4.03 \times 10^3 \end{pmatrix} \mathbf{F}_x$$

$$\frac{d}{dt} \begin{pmatrix} [N] - 1.16 \times 10^{-11} \\ [NO] - 2.78 \times 10^{-6} \end{pmatrix} = \begin{pmatrix} -0.766 & -0.643 \\ 0.643 & -0.766 \end{pmatrix} \mathbf{Q}$$

$$\begin{pmatrix} -9.67 \times 10^8 & 3.38 \times 10^3 \\ 0 & -1.19 \times 10^3 \end{pmatrix} \mathbf{U}$$

$$\begin{pmatrix} -0.766 & 0.643 \\ -0.643 & -0.766 \end{pmatrix} \mathbf{Q}^T$$

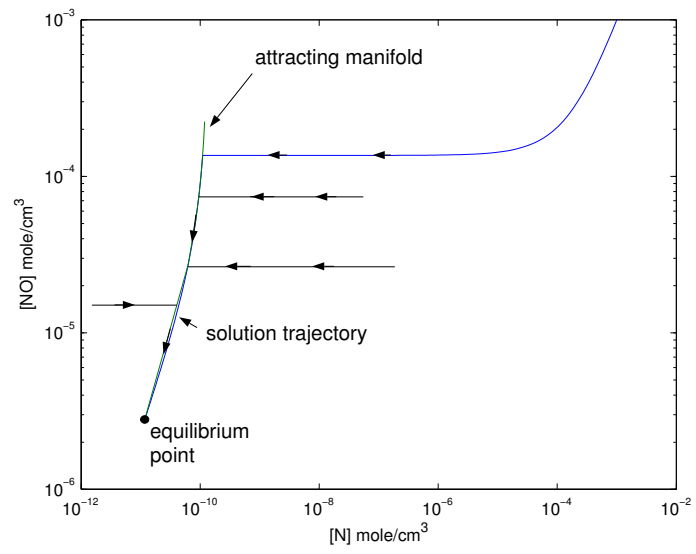
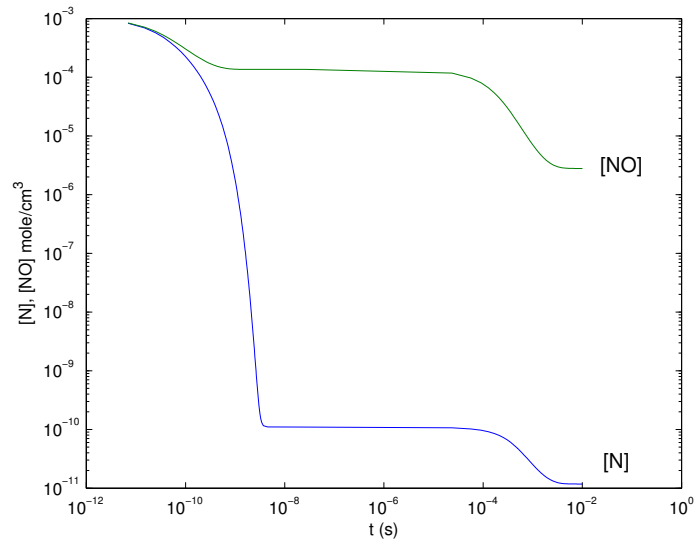
$$\begin{pmatrix} [N] - 1.16 \times 10^{-11} \\ [NO] - 2.78 \times 10^{-6} \end{pmatrix}$$

- Condition number (stiffness ratio) = $\left| \frac{-9.67 \times 10^8}{-1.19 \times 10^3} \right| = 8.1 \times 10^5$.
- Locally the ILDM is defined by

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

$$(-0.766 \quad 0.643) \begin{pmatrix} F_1([N], [NO]) \\ F_2([N], [NO]) \end{pmatrix} = 0.$$

- Use arc length continuation methods to define complete ILDM
- The physical equilibrium has negative eigenvalues: stable.
- The non-physical equilibria have positive eigenvalues: unstable.



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

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

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

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

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

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

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

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

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

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

$N = 9$ 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:

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

Δ_x is either Godunov *or* wavelet discretization operator.

2. Reaction source term step:

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

- 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:

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

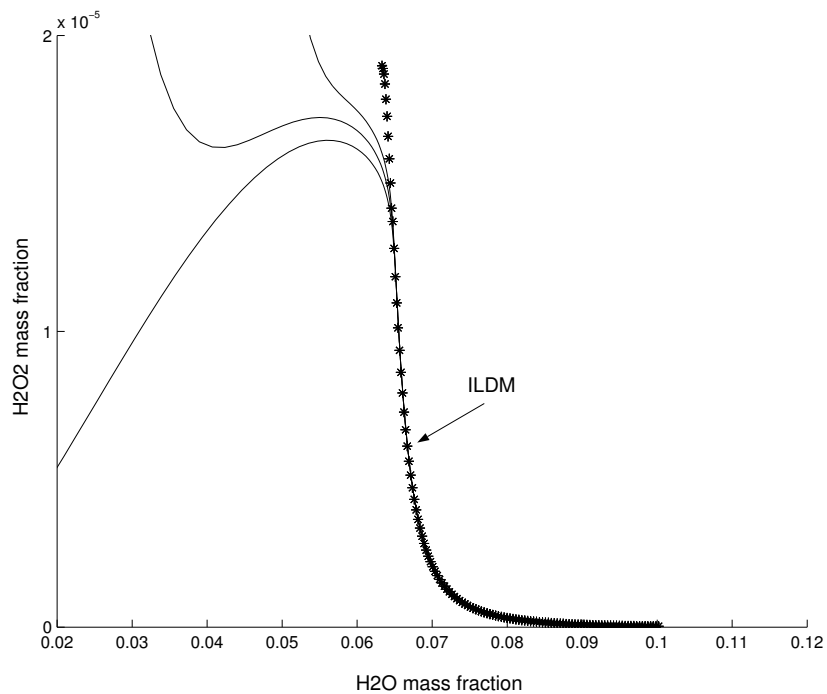
- Equations reduce to

$$\rho = \rho_o, \quad u = u_o, \quad e = e_o,$$
$$\frac{dY_i}{dt} = \frac{\omega}{\rho_o}.$$

- 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

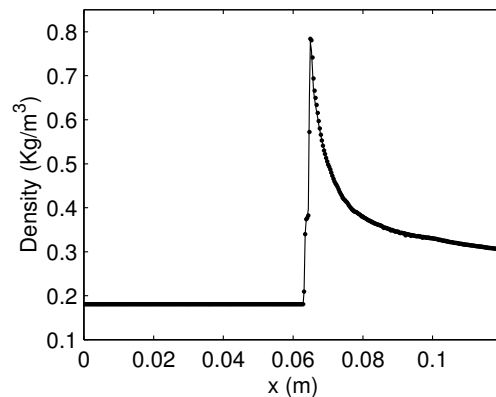
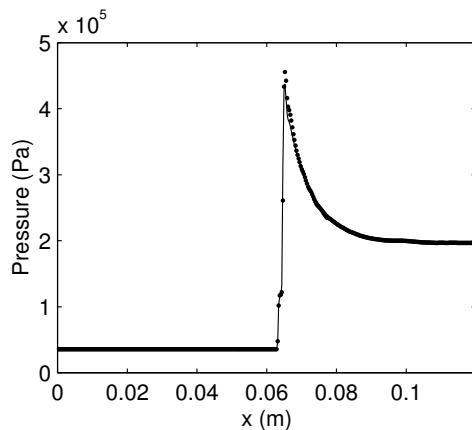
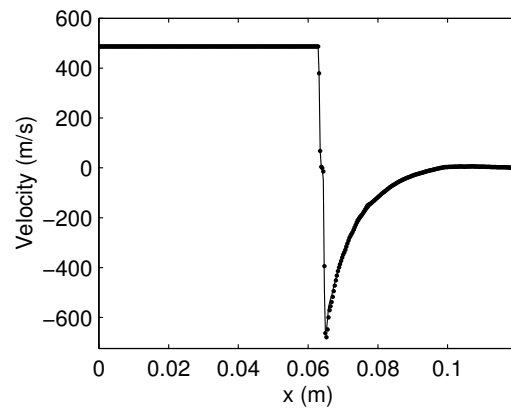
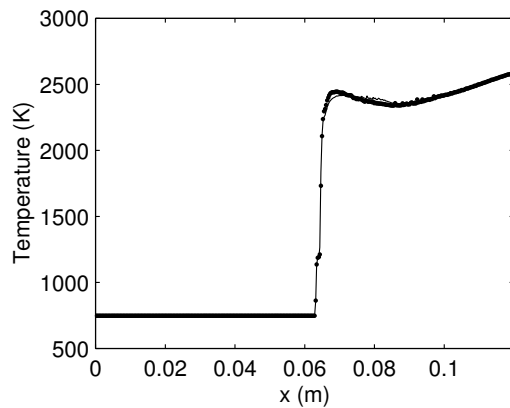
Sample ILDM for $H_2 - O_2$

