An Eigenvalue-Based Estimate of Reaction Zone Thicknesses in Gas Phase Detonations

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30th International Symposium on Combustion
Chicago, Illinois

30 July 2004

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Motivation

- Detailed kinetics models are widely used in detonation simulations.
- The finest length scale predicted by such models is usually not clarified and often not resolved.
- Tuning computational results to match experiments without first harmonizing with underlying mathematics renders predictions unreliable.

Model: Reactive Euler Equations

- one-dimensional
- steady
- inviscid
- detailed Arrhenius kinetics
- calorically imperfect ideal gas mixture

Model: Reactive Euler Equations

$$
\begin{aligned}
\rho u &= \rho_o D, \\
\rho u^2 + p &= \rho_o D^2 + p_o, \\
e + \frac{u^2}{2} + \frac{p}{\rho} &= e_o + \frac{D^2}{2} + \frac{p_o}{\rho_o}, \\
\frac{dY_i}{dx} &= f_i \equiv \frac{\dot{\omega}_i M_i}{\rho_o D}.
\end{aligned}
$$

Supplemented by state equations and the law of mass action.

Reduced Model

Algebraic reductions lead to a final form of

$$\frac{dY_i}{dx} = f_i(Y_1, \ldots, Y_{N-L})$$

with

- N: number of molecular species
- L: number of atomic elements

Eigenvalue Analysis of Local Length Scales

Local behavior is modelled by

$$\frac{d\mathbf{Y}}{dx} = \mathbf{J} \cdot (\mathbf{Y} - \mathbf{Y}^*) + \mathbf{b}, \qquad \mathbf{Y}(x^*) = \mathbf{Y}^*,$$

whose solution has the form

$$\mathbf{Y}(x) = \mathbf{Y}^* + \left(\mathbf{P} \cdot e^{\mathbf{\Lambda}(x - x^*)} \cdot \mathbf{P}^{-1} - \mathbf{I} \right) \cdot \mathbf{J}^{-1} \cdot \mathbf{b}.$$

Here $\mathbf{\Lambda}$ has eigenvalues λ_i of Jacobian $\mathbf{J}$ in its diagonal.

