Application of Intrinsic Low Dimensional Manifolds to Nitramine Combustion

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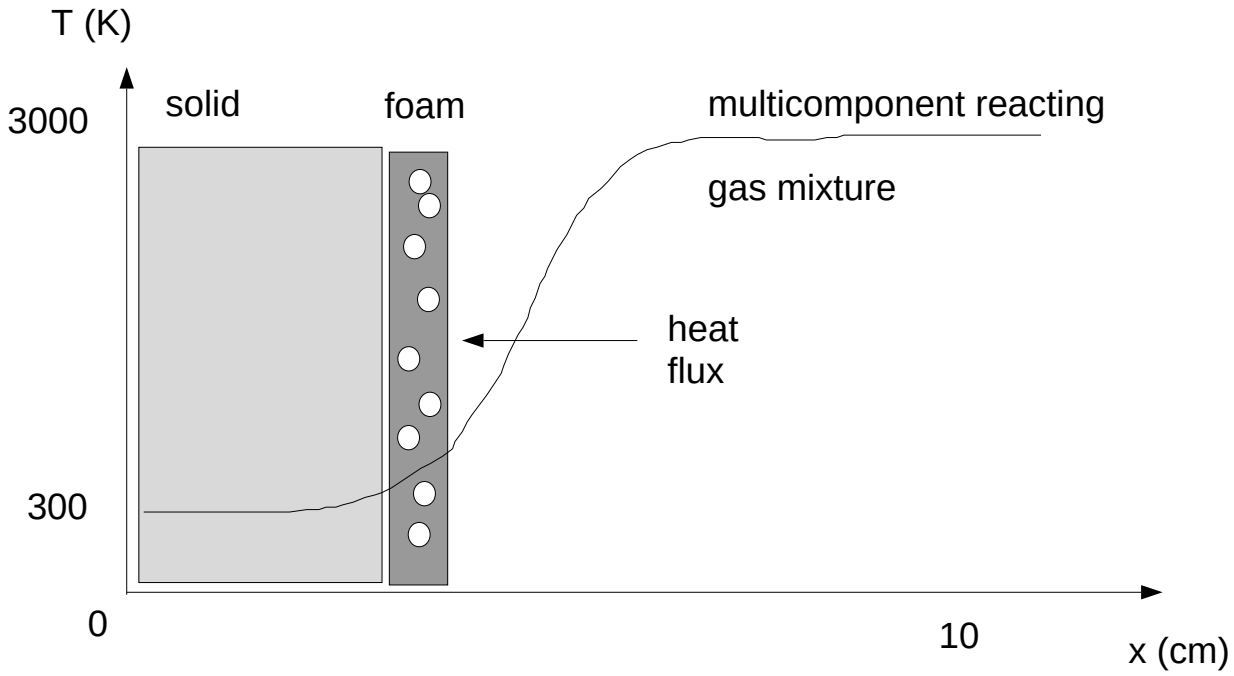
Outline

- Introduction to issues in nitramine (e.g. HMX or RDX) combustion
- Intrinsic Low Dimensional Manifold (ILDM) technique (Maas & Pope, 1992)
- Wavelet Adaptive Multilevel Representation (WAMR) technique (Paolucci & Vasilyev)
- Results for one-dimensional viscous $H_2/O_2/Ar$ detonation with detailed kinetics
- Preliminary results for HMX gas phase combustion
- Conclusions

RDX/HMX COMBUSTION

- part of ongoing theoretical/experimental LANL study of low pressure $\sim 10\ atm$ combustion of explosives (Son, Liau, et al.),
- similar to solid propellant combustion,
- preheat zone in semi-infinite solid,
- two-phase bubbly liquid foam layer,
- gaseous flame region,
- gas phase reactions greatest computational burden in simulations.



Some Important Questions

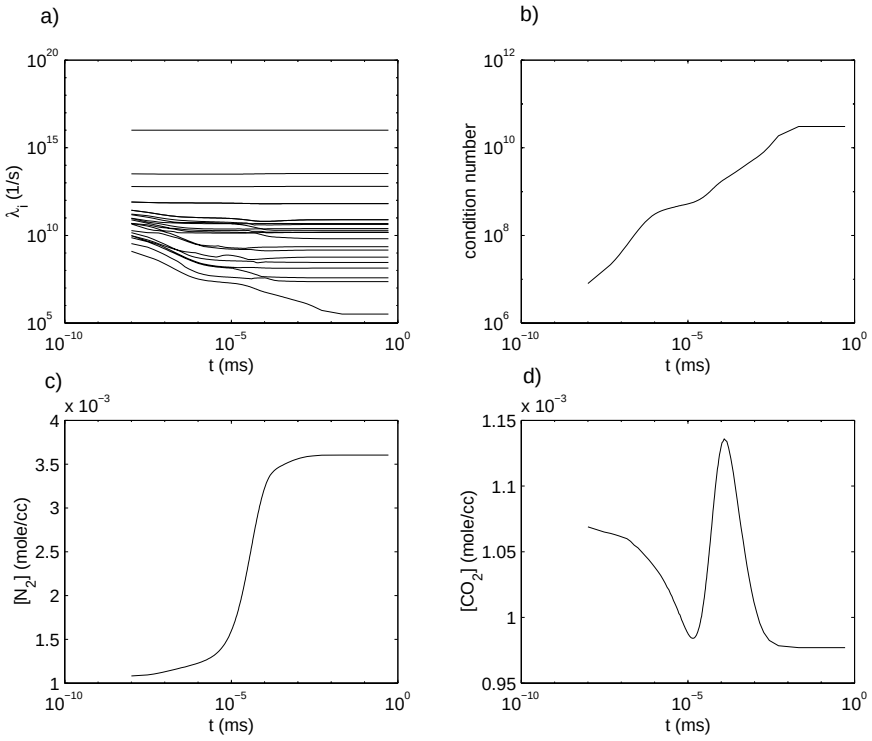
- Do we have resolved, accurate solutions for HMX combustion?
- How can ILDM improve the calculation of HMX combustion?
- How can ILDM, derived for well-stirred systems, be used rationally in systems in which convection and diffusion are important?