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

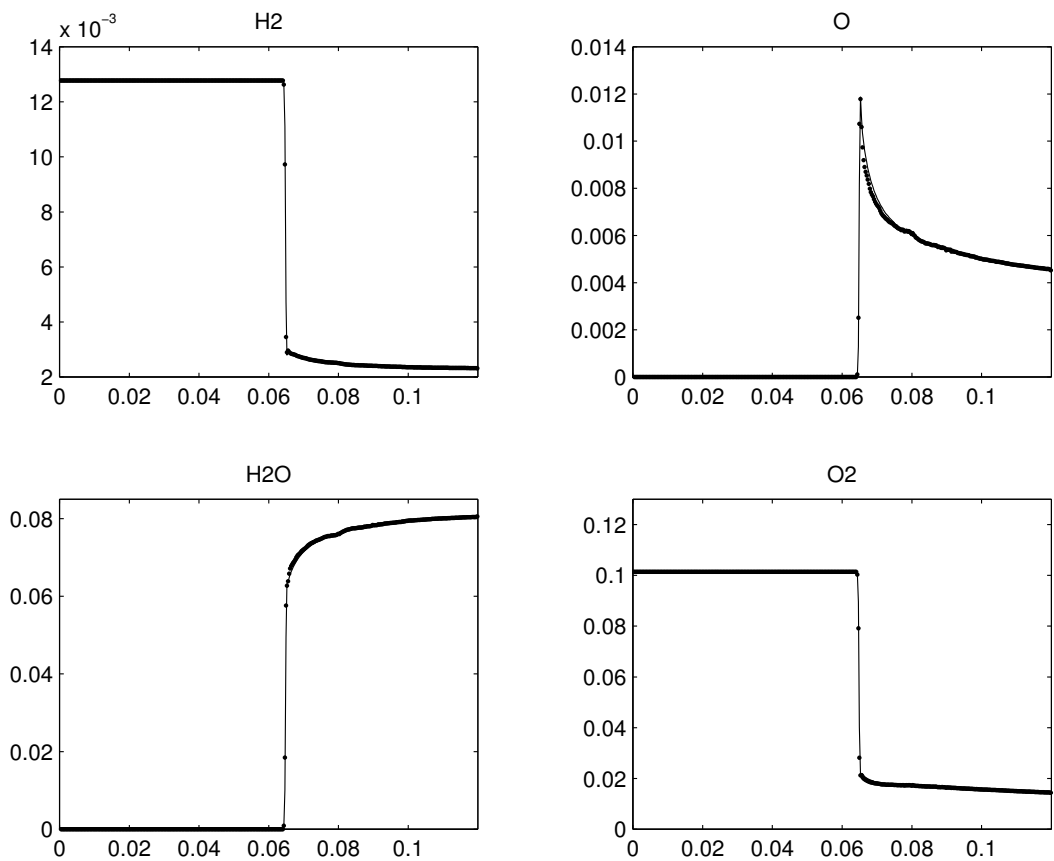


Inviscid $H_2 - O_2$ Ignition Delay with and without ILDM

- 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).

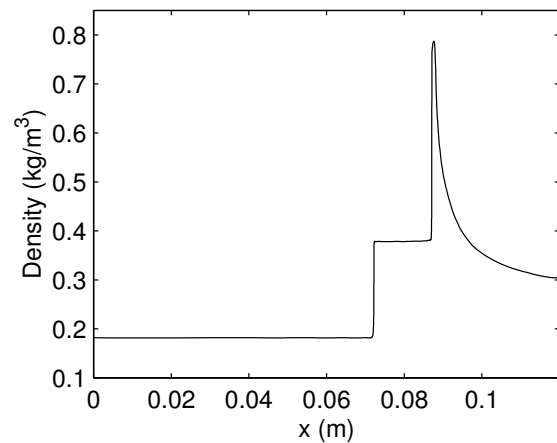
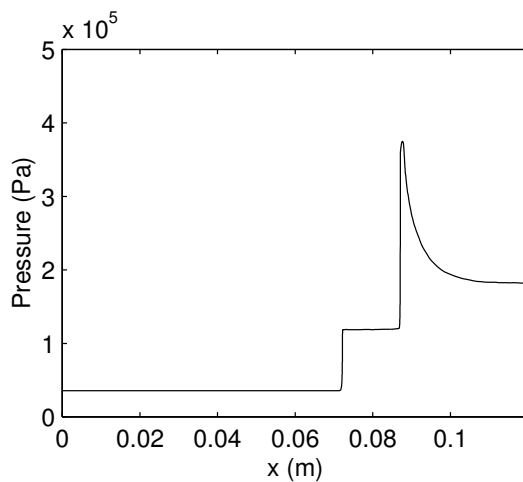
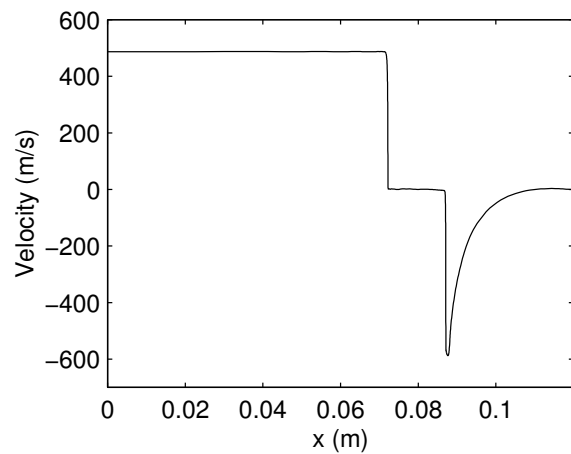
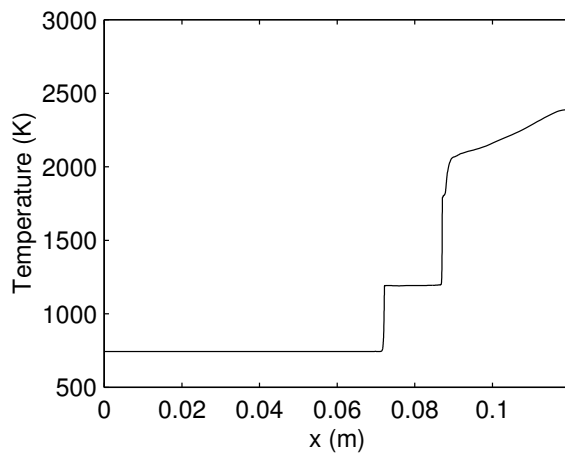