The length scales are given by

$$\ell_i(x) = \frac{1}{|\lambda_i(x)|}.$$

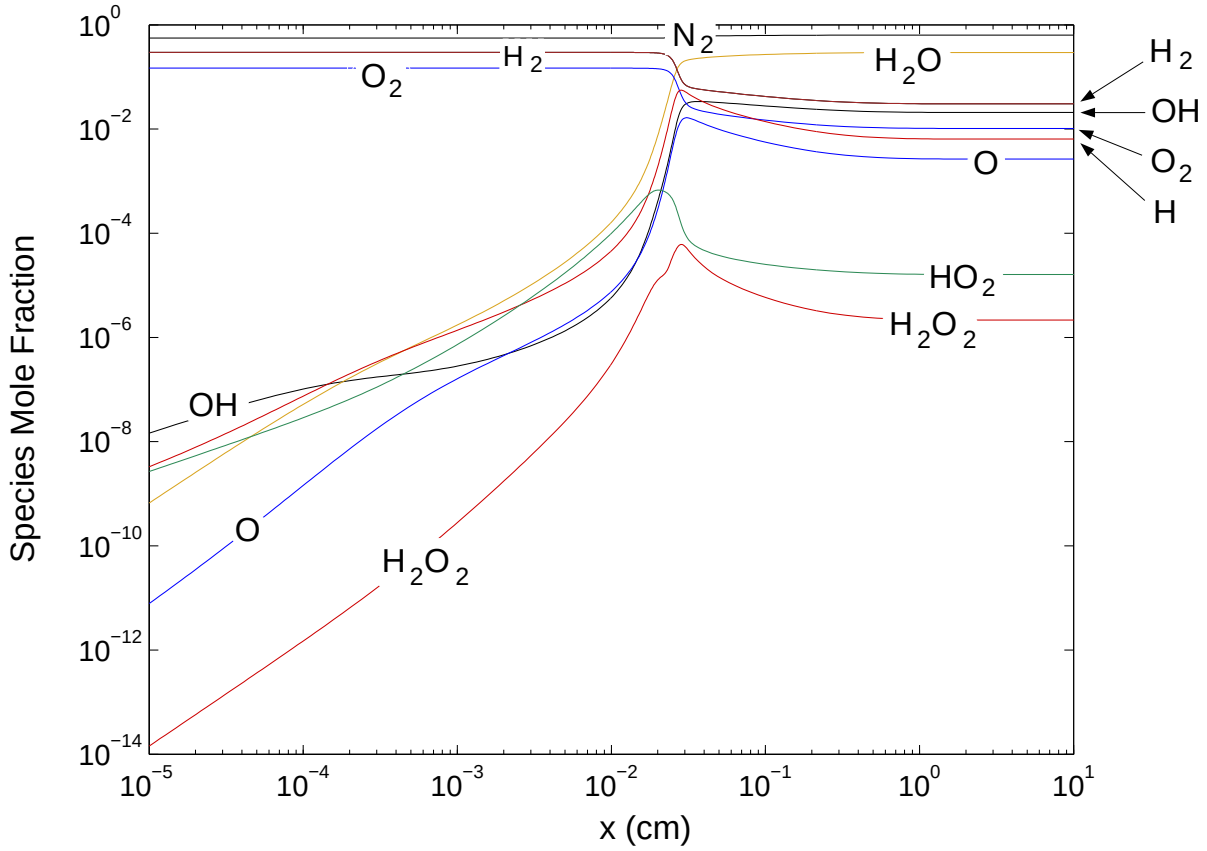
Computational Methods

- A standard ODE solver (DLSODE) was used to integrate the equations.
- Standard IMSL subroutines were used to evaluate the local Jacobians and eigenvalues at every step.
- The Chemkin software package was used to evaluate kinetic rates and thermodynamic properties.
- Computation time was typically two minutes on a $900\ MHz$ Sun Blade 1000.

Physical System

- Hydrogen-air detonation: $2H_2 + O_2 + 3.76N_2$.
- $N = 9$ molecular species, $L = 3$ atomic elements, $J = 19$ reversible reactions.
- $p_o = 1\ atm$.
- $T_o = 298\ K$.
- Identical to system studied by both Shepherd (1986) and Mikolaitis (1987).