Motivation for ILDM

- Detailed finite rate kinetics critical in reactive fluid mechanics
- 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).
- chemical time scales typically more demanding than convection-diffusion
- Reduced kinetics necessary given current computational resources.

RDX GAS PHASE COMBUSTION SIMULATION

- very similar to HMX
- Uses Yetter's 45 species, 232 reaction detailed kinetics mechanism,
- Constant pressure
- well-stirred
- fastest time scales $\sim 10^{-16}$ s!
- stiffness ratio (fastest time scale/slowest time scale) $\sim 10^{11}$



Compressible Reactive Navier-Stokes Equations

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

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

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

$$\frac{\partial}{\partial t}(\rho y_l) + \frac{\partial}{\partial x}(\rho u y_l + j_l) = 0, \qquad (l = 1, \ldots, L-1), \qquad \text{elements}$$

$$\frac{\partial}{\partial t}(\rho Y_i) + \frac{\partial}{\partial x}(\rho u Y_i + J_i) = \dot{\omega}_i M_i, \qquad (i = 1, \ldots, N-L), \qquad \text{species}$$

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

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

$$J_i = -\rho\mathcal{D}\frac{\partial Y_i}{\partial x}, \qquad (i = 1, \ldots, N), \qquad \text{Fick's law}$$

$$y_l = m_l \sum_{i=1}^{N} \frac{\phi_{il}}{M_i} Y_i, \qquad (l = 1, \ldots, L-1), \qquad \text{element mass fraction}$$

$$j_l = m_l \sum_{i=1}^{N} \frac{\phi_{il}}{M_i} J_i, \qquad (l = 1, \ldots, L-1), \qquad \text{element mass flux}$$

$$\sum_{i=1}^{N} Y_i = 1, \qquad \text{mass fraction constraint}$$

$$\sum_{l=1}^{L} y_l = 1, \qquad \text{element mass fraction constraint}$$

$$\dot{\omega}_i = \sum_{j=1}^{J} a_j T^{\beta_j} \exp\left(\frac{-E_j}{\Re T}\right)\left(\nu''_{ij} - \nu'_{ij}\right)\prod_{k=1}^{N}\left(\frac{\rho Y_k}{M_k}\right)^{\nu'_{kj}}, \qquad (i = 1, \ldots, N-L) \qquad \text{law of mass action}$$

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

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

N species, L elements, J reactions

$3N + L + 6$ equations in $3N + L + 6$ unknowns

Focus on element conservation

- $L-1$ explicit element conservation equations formed along with $N-L$ species evolution equations, instead of the typical $N-1$ species equations,
- facilitates a proper use of ILDM in upcoming operator splitting,
- In general element mass fractions change due to mass diffusion

$$\rho\frac{dy_l}{dt} = -\frac{\partial j_l}{\partial x}.$$

- With simple Fick's Law with no preferential diffusion

$$\rho\frac{dy_l}{dt} = \mathcal{D}\frac{\partial}{\partial x}\left(\rho\frac{\partial y_l}{\partial x}\right).$$

- In uniformly premixed problem with no boundary influences then, all element concentrations are constant for all time:

$$\frac{dy_l}{dt} = 0.$$

Operator Splitting Technique

- Equations are of form

$$\frac{\partial}{\partial t}\mathbf{q}(x,t) + \frac{\partial}{\partial x}\mathbf{f}(\mathbf{q}(x,t)) = \mathbf{g}(\mathbf{q}(x,t)), \qquad \mathbf{q},\mathbf{f},\mathbf{g} \in \Re^{N+2}.$$

  where

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

- $\mathbf{f}$ 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 any spatial discretization operator, here a wavelet 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:

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

$$l = 1, \ldots, L-1, \qquad i = 1, \ldots, N-L.$$

- Equations reduce to

$$\rho = \rho_o, \qquad u = u_o, \qquad e = e_o, \qquad y_l = y_{lo},$$

$$\frac{dY_i}{dt} = \frac{\dot{\omega}_i M_i}{\rho_o}, \qquad i = 1, \ldots, N-L$$

- $\dot{\omega}_i$ has dependency on ρ, e, y_l, and Y_i

- ODEs for Y_i are stiff, usually solved with implicit methods.

- ODEs for Y_i can be attacked with manifold methods to remove stiffness with ILDM with ρ, e, $y_l, \ldots, y_{L-1}$ parameterization.

