Simulations Using Detailed Kinetics

Demand Proper Resolution

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Sixth International Conference on Chemical Kinetics
Gaithersburg, Maryland
26 July 2005

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Chemical Kinetics and Aerospace Engineering?

"It is known that numerical solutions of conservation laws with stiff source terms may be erroneous...These purely numerical problems are caused by the smearing effect of the conservation law solver...This can produce totally nonphysical solutions... Using a sufficiently fine mesh it is always possible to avoid nonphysical solutions....a sufficient spatial resolution is as important as a temporal resolution."

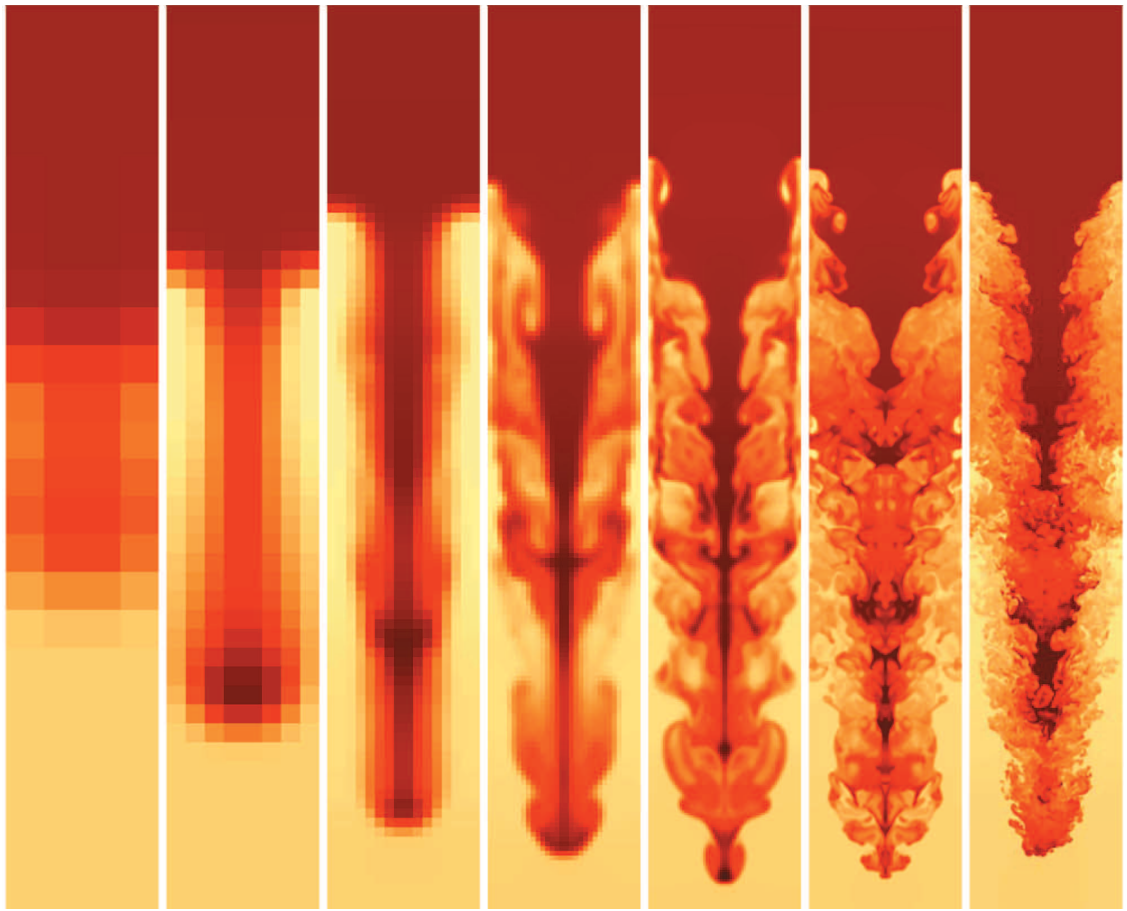
Randall LeVeque, University of Washington, *SIAM Journal of Scientific Computing*, 2000.