Inviscid $H_2 - O_2$ Ignition Delay with and without ILDM



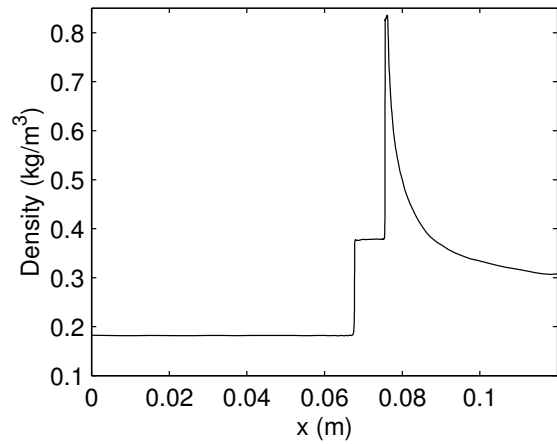
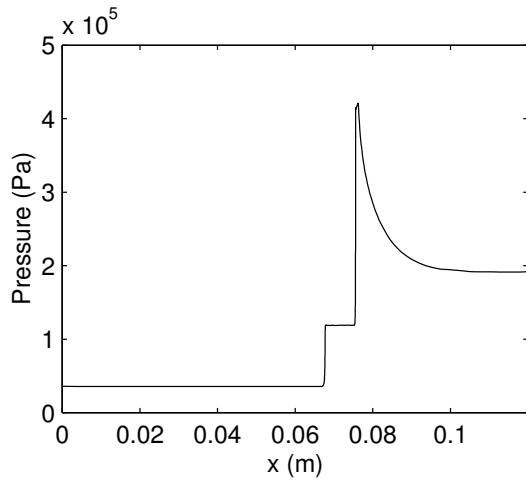
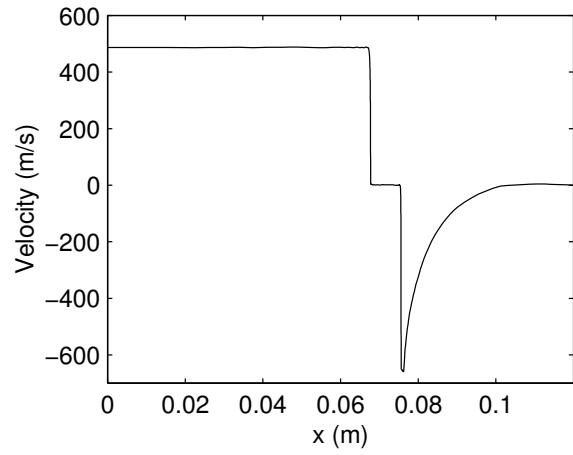
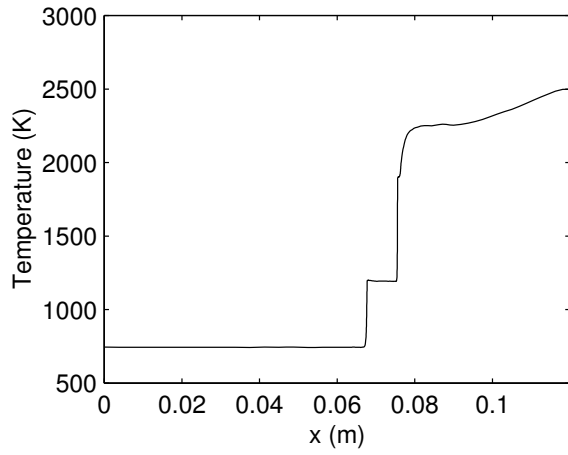
Viscous $H_2 - O_2$ Ignition Delay with Wavelets

- 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!*
- $t = 180 \mu s$.



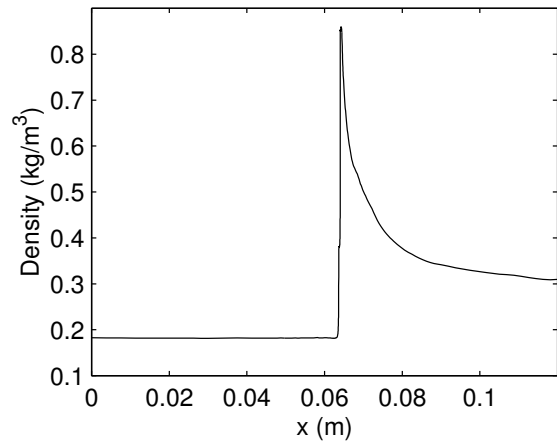
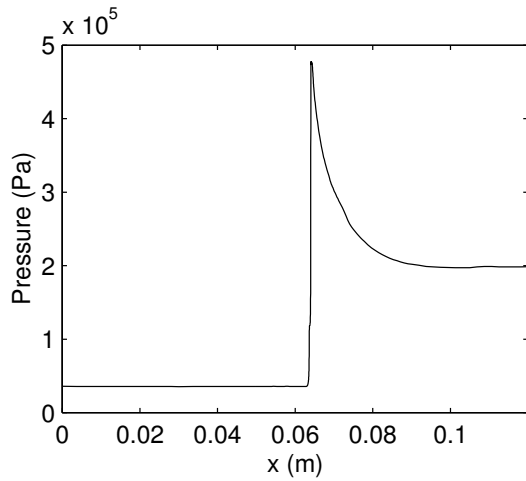
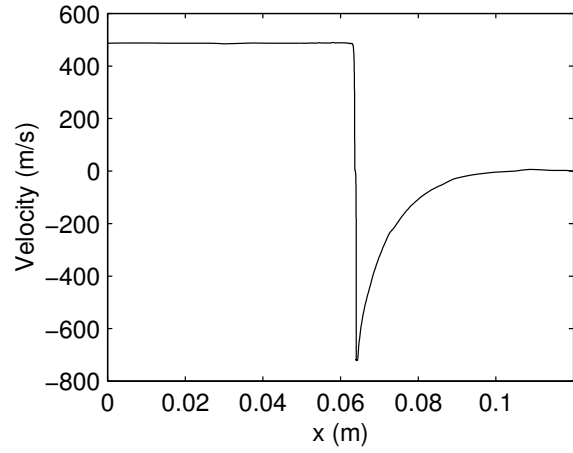
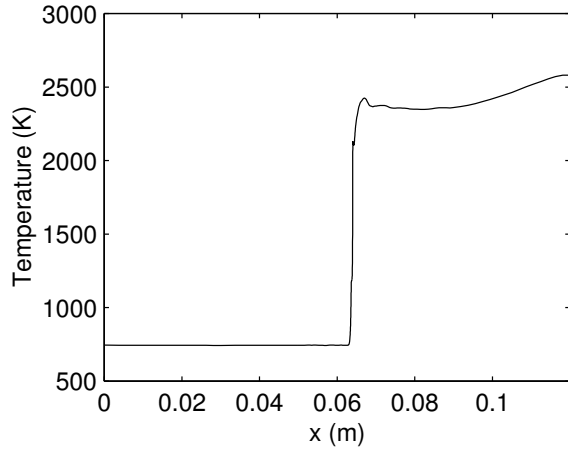
Viscous $H_2 - O_2$ Ignition Delay with Wavelets

- $t = 190 \mu s$



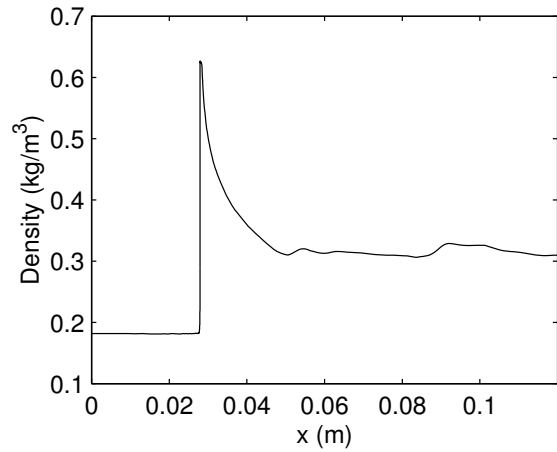
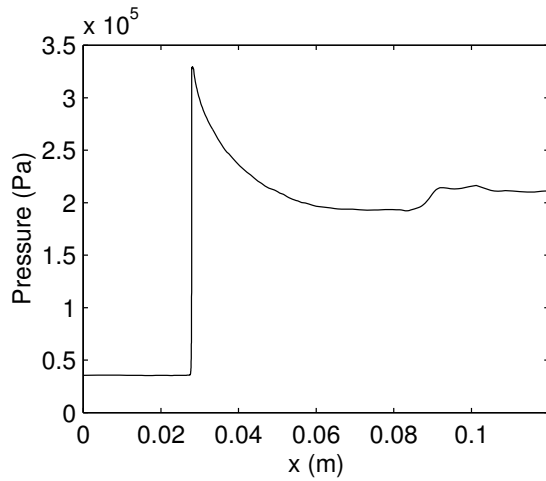
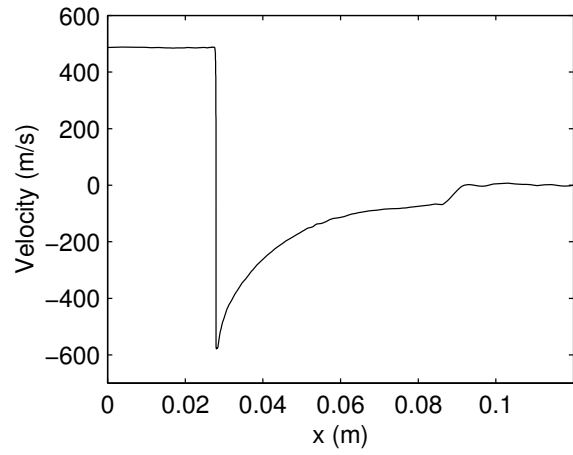
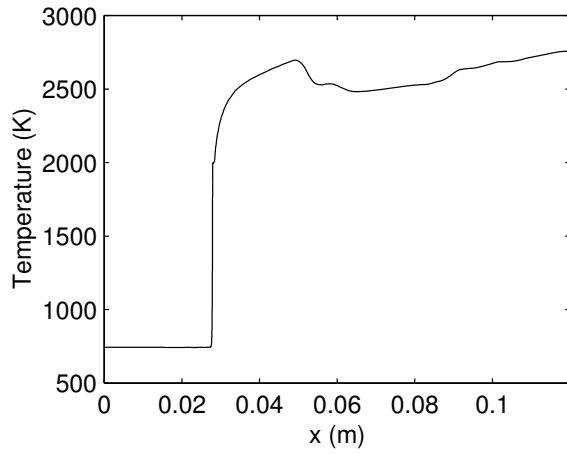
Viscous $H_2 - O_2$ Ignition Delay with Wavelets