Intrinsic Low-Dimensional Manifold Method (ILDM)

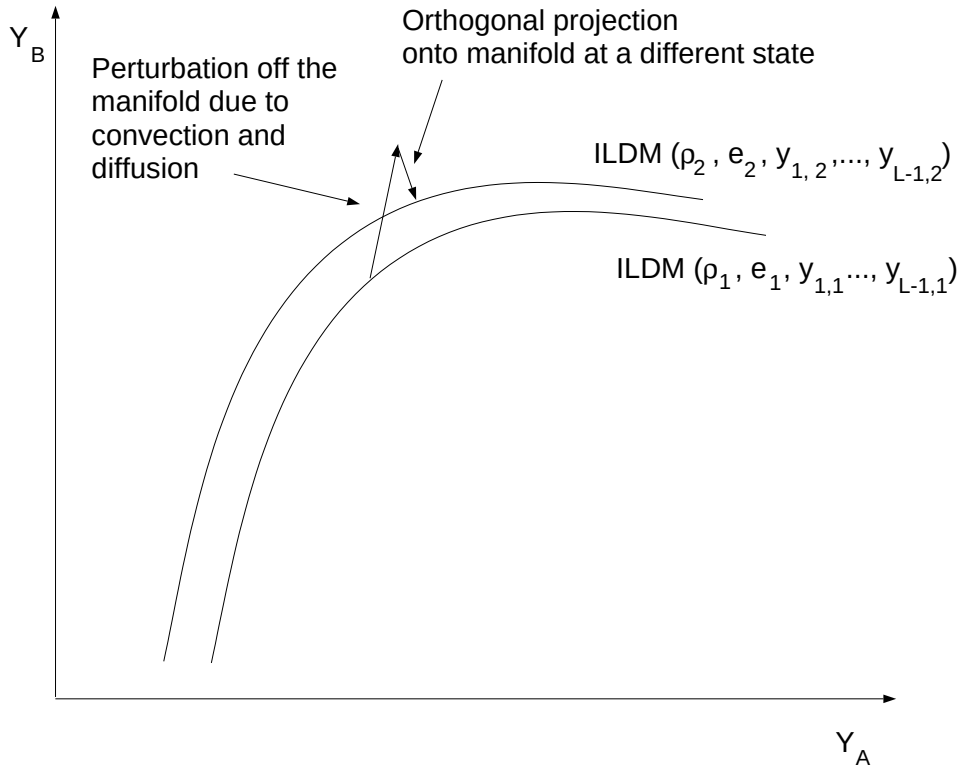
- Uses a dynamical systems approach,
- Does not require imposition of *ad hoc* partial equilibrium or steady state assumptions,
- Fast time scale phenomena are systematically equilibrated,
- Slow time scale phenomena are resolved in time,
- Computation time reduced by factor of ~ 10 for non-trivial combustion problems; manifold gives much better roadmap to find solution relative to general implicit solution techniques (Norris, 1998)

Necessary Dimension of ILDM

- Spatial discretization of PDEs results in a set of adiabatic, isochoric well-stirred reactors,
- N species with L elements at constant e and ρ gives rise to a $(N-L)$-dimensional phase space (same as composition space),
- To resolve M slow time scales, we identify M-dimensional subspaces (manifolds), $M < (N-L)$, embedded within the $(N-L)$-dimensional phase space on which the M slow time scale events evolve,
  - Fast time scale events rapidly move to the manifold,
  - Slow time scale events move on the manifold,
  - Because of convection-diffusion, e, ρ, y_l vary, requiring a $K = M + L + 1$-dimensional manifold.
  - If y_l conserved (premixed with no preferential diffusion), dimension of manifold is reduced by $L - 1$.
  - e.g., for $M = 1$ in premixed $H_2/O_2/Ar$ with no preferential diffusion, we need $K = 3$.
  - e.g., for $M = 1$ in non-premixed HMX (with H, O, C, and N) in Ar, we need $K = 7$. For isobaric, $K = 6$.

Implementation of ILDMs with Convection-Diffusion

- To minimize phase error, must integrate full equations until sufficiently close to ILDM
- When near ILDM, M slow equations are integrated, other variables found by table lookup
- Convection-diffusion step *applied to all variables* perturbs system from ILDM
- In next reaction step, orthogonally project to ILDM at *different* value of ρ, e, $y_1, \ldots, y_{N-1}$.



Formulation of General Manifolds

- A well-stirred adiabatic, isochoric chemically reactive system of N species in L elements is modeled by a set of non-linear ordinary differential equations:

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

$$\mathbf{x}: \text{ species concentration}; \mathbf{x} \in \Re^{N-L}$$

- 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:

$$\mathbf{F}_{\mathbf{x}} = \mathbf{Q} \cdot \mathbf{U} \cdot \mathbf{Q}^T$$

$$\mathbf{Q} = \begin{pmatrix} \vdots & \vdots & & \vdots \\ q_1 & q_2 & \cdots & q_{N-L} \\ \vdots & \vdots & & \vdots \end{pmatrix}, \quad \mathbf{U} = \begin{pmatrix} \lambda_1 & u_{1,2} & \cdots & u_{1,N-L} \\ 0 & \lambda_2 & \cdots & u_{2,N-L} \\ 0 & \cdots & \ddots & \vdots \\ 0 & \cdots & 0 & \lambda_{N-L} \end{pmatrix}, \quad \mathbf{Q}^T = \begin{pmatrix} \cdots & q_1^T & \cdots \\ \cdots & q_2^T & \cdots \\ & \vdots & \\ \cdots & q_{N-L}^T & \cdots \end{pmatrix}$$

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, $\Re^{N-L}$.
- We then define M slow time scales, $M < N - L$.
- Next define a non-square matrix $\mathbf{W}$ which has in its rows the Schur vectors associated with the fast time scales:

$$\mathbf{W} = \begin{pmatrix} \cdots & \cdots & q_{M+1}^T & \cdots & \cdots \\ \cdots & \cdots & q_{M+2}^T & \cdots & \cdots \\ & & \vdots & & \\ \cdots & \cdots & q_{N-L}^T & \cdots & \cdots \end{pmatrix}.$$