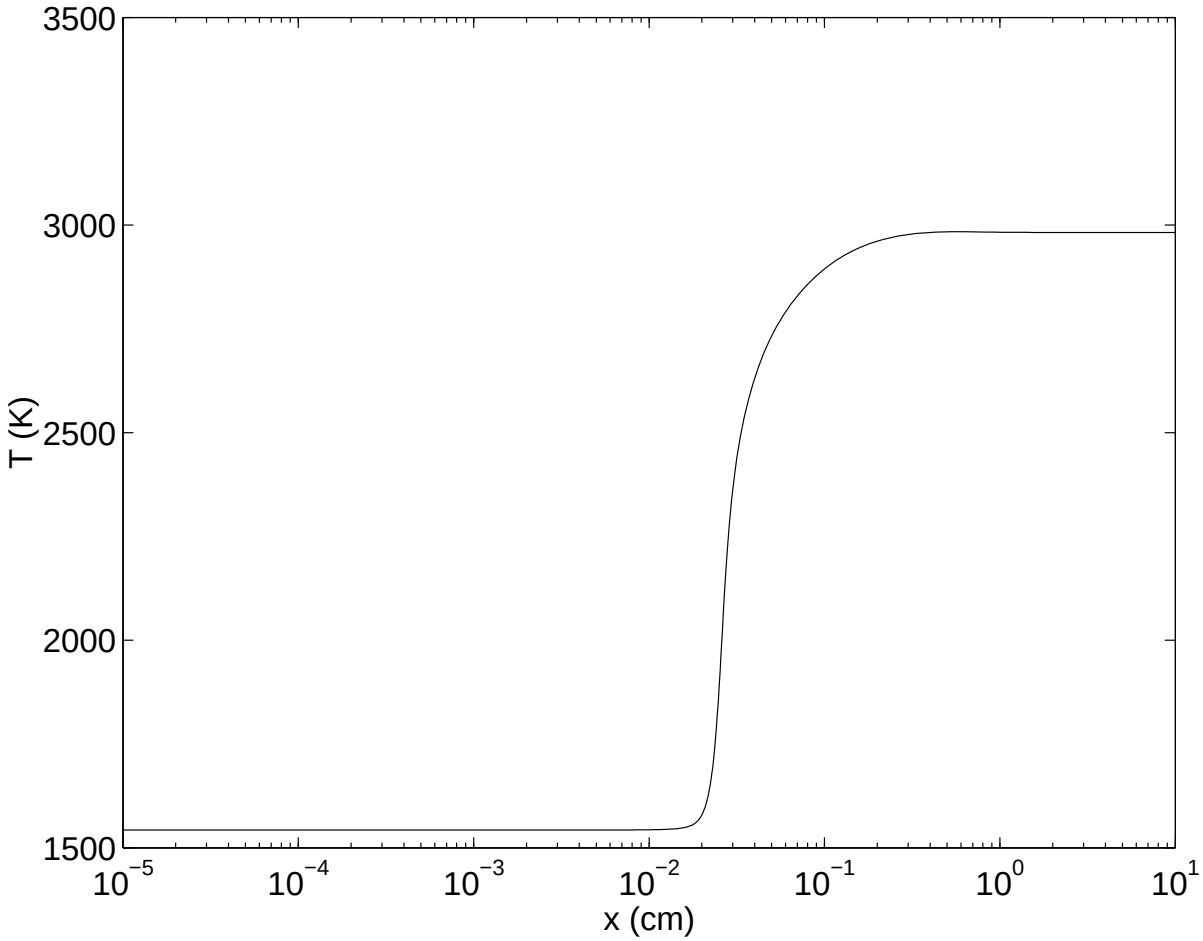
Mole Fractions versus Distance



- significant evolution at fine length scales

  $x < 10^{-3}\, cm.$