- $t = 200 \mu s$



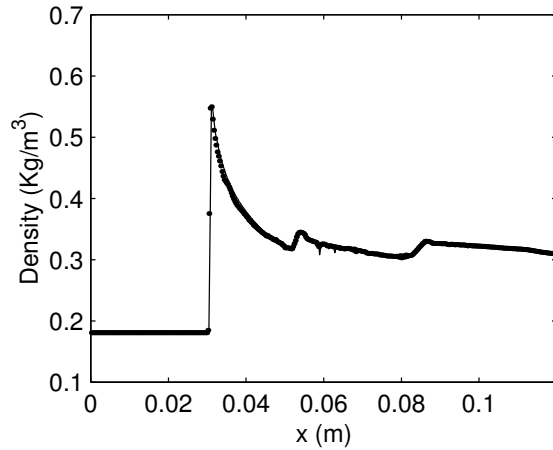
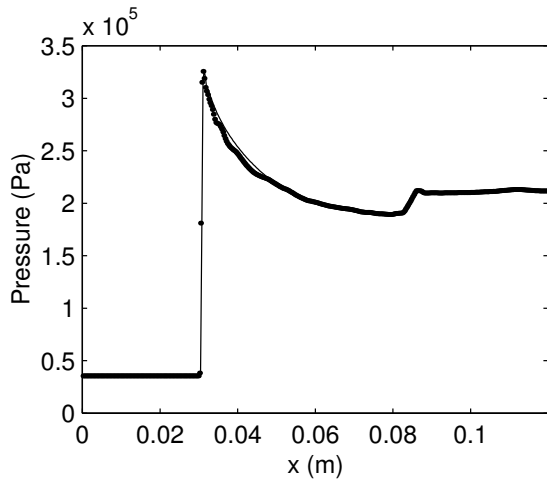
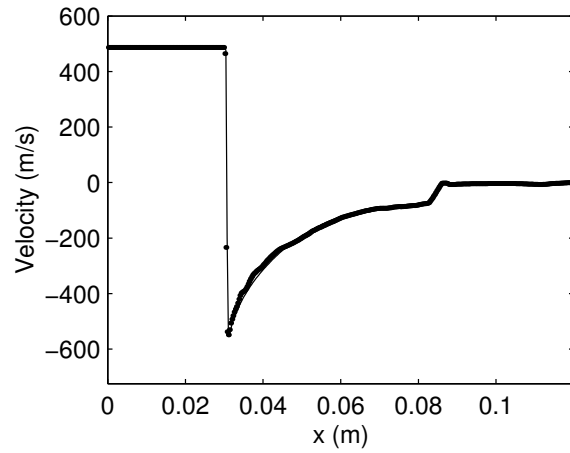
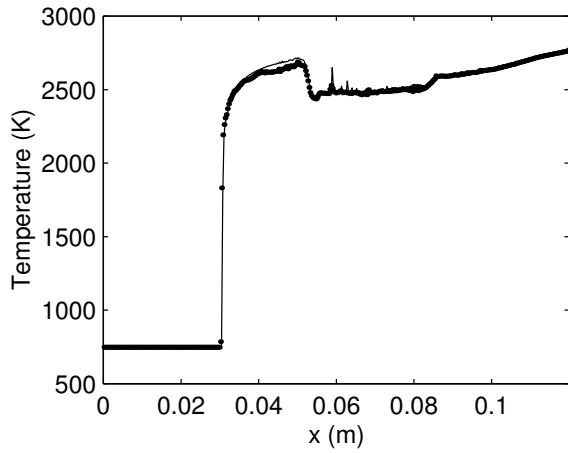
Viscous $H_2 - O_2$ Ignition Delay with Wavelets

• $t = 230 \mu s$



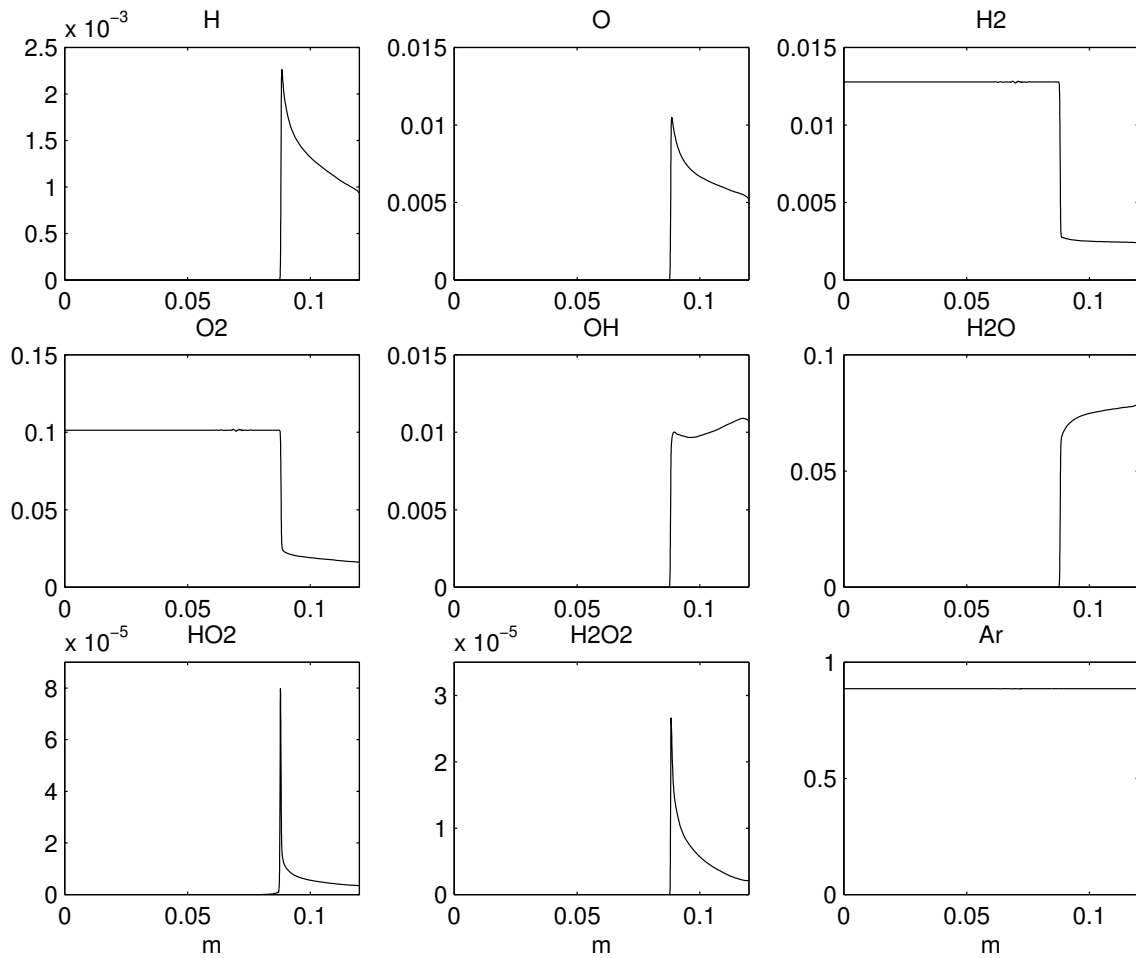
Comparison with Inviscid/ILDM Result at Same Time