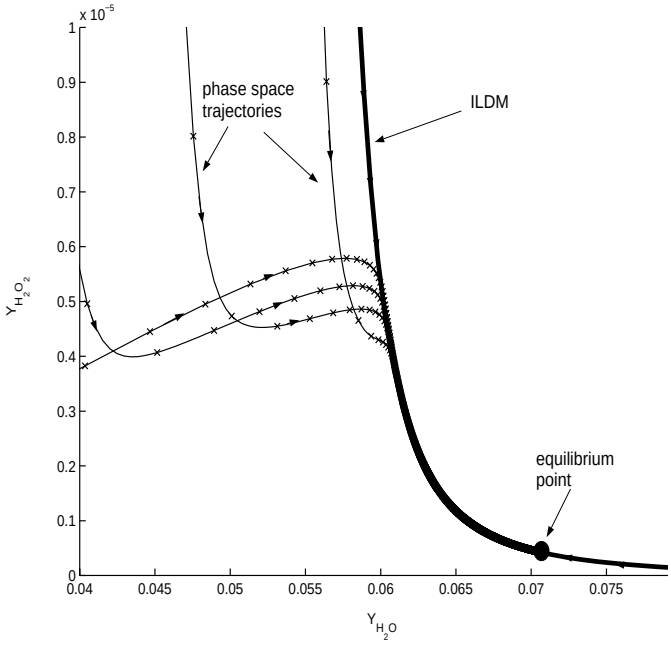
- Letting the fast time scale events equilibrate defines the manifold:

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

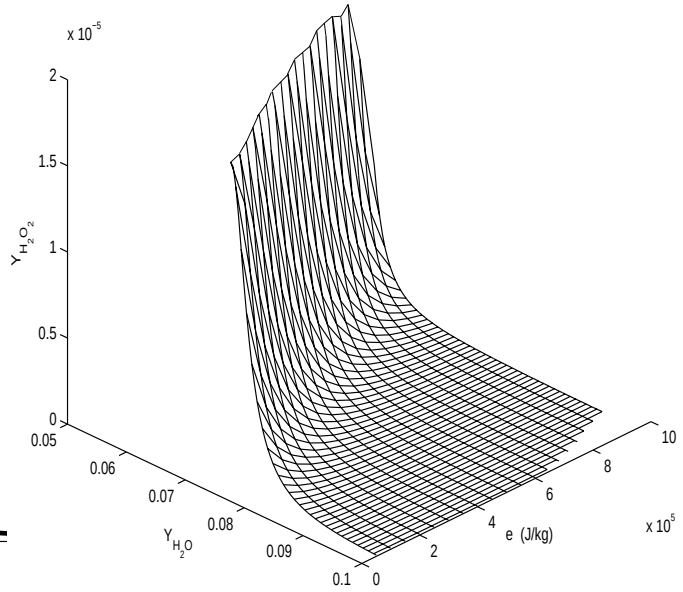
Sample ILDM for $H_2/O_2/Ar$

- Based on $N = 9$, $J = 37$ mechanism of Maas and Warnatz,
- Projection in Y_{H_2O}, $Y_{H_2O_2}$ plane and Y_{H_2O}, $Y_{H_2O_2}$, e space
- Adiabatic ($e = 8 \times 10^5\ J/kg$), isochoric ($\rho = 5.0 \times 10^{-4}\ kg/m^3$), $y_H = 0.01277$, $y_O = 0.10137$, $y_{Ar} = 0.88586$,
- We can get 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.