"...the flow is extremely complex and quite sensitively dependent on the computational resolution...The take-home message is that resolution matters..."

Leo Kadanoff, University of Chicago, on results obtained in DOE Accelerated Supercomputing Initiative (ASCI), *Computing in Science and Engineering*, 2004.

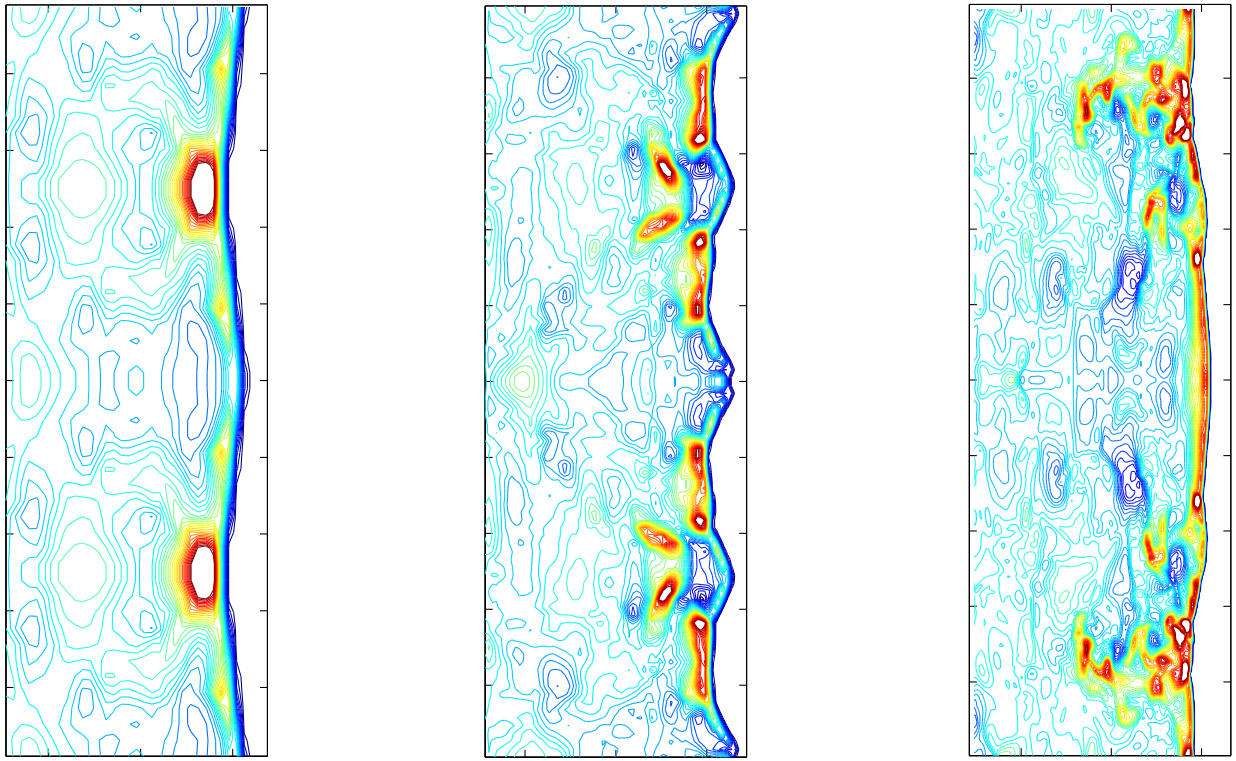
“Resolution Matters” in Fluid Mechanics:

Kadanoff (2004)