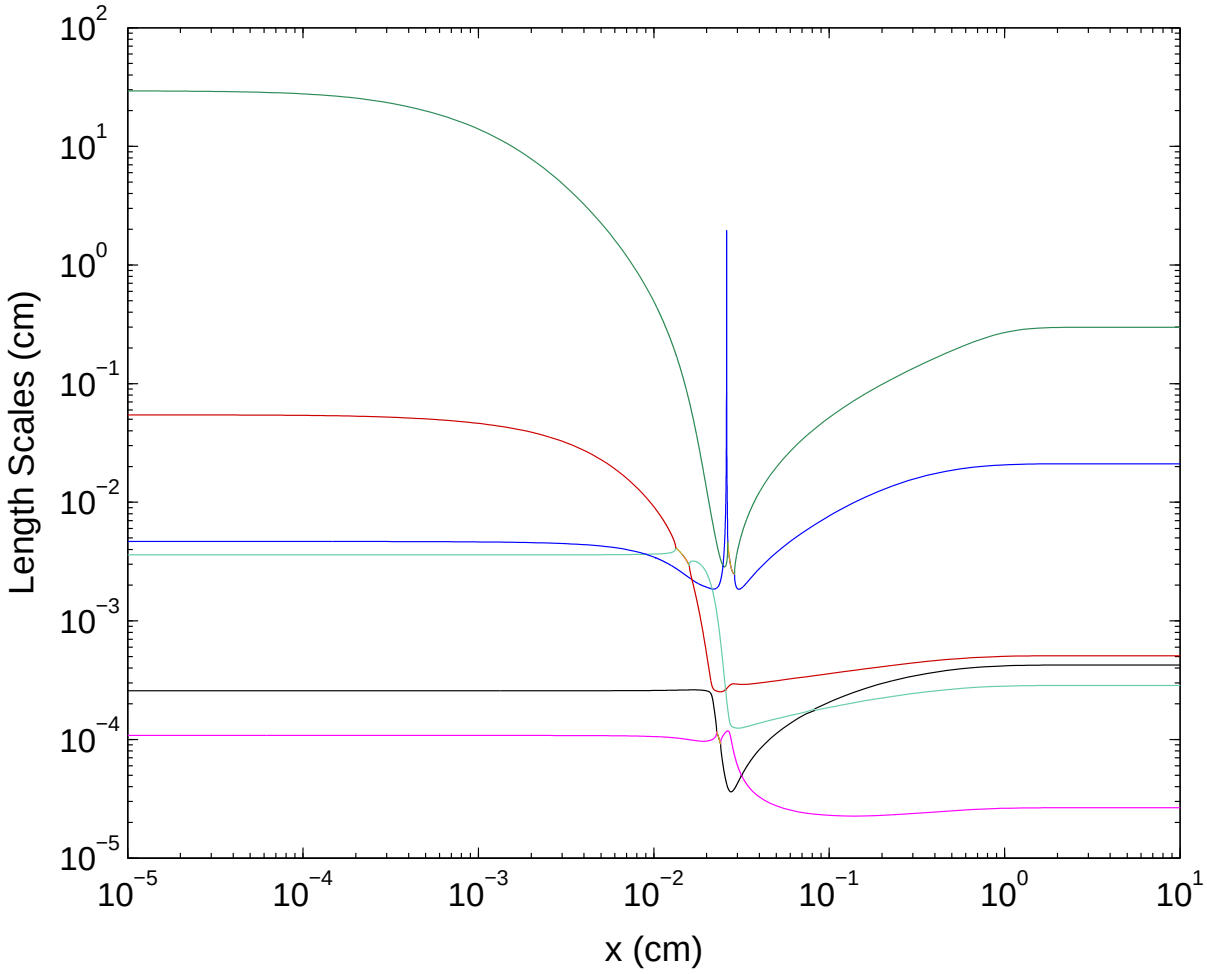
Temperature Profile



- Temperature flat in the post-shock induction zone $0 < x < 2.6 \times 10^{-2}\, cm$.