2-D projection

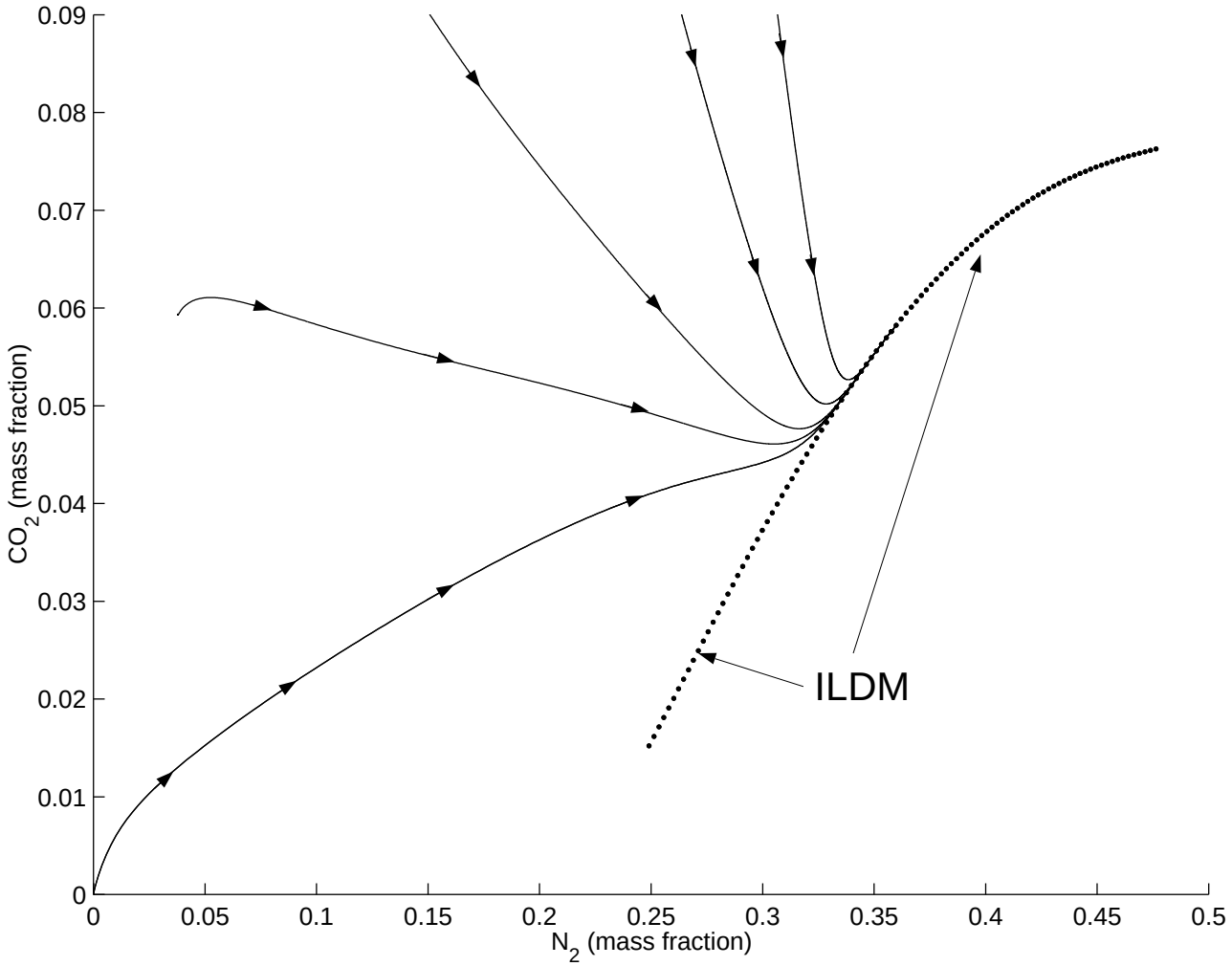


3-D projection



Sample 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 of ILDM in Y_{N_2}, Y_{CO_2} plane,
- Solution trajectories relax to ILDM on fast time scale.



Wavelet Adaptive Multilevel Representation (WAMR) Technique

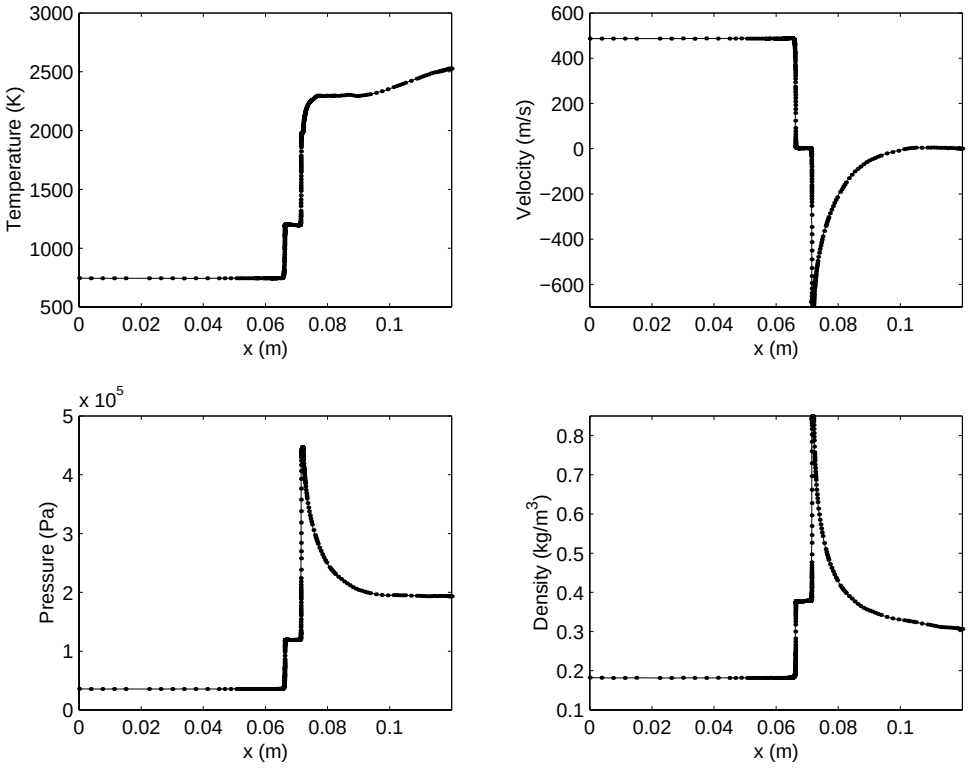
- Summary of standard spatial discretization techniques
  - Finite difference-good spatial localization, poor spectral localization, and slow convergence,
  - Finite element- good spatial localization, poor spectral localization, and slow convergence,
  - Spectral–good spectral localization, poor spatial 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,
  - 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.

Ignition Delay in Premixed $H_2/O_2/Ar$

- 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.