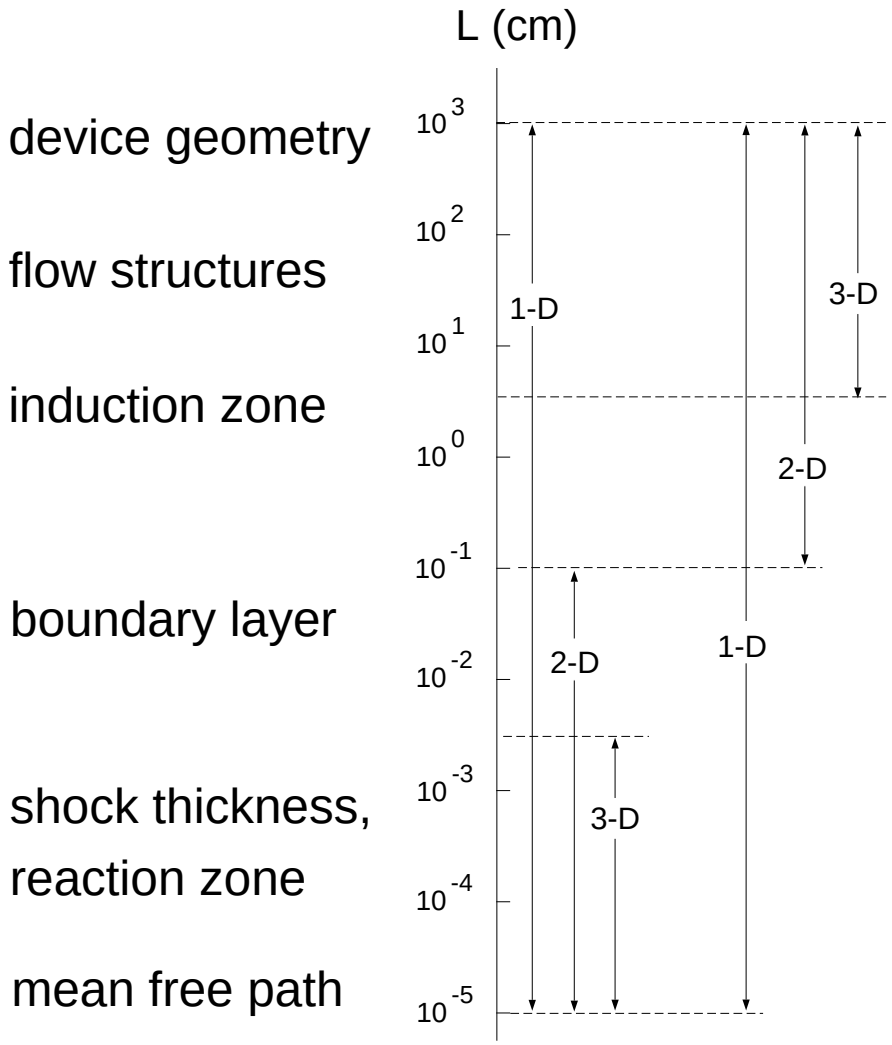


”Resolution Matters” in Combustion:

Singh, Powers, Paolucci (1999)