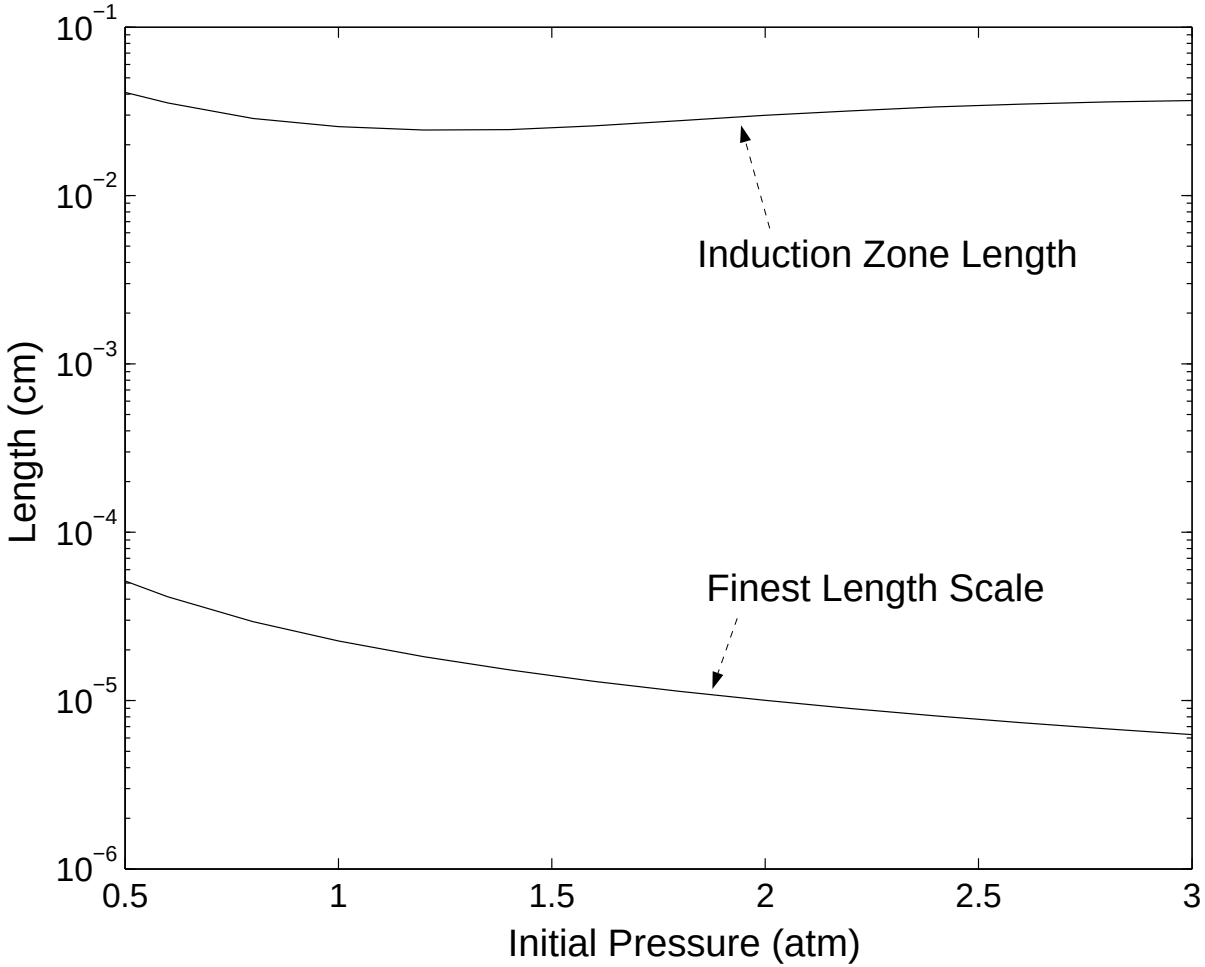
- Thermal explosion followed by relaxation to