• $t = 230 \mu s$



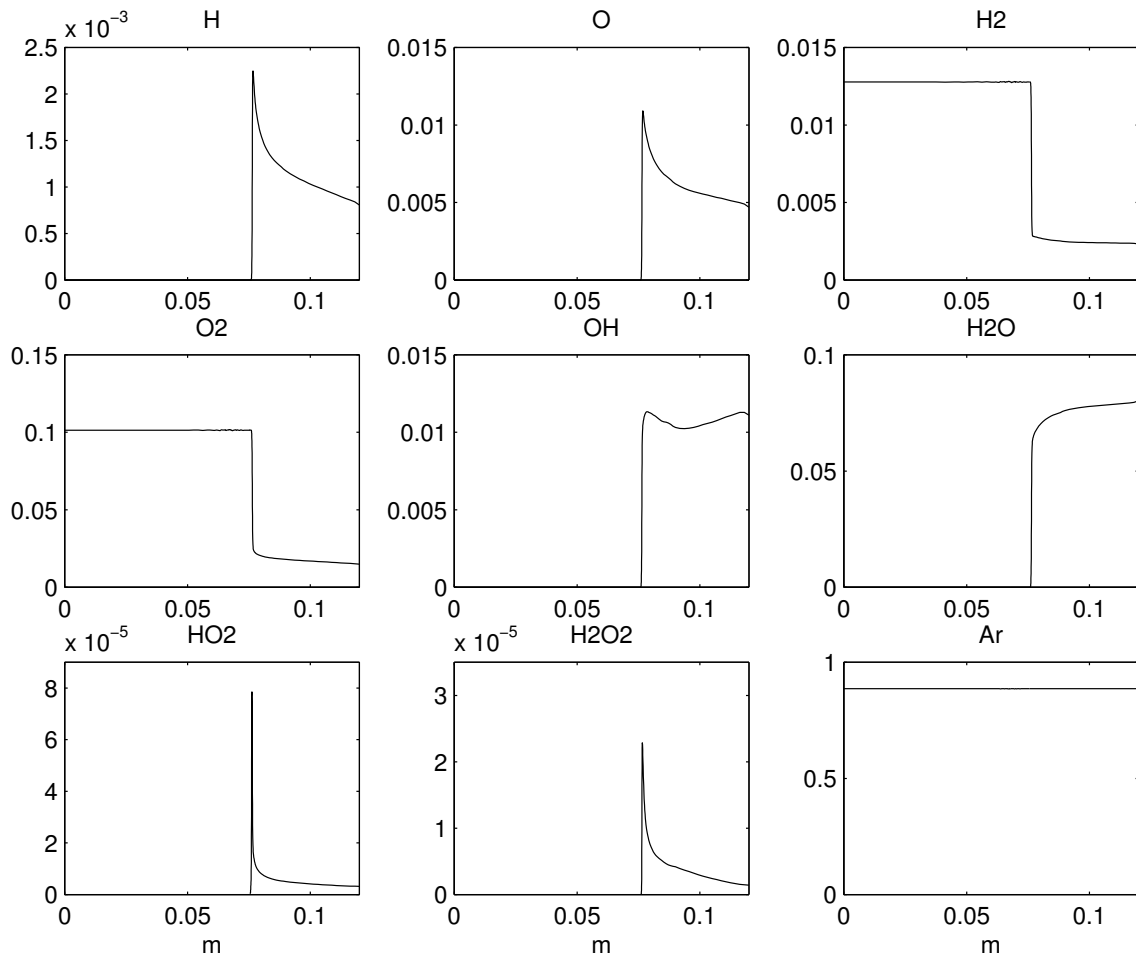
Viscous $H_2 - O_2$ Ignition Delay with Wavelets

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



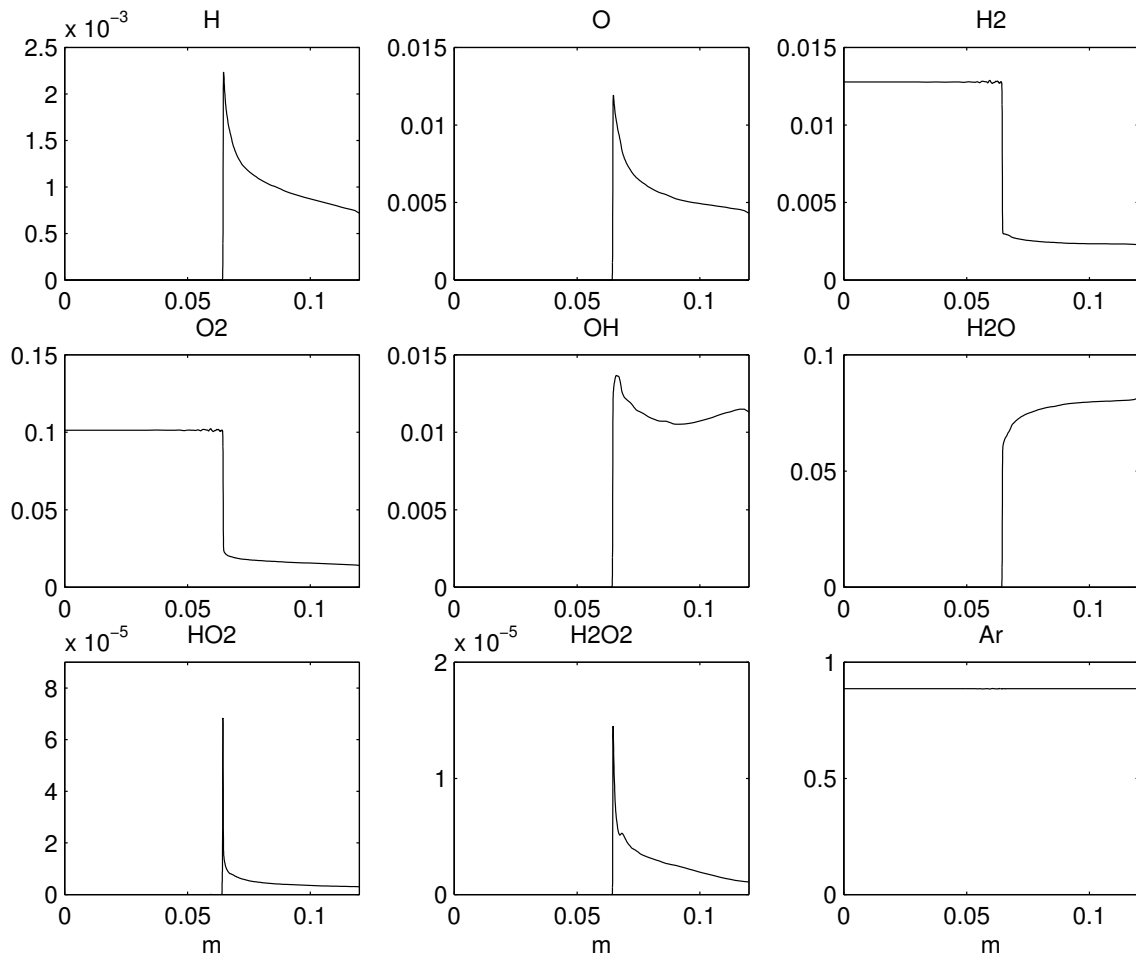
Viscous $H_2 - O_2$ Ignition Delay with Wavelets