Estimate of Present Computational Capability



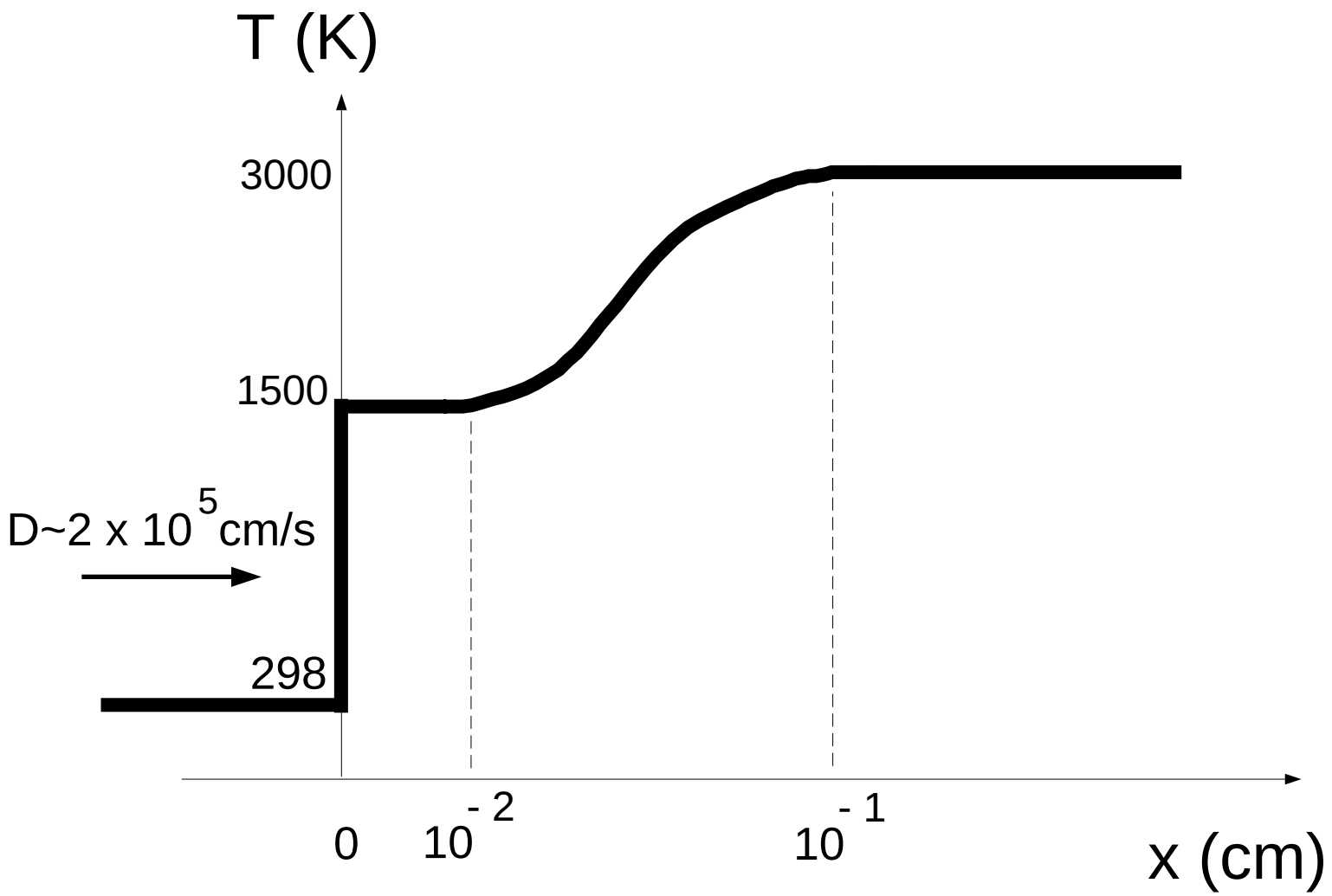
Motivation

- Detailed kinetics are widely used in reactive flow.
- Applications exist for propulsion, combustion, atmospheric chemistry, chemical vapor deposition, etc.
- The finest length scale predicted by such models is usually neither clarified nor resolved.
- Tuning computational results to match experiments without first harmonizing with underlying mathematics renders predictions unreliable.

Literature Review: $H_2/O_2/N_2$ Detonation

- Westbrook, *Combust. Sci. Tech.*, 1982.
- Shepherd, *Dynamics of Explosions*, 1986.
- Mikolaitis, *Combust. Sci. Tech.*, 1987.
- Oran, *et al.*, *Combust. Flame*, 1998.
- Paolucci, *et al. Combust. Theory Model.*, 2001.
- Hayashi, *et al.*, *Proc. Combust. Institute*, 2002.
- Law, *et al.*, *J. Propul. Power*, 2003.
- Powers and Paolucci, *AIAA J.*, 2005.