Eigenvalue Analysis: Length Scale Evolution



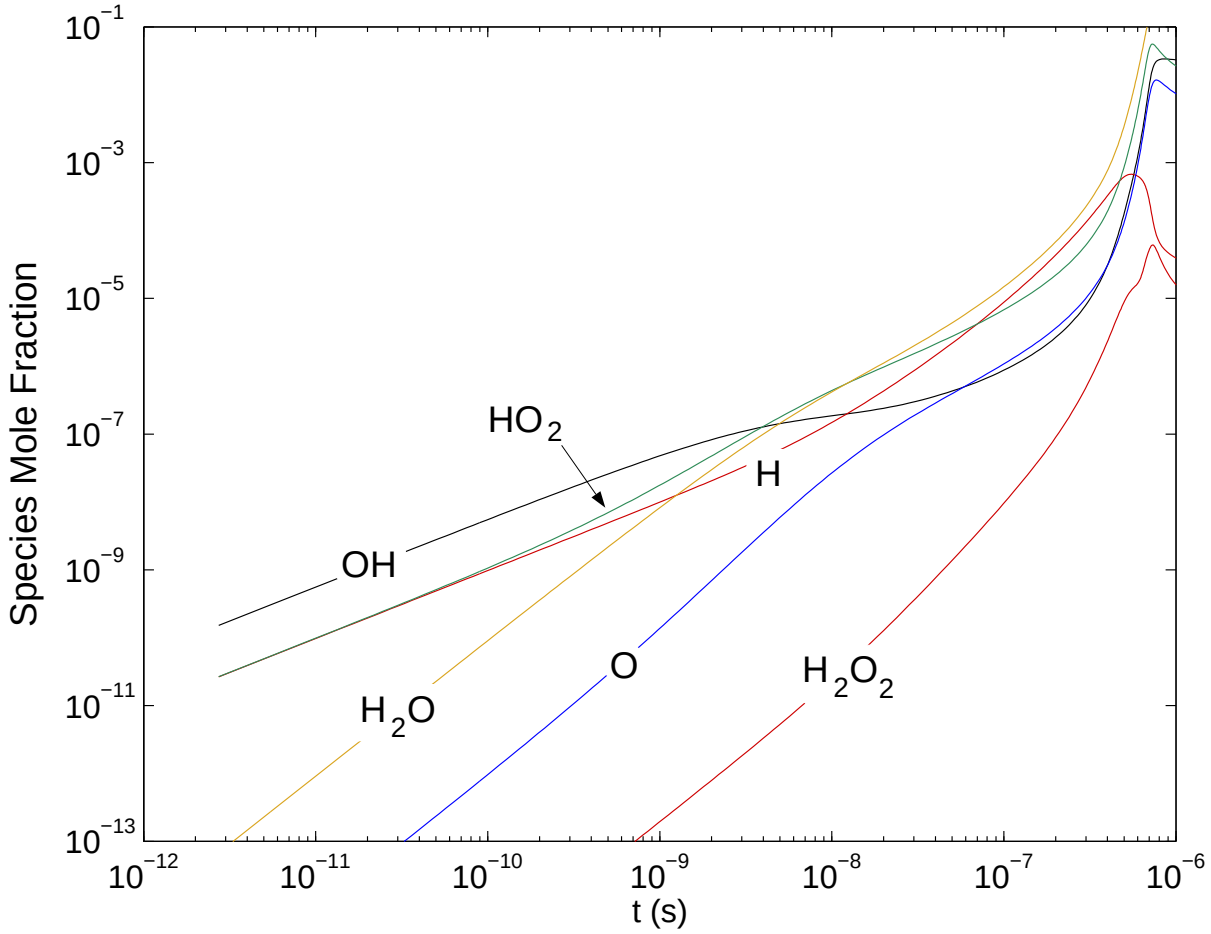
- Finest length scale: $2.3 \times 10^{-5}\ cm$.
- Coarsest length scale $3.0 \times 10^{1}\ cm$.