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



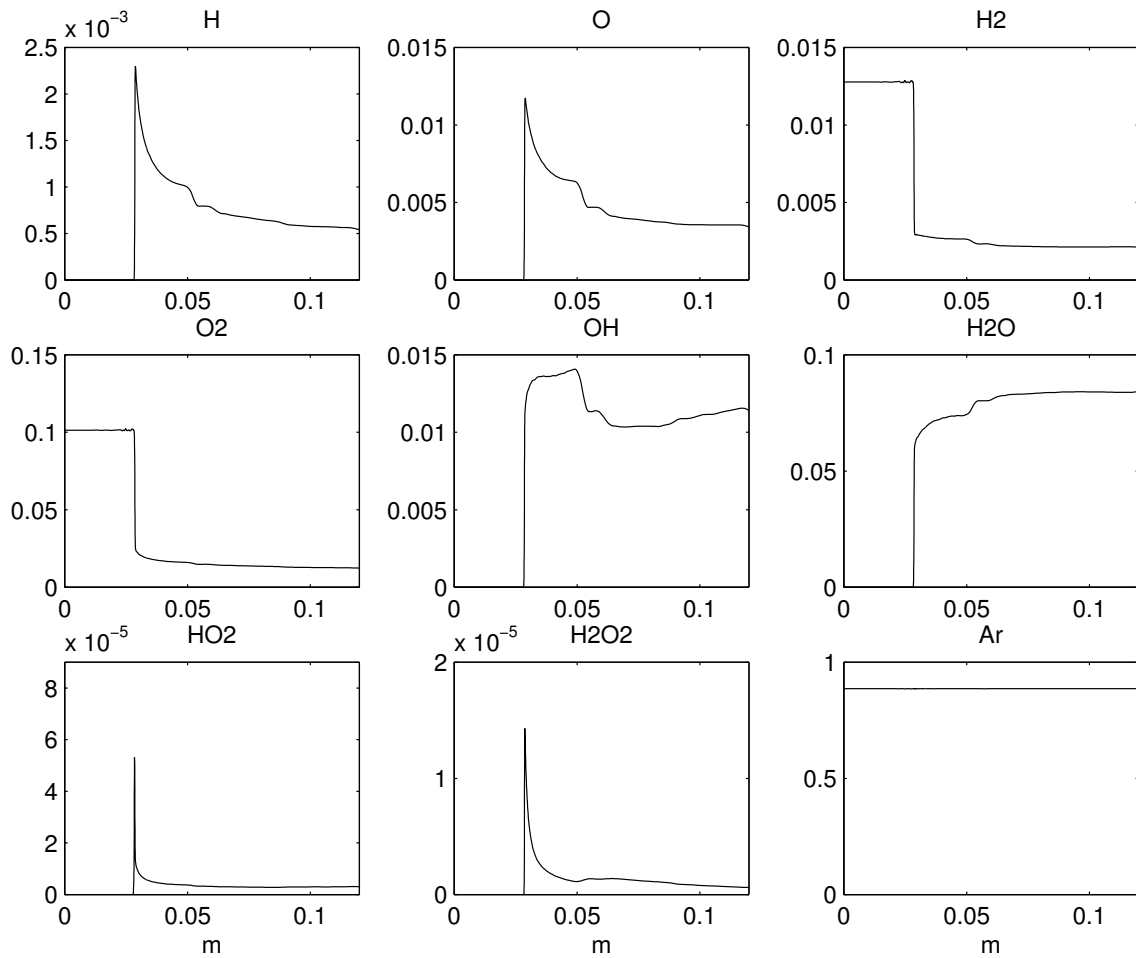
Viscous $H_2 - O_2$ Ignition Delay with Wavelets

- $t = 200 \mu s$
- species mass fractions plotted vs. distance



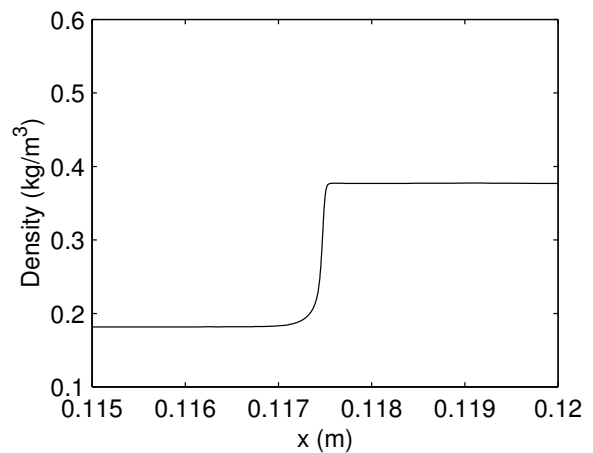
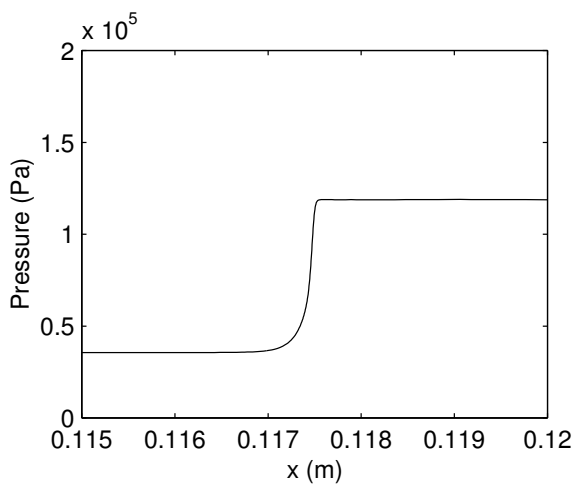
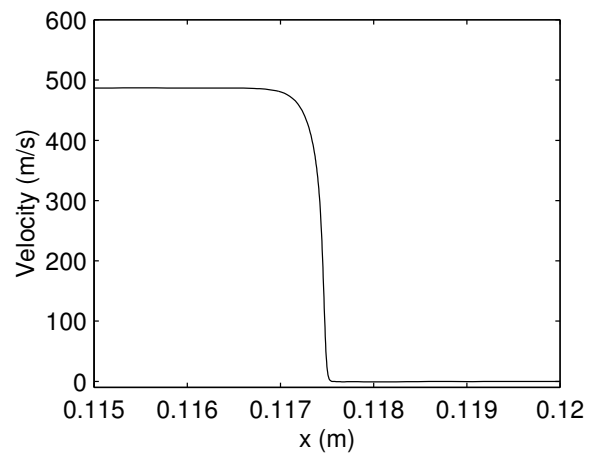
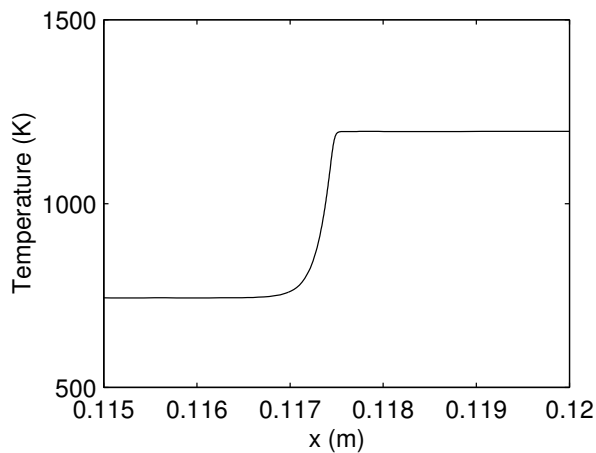
Viscous $H_2 - O_2$ Ignition Delay with Wavelets

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



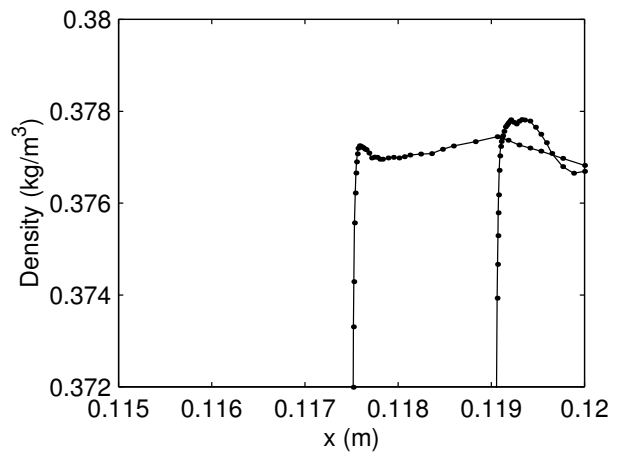
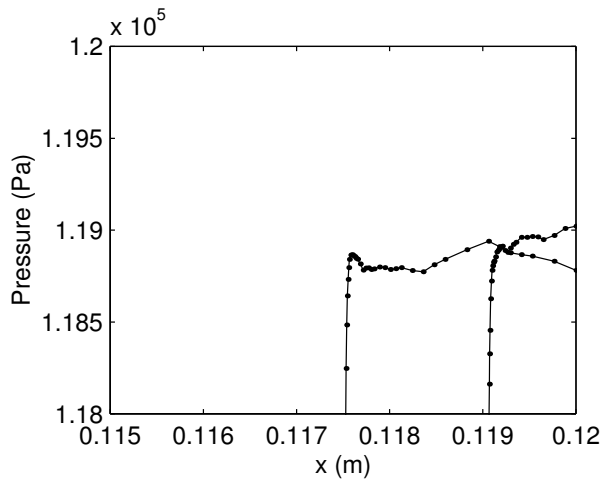
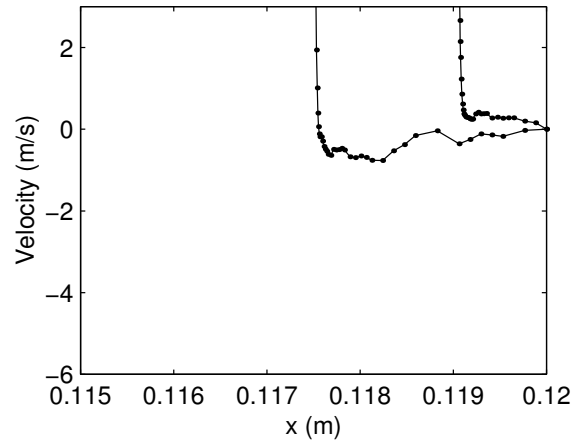
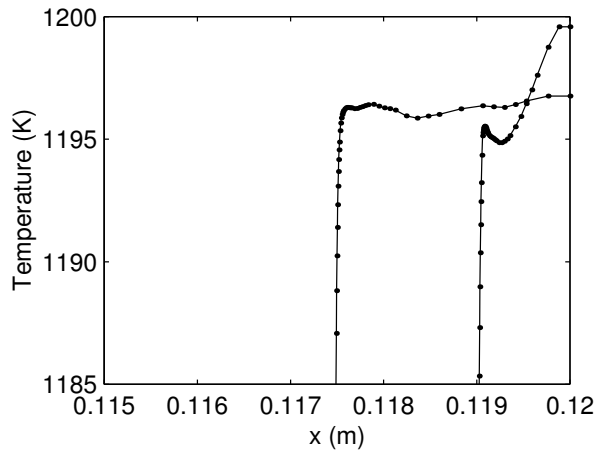
Post Reflection Entropy Layer?: Viscous Wavelet Results