Schematic of Steady Detonation



Model: Reactive Euler Equations

- convection and reaction; no diffusion
- 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 EOS and 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 modeled by

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

whose solution is

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

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

Length scales 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.

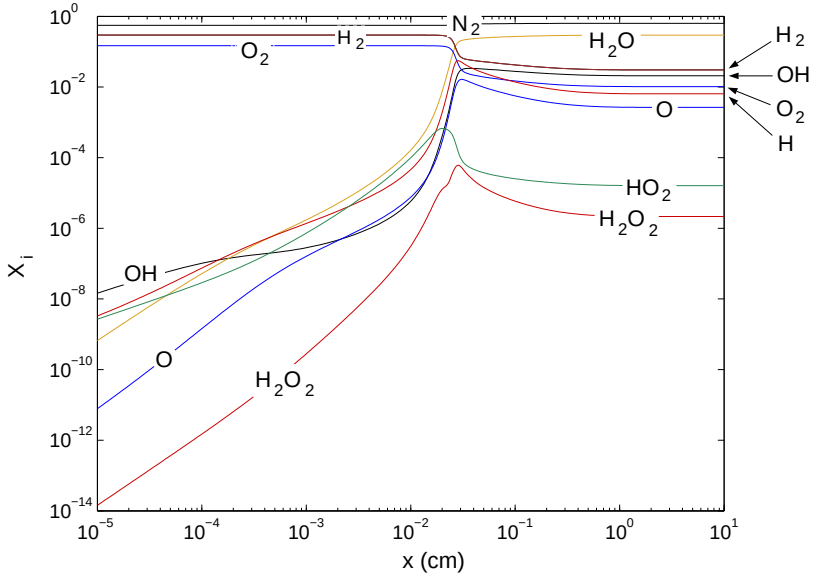
Physical System

- 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 Shepherd (1986).

Detailed Kinetics Model

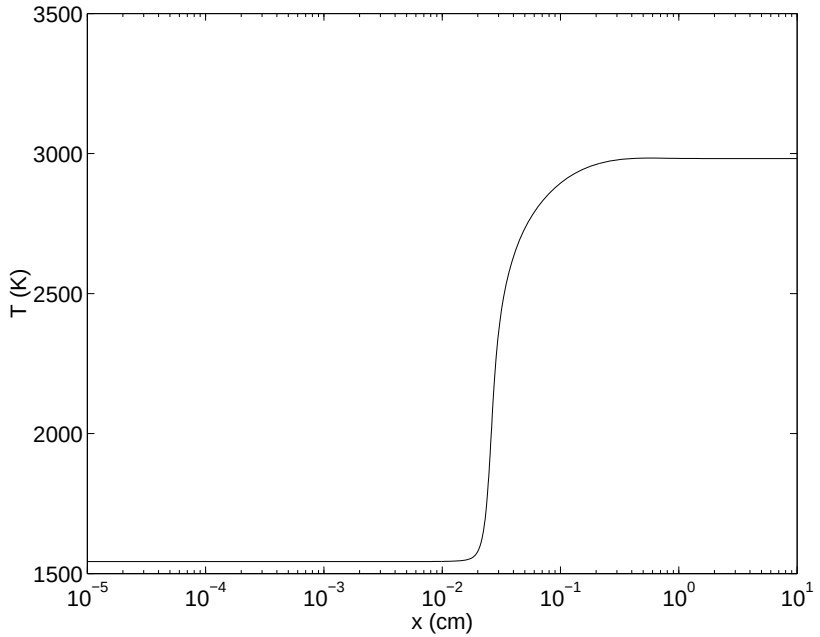
j	Reaction	A_j	β_j	E_j
1	$H_2 + O_2 \rightleftharpoons OH + OH$	1.70×10^{13}	0.00	47780
2	$OH + H_2 \rightleftharpoons H_2O + H$	1.17×10^{9}	1.30	3626
3	$H + O_2 \rightleftharpoons OH + O$	5.13×10^{16}	-0.82	16507
4	$O + H_2 \rightleftharpoons OH + H$	1.80×10^{10}	1.00	8826
5	$H + O_2 + M \rightleftharpoons HO_2 + M$	2.10×10^{18}	-1.00	0
6	$H + O_2 + O_2 \rightleftharpoons HO_2 + O_2$	6.70×10^{19}	-1.42	0
7	$H + O_2 + N_2 \rightleftharpoons HO_2 + N_2$	6.70×10^{19}	-1.42	0
8	$OH + HO_2 \rightleftharpoons H_2O + O_2$	5.00×10^{13}	0.00	1000
9	$H + HO_2 \rightleftharpoons OH + OH$	2.50×10^{14}	0.00	1900
10	$O + HO_2 \rightleftharpoons O_2 + OH$	4.80×10^{13}	0.00	1000
11	$OH + OH \rightleftharpoons O + H_2O$	6.00×10^{8}	1.30	0
12	$H_2 + M \rightleftharpoons H + H + M$	2.23×10^{12}	0.50	92600
13	$O_2 + M \rightleftharpoons O + O + M$	1.85×10^{11}	0.50	95560
14	$H + OH + M \rightleftharpoons H_2O + M$	7.50×10^{23}	-2.60	0
15	$H + HO_2 \rightleftharpoons H_2 + O_2$	2.50×10^{13}	0.00	700
16	$HO_2 + HO_2 \rightleftharpoons H_2O_2 + O_2$	2.00×10^{12}	0.00	0
17	$H_2O_2 + M \rightleftharpoons OH + OH + M$	1.30×10^{17}	0.00	45500
18	$H_2O_2 + H \rightleftharpoons HO_2 + H_2$	1.60×10^{12}	0.00	3800
19	$H_2O_2 + OH \rightleftharpoons H_2O + HO_2$	1.00×10^{13}	0.00	1800