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

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



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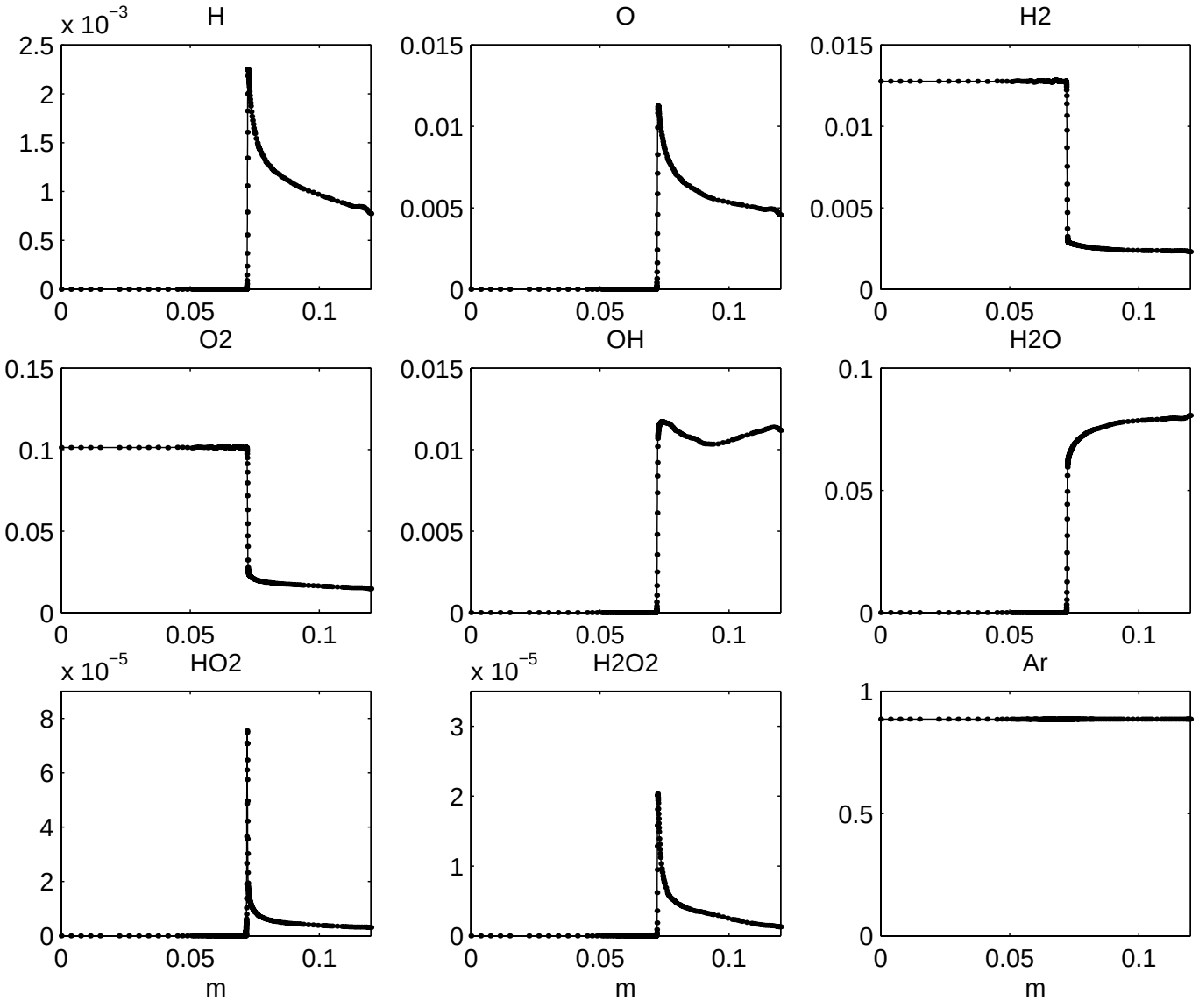
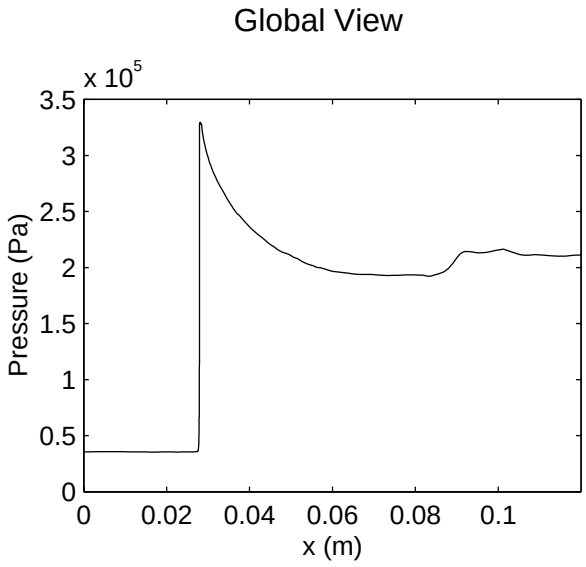
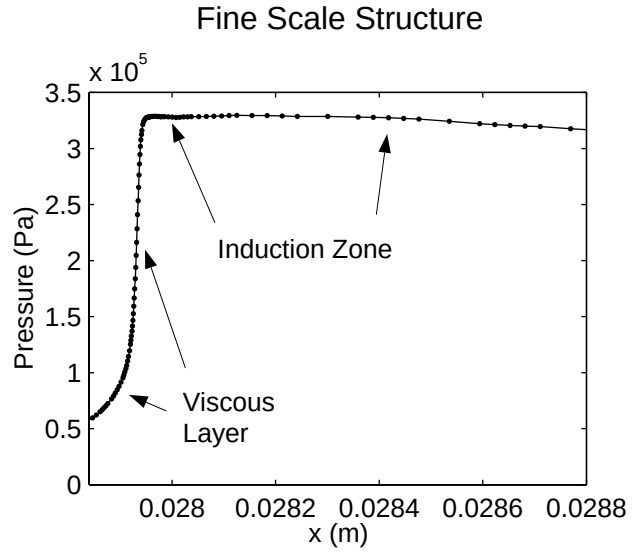


Viscous $H_2 - O_2$ Ignition Delay with Wavelets

Global and Fine Scale Structures

- $t = 230\ \mu s$, Induction zone length: $\sim 470\ \mu m$, Viscous shock thickness: $\sim 50\ \mu m$ (should use smaller μ),
- No significant reaction in viscous shock zone.