- 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

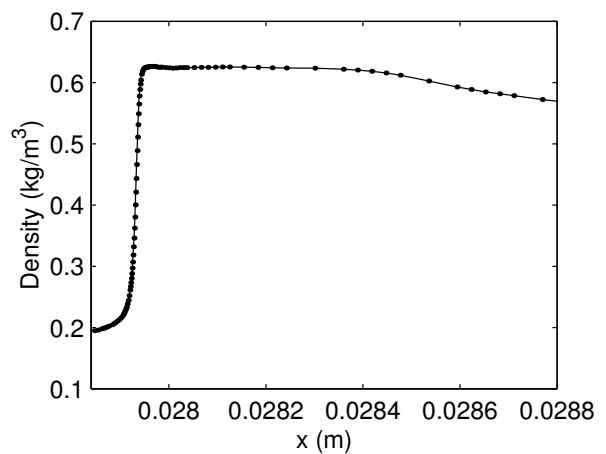
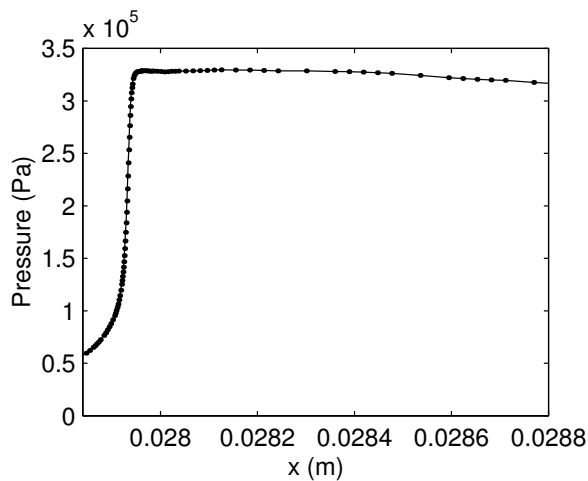
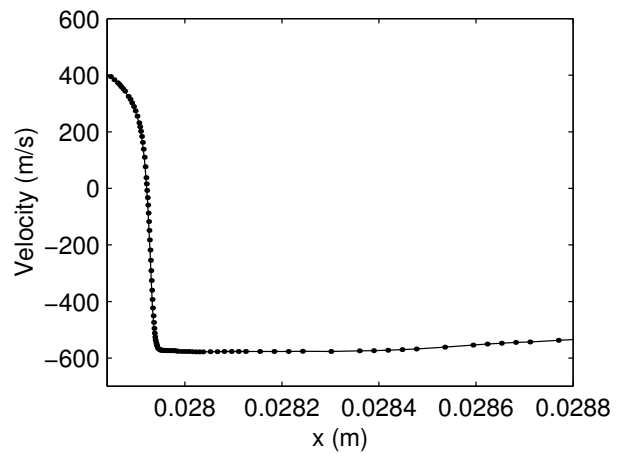
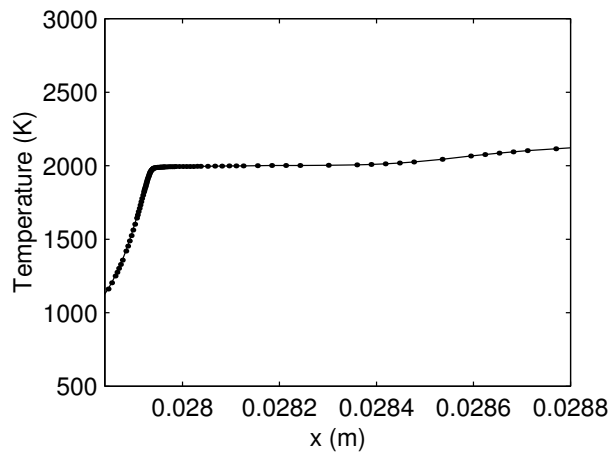
- small entropy layer evident on finer scale,
- temperature rise $\sim 5\text{ K}$; dissipates quickly,
- inviscid calculations before adjustment give persistent temperature rise of $\sim 20\text{ K}$; reaction acceleration small.



Viscous $H_2 - O_2$ Ignition Delay with Wavelets

Close-up: Viscous Shock Structure and Induction Zone

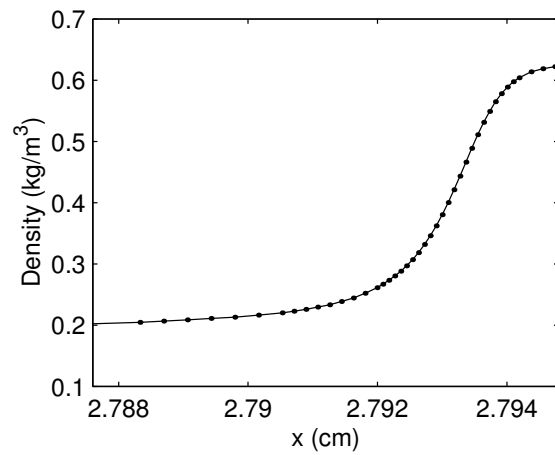
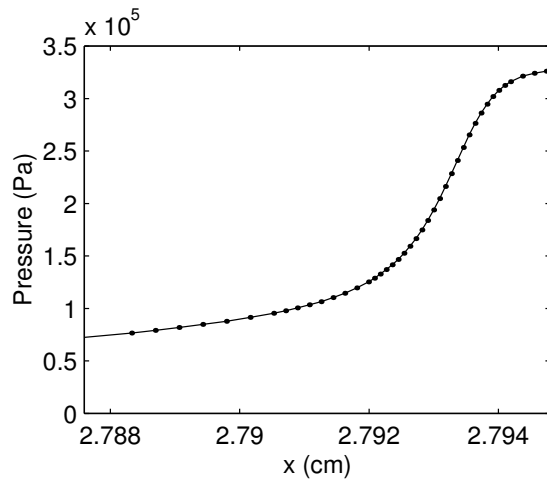
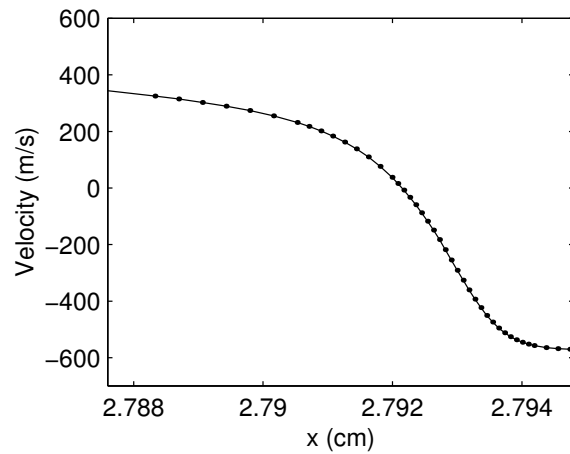
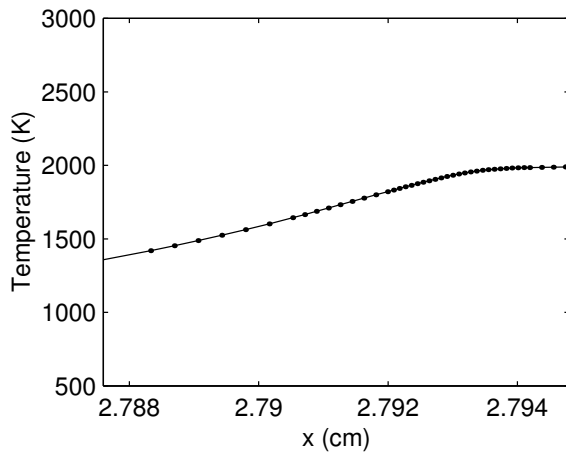
- $t = 230 \mu s$,
- Induction zone length: $\sim 470 \mu m$,
- No significant reaction in viscous shock zone.