Mole Fractions versus Distance



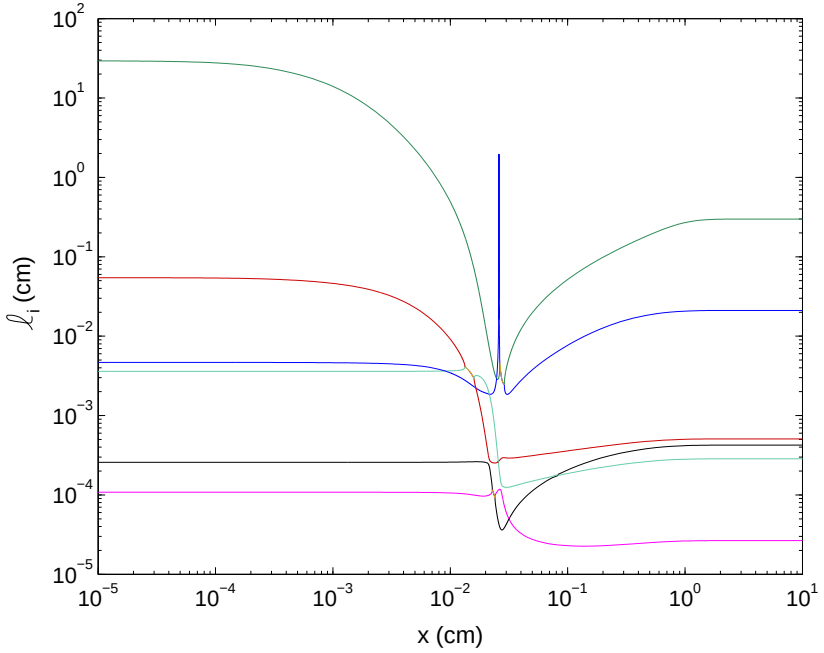
- significant evolution at fine length scales $x < 10^{-3}\ cm$.
- results agree with those of Shepherd.