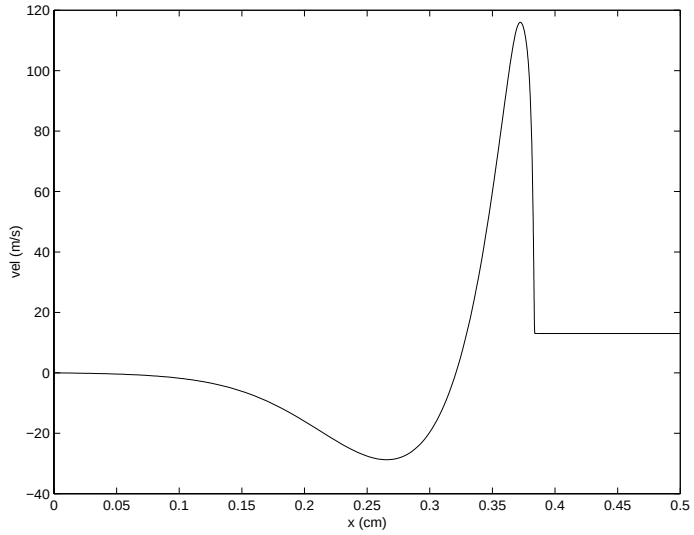


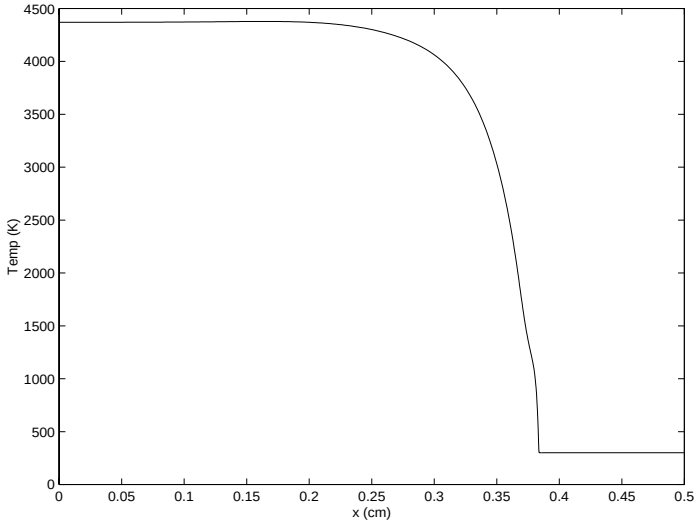


Preliminary HMX calculations with Convection Diffusion

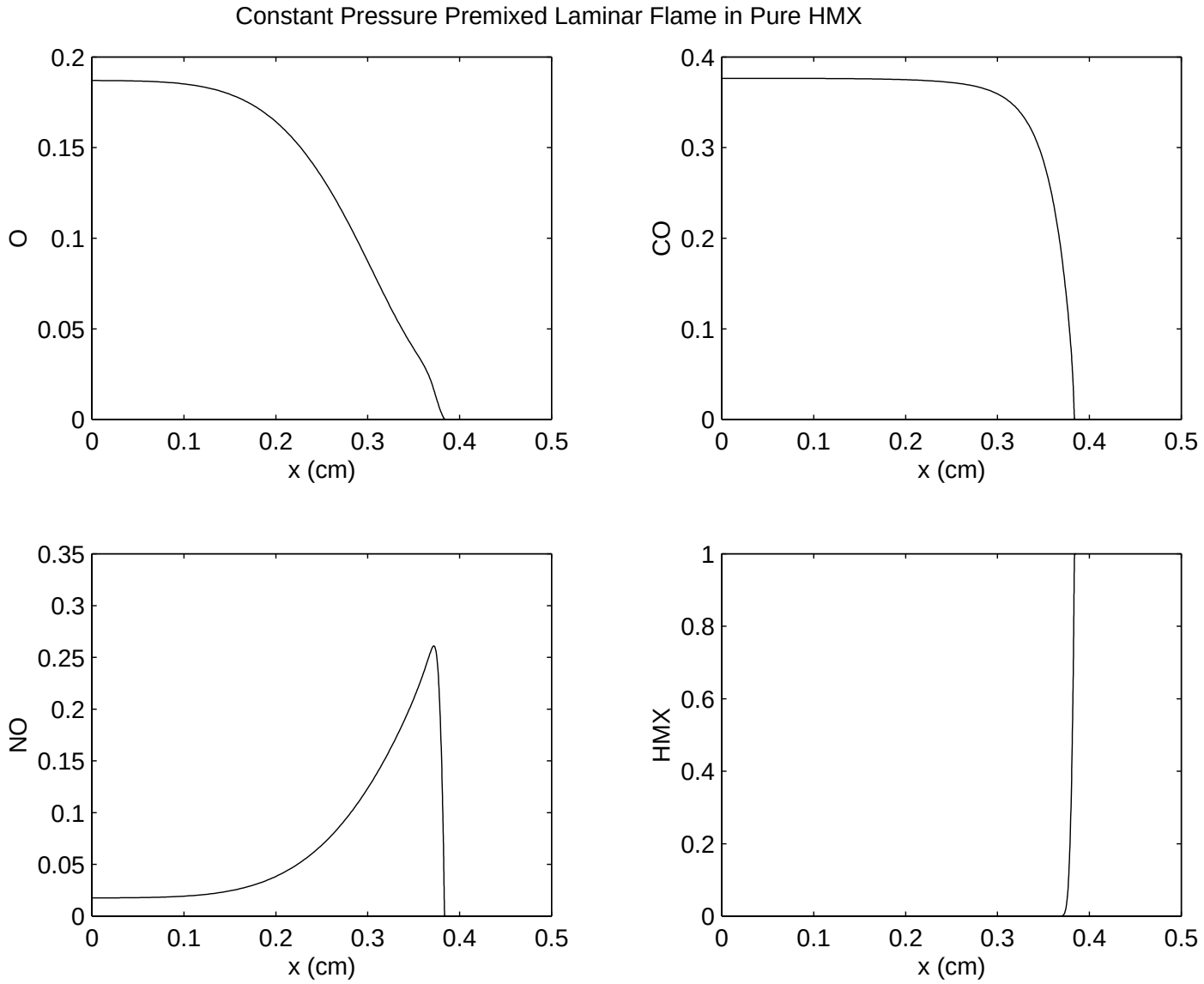
- Manifold methods not yet implemented,
- We consider constant pressure (0.75 atm) flame propagation into pure HMX pyrolysis product gas,
- This preliminary problem has invariant element concentration to facilitate construction of low-dimensional ILDM.
- Fundamental length scales dictated by flame speed which balances effects of reaction and diffusion,
- Range of intrinsic length scales are severe for HMX flames: sub-nanometer to millimeter
- Typical geometric length scales of devices may be meters
- Preliminary calculations done on very small geometric domain with uniform grid (250 cells, and not all scales are resolved),
- Explicit convection diffusion step and implicit reaction step
- *For full problem, adaptive technique required with current computational resources.*