Influence of Initial Pressure



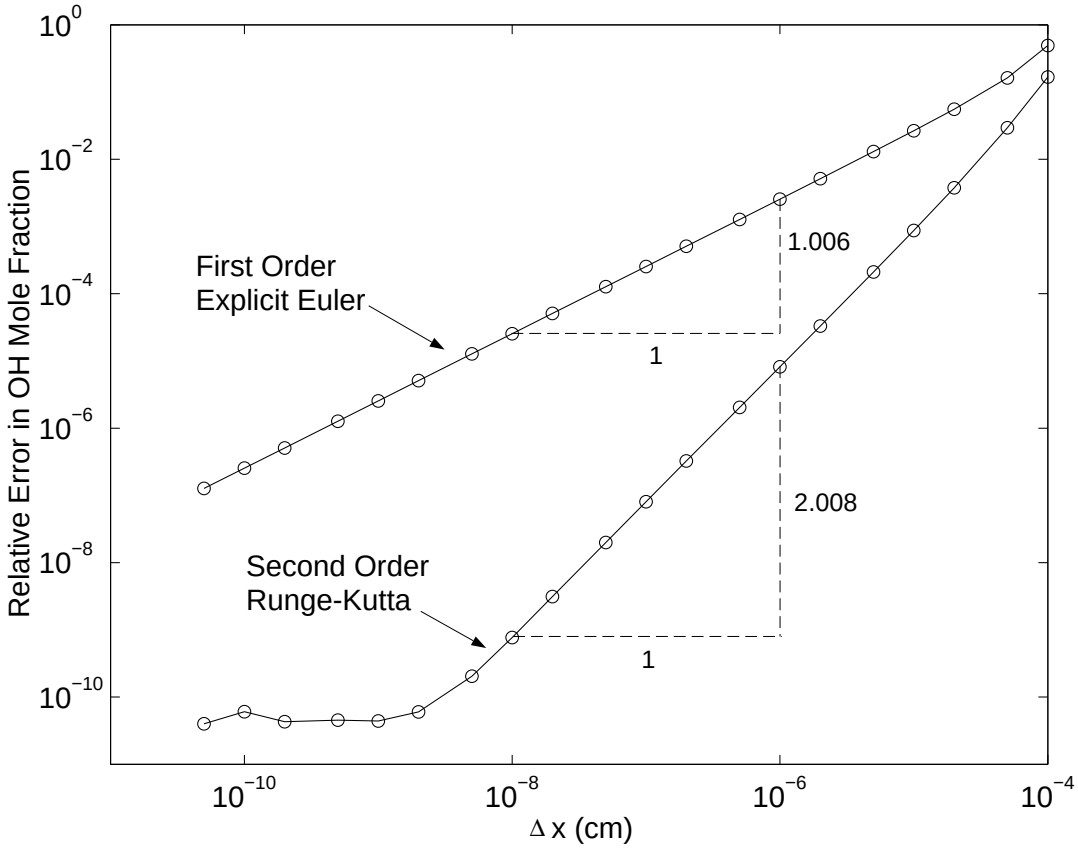
- Induction zone length and finest length scale are sensitive to initial pressure.
- Finest length scale three orders of magnitude