Temperature Profile



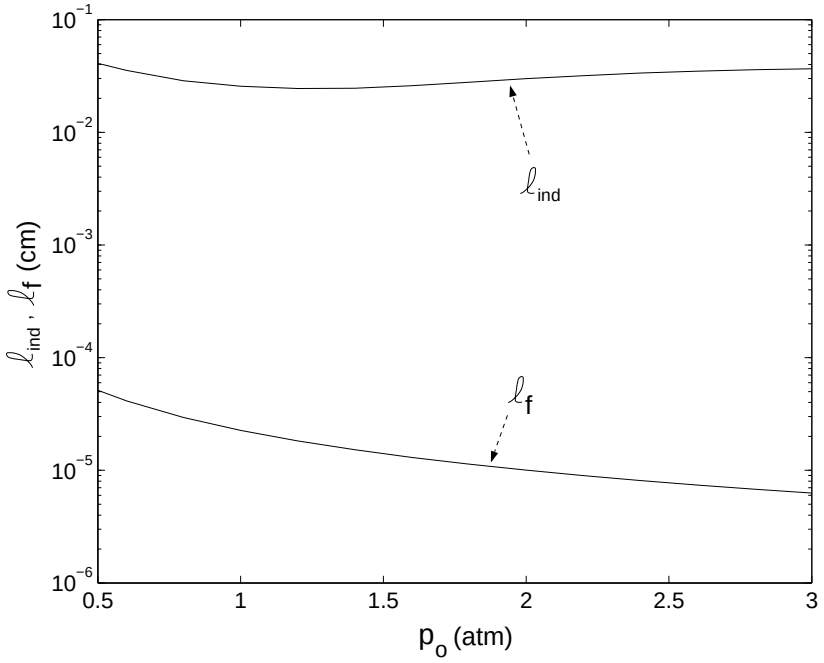
- Temperature flat in the post-shock induction zone $0 < x < 2.6 \times 10^{-2}\ cm$.
- Thermal explosion followed by relaxation to equilibrium at $x \sim 10^{0}\ cm$.

Eigenvalue Analysis: Length Scale Evolution



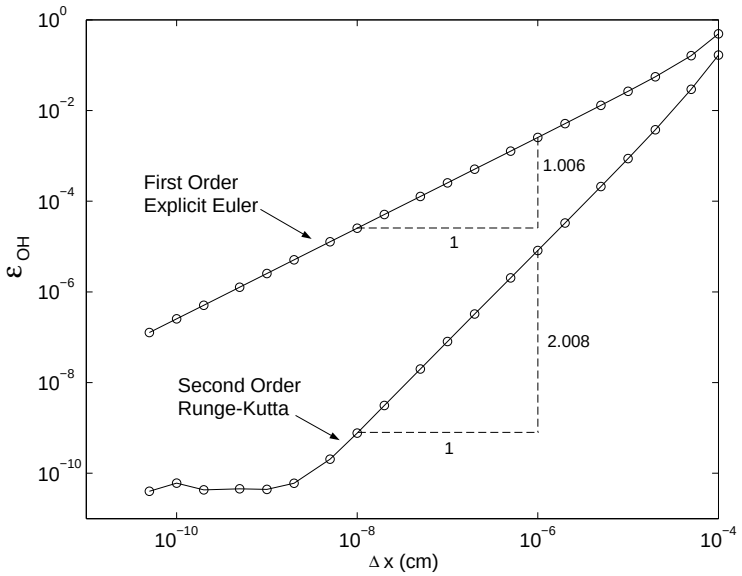
- Finest length scale: $2.3 \times 10^{-5}\ cm$.
- Coarsest length scale $3.0 \times 10^{1}\ cm$.
- Finest length scale similar to that necessary for numerical stability of ODE solver.