Premixed laminar flame in gas phase HMX: temperature and velocity

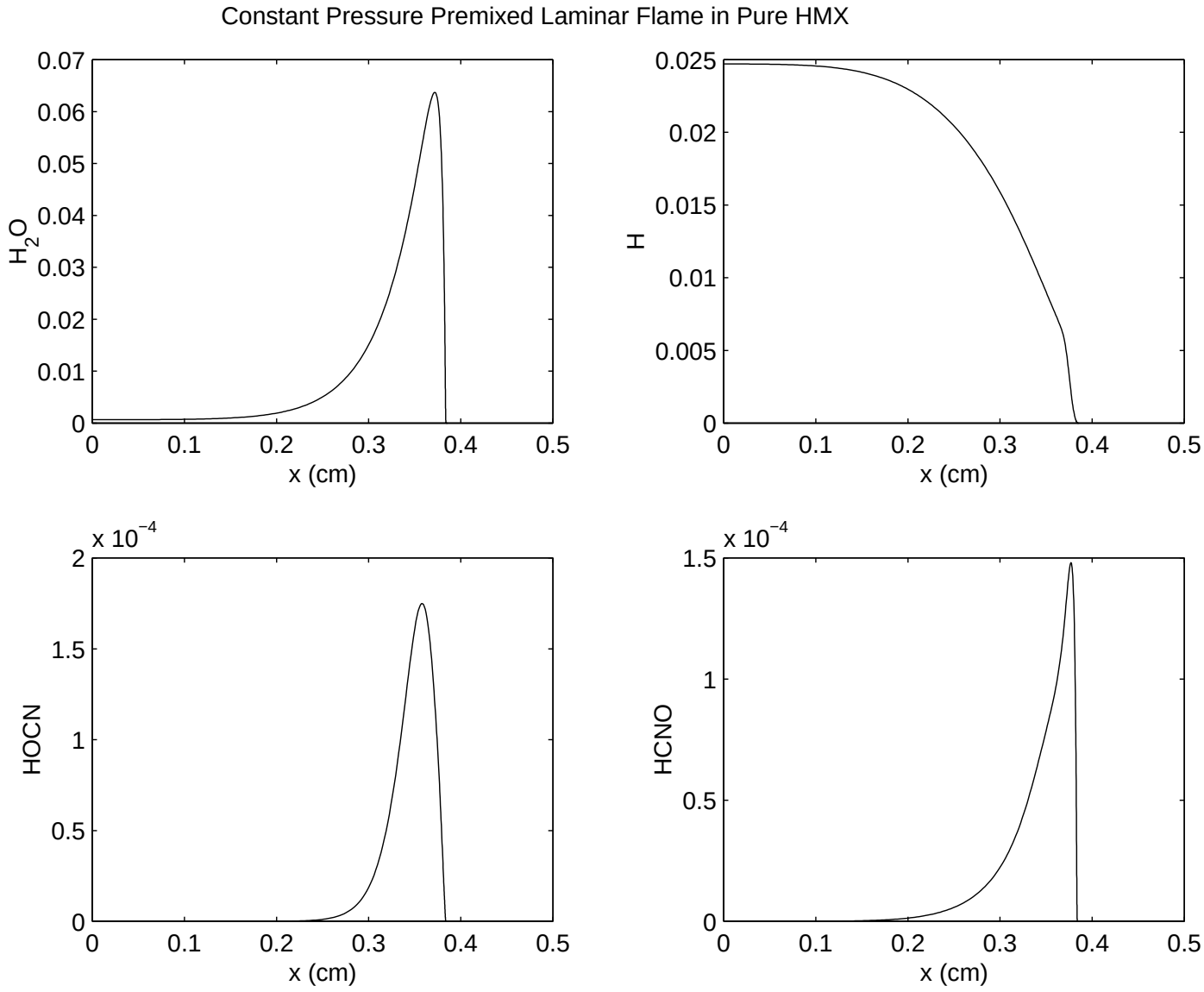




Premixed laminar flame in gas phase HMX: major species



Premixed laminar flame in gas phase HMX: minor species



Conclusions

- Given present computational resources, accurate solution for HMX gas phase chemistry with detailed kinetics will require some means to reduce chemical stiffness as well as an adaptive multilevel scheme for spatial resolution.
- A high dimension ILDM (at least $K = 6$) coupled with a WAMR technque is a promising candidate.
- Such schemes have been demonstrated on simpler systems and are currently being applied to HMX.