Viscous $H_2 - O_2$ Ignition Delay with Wavelets

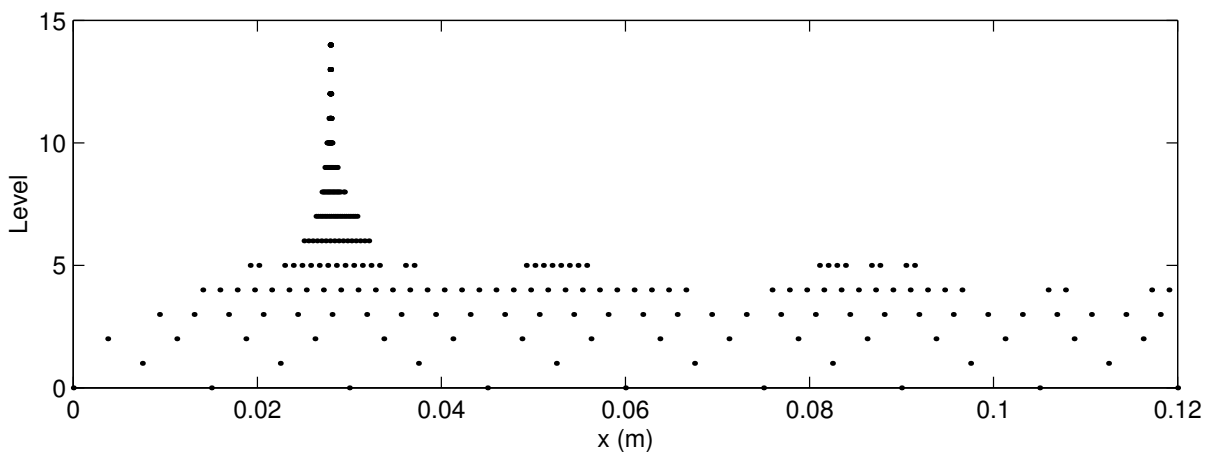
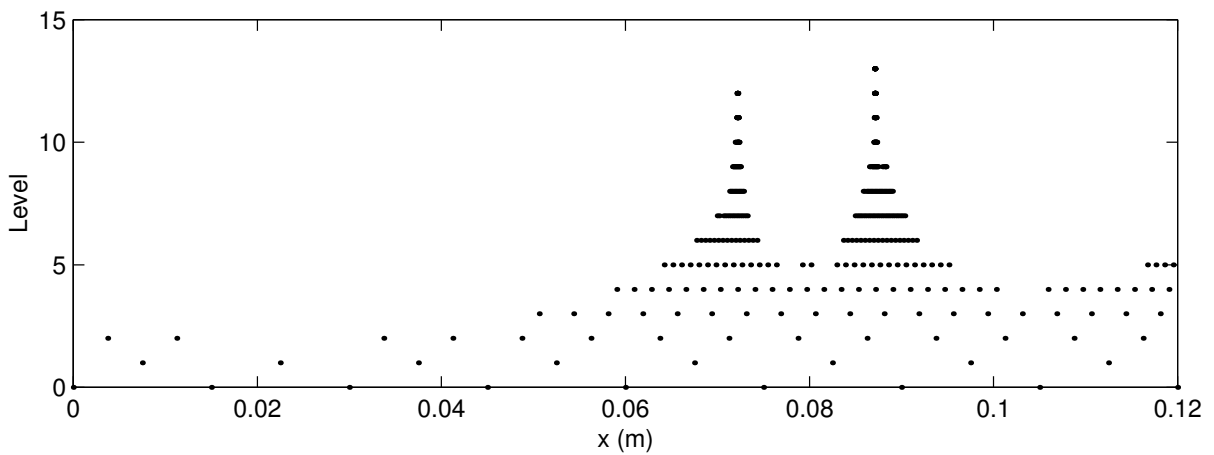
Closer-up: Viscous Shock Structure Only

- $t = 230 \mu s$
- 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)

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

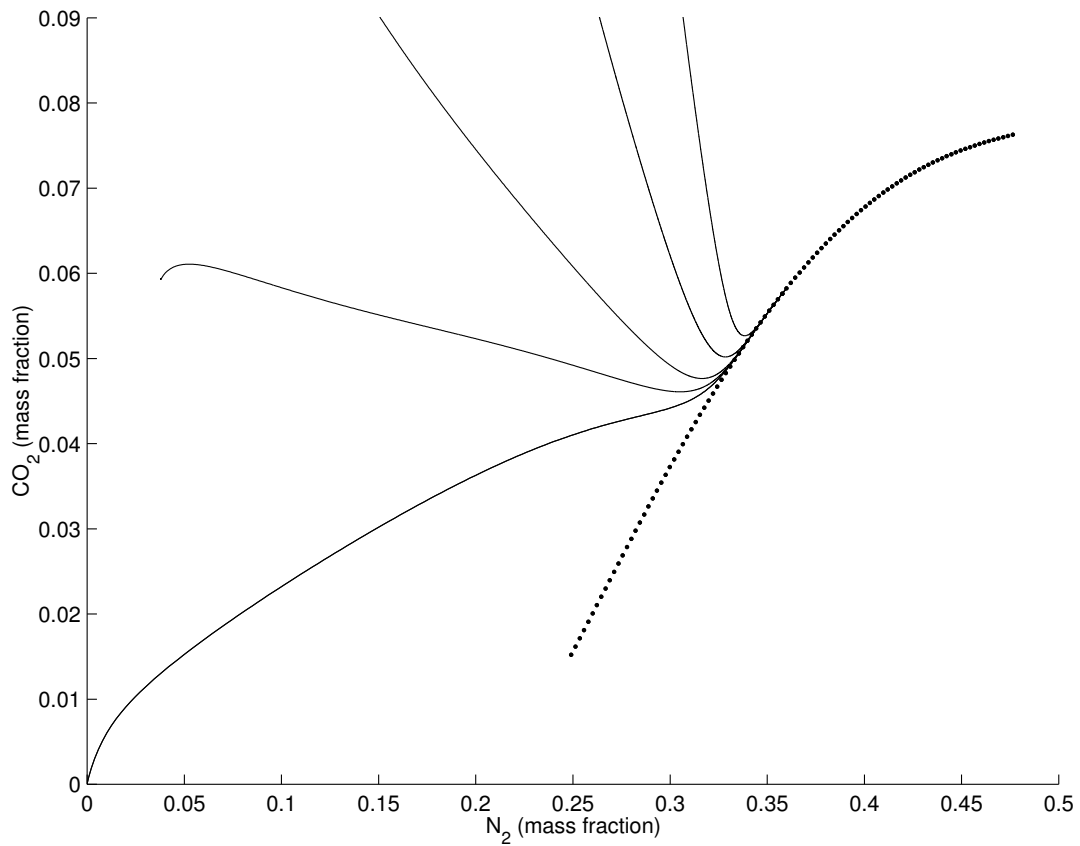
$$0 < \chi_C < 10^1; 0 < \chi_H < 10^1; 0 < \chi_N < 10^1; 0 < \chi_O < 10^1.$$

(Liau, 1999)

- Three-dimensional manifold for preliminary premixed problem?

ILDDM for Gas Phase HMX System

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