Influence of Initial Pressure



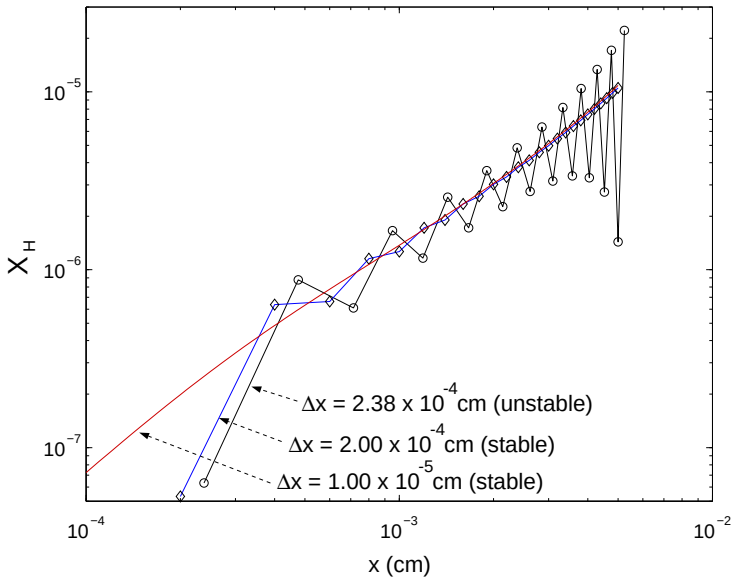
- Induction zone length and finest length scale are sensitive to initial pressure.
- Finest length scale three orders of magnitude smaller than induction zone length.

Grid Convergence



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

Numerical Stability



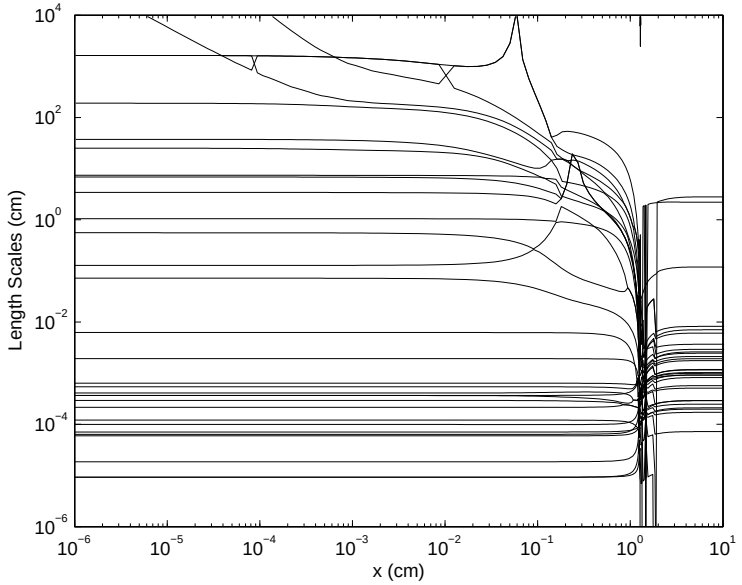
- Discretizations finer than finest physical length scale are numerically stable.
- Discretizations coarser than finest physical length scale are numerically unstable.

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}
Jameson, *et al.*, 1998	2.35×10^{-2}	4.74×10^{-5}	3.20×10^{-3}
Hayashi, *et al.*, 2002	1.50×10^{-2}	1.23×10^{-5}	5.00×10^{-4}
Hu, *et al.*, 2004	1.47×10^{-1}	2.17×10^{-4}	2.50×10^{-3}
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}
Jeung, *et al.*, 1998	1.80×10^{-2}	5.61×10^{-7}	5.94×10^{-2}

All are under-resolved, some severely.

Methane-Air Detonation with GRI 3.0



- 53 species, 219 reactions
- Results similar to H_2-air, but more length scales
- Induction zone around $10^0\ cm$
- Finest scale around $10^{-5}\ cm$

Conclusions

- Detonation calculations are often under-resolved, by as much as five 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 artificially stabilizes instabilities.
- For a repeatable scientific calculation of detonation, the finest physical scales must be resolved.