Verification: Comparison with Mikolaitis



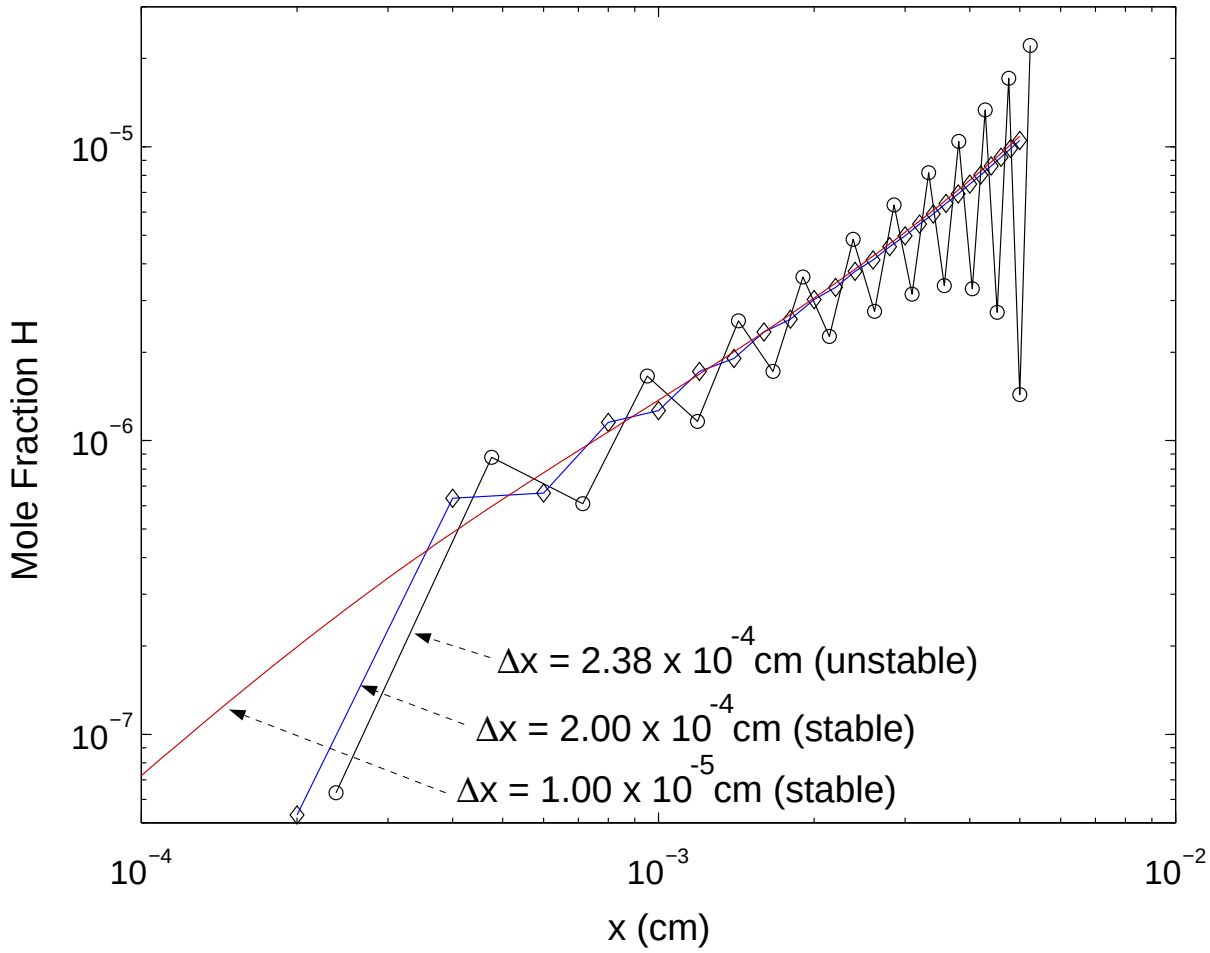
- Lagrangian calculation allows direct comparison with Mikolaitis' results.

Grid Convergence



- Finest length scale must be resolved to converge at proper order.
- Results are converging at proper order for first

Numerical Stability



- Discretizations finer than finest physical length scale are numerically stable.
- Discretizations coarser than finest physical

Examination of Recently Published Results

Ref.	$\ell_{ind}\ (cm)$	$\ell_f\ (cm)$	$\Delta x\ (cm)$
Oran, *et al*, 1998	1.47×10^{-1}	2.17×10^{-4}	3.88×10^{-3}
Shepherd, *et al.*, 2003	1.46×10^{-1}	2.16×10^{-4}	AMR
Hayashi, *et al.*, 2002	1.50×10^{-2}	1.23×10^{-5}	5.00×10^{-4}
Powers, *et al.*, 2001	1.54×10^{-2}	2.76×10^{-5}	8.14×10^{-5}
Fedkiw, *et al.*, 1997	1.54×10^{-2}	2.76×10^{-5}	3.00×10^{-2}
Ebrahimi and Merkle, 2002	5.30×10^{-3}	7.48×10^{-6}	1.00×10^{-2}
Sislian, *et al.*, 1998	1.38×10^{-1}	2.23×10^{-4}	1.00×10^{0}

All are under-resolved, some severely.

Conclusions

- Detonation calculations are often under-resolved, by as much as four orders of magnitude.
- Equilibrium properties are insensitive to resolution, while transient phenomena can be sensitive.
- Sensitivity of results to resolution is not known *a priori*.
- Numerical viscosity stabilizes instabilities.
- For a repeatable scientific calculation of detonation, the finest physical scales must be resolved.

Moral

You either do detailed kinetics with the proper resolution,

or

you are fooling yourself and others, in which case you should stick with reduced kinetics!