High Accuracy Shock-Fitted Computation of Unsteady Detonation with Detailed Kinetics

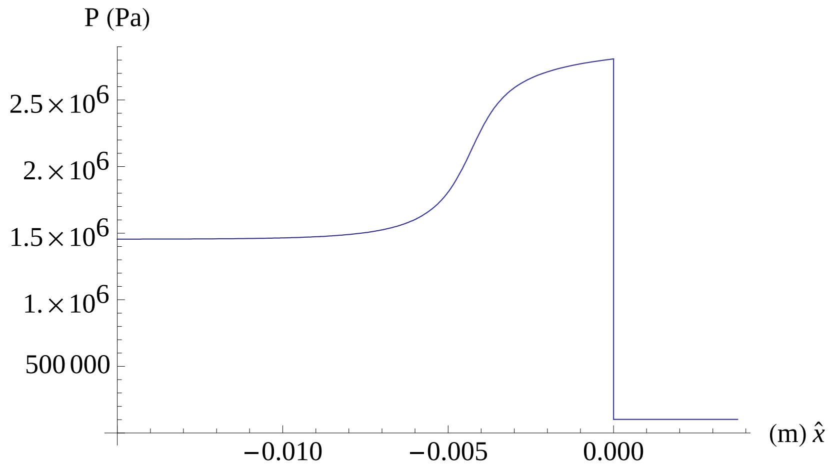
Tariq D. Aslam (aslam@lanl.gov)
Los Alamos National Laboratory; Los Alamos, NM
Joseph M. Powers (powers@nd.edu)
University of Notre Dame; Notre Dame, IN

10^{th} US National Congress on Computational Mechanics
Columbus, Ohio
18 July 2009

Outline

- Gas phase detonation introduction
- Length scale requirements from steady traveling wave solutions for H_2-air (review)
- Unsteady dynamics of ozone detonation

Fundamentals of Detonation



- *Detonation*: shock-induced combustion process
- *applications*: aerospace propulsion, safety, military, internal combustion engines, etc.

Length and Time Scale Discussion

Simplistic linear advection-reaction model:

$$\underbrace{\frac{\partial \psi}{\partial t}}_{\text{evolution}} + \underbrace{u_o \frac{\partial \psi}{\partial x}}_{\text{advection}} = \underbrace{-k\psi}_{\text{reaction}}$$

$$\frac{d\psi}{dt} = -k\psi : \qquad \text{time scale} \qquad \tau = \frac{1}{k}$$

$$u_o \frac{d\psi}{dx} = -k\psi : \qquad \text{length scale} \qquad \ell = \frac{u_o}{k}$$

Fast reaction (large k) induces small length and time scales.

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.
- See Powers and Paolucci, *AIAA Journal*, 2005.
- We explore the transient behavior of detonations with *fully resolved* detailed kinetics.

Verification and Validation

- *verification:* solving the equations right (math).
- *validation:* solving the right equations (physics).
- Main focus here on verification
- Some limited validation possible, but detailed validation awaits more robust measurement techniques.
- Verification and validation always necessary but never sufficient: finite uncertainty must be tolerated.

Model: Steady 1D Reactive Euler Equations

$$\rho u = \rho_o D,$$

$$\rho u^2 + p = \rho_o D^2 + p_o,$$

$$e + \frac{u^2}{2} + \frac{p}{\rho} = e_o + \frac{D^2}{2} + \frac{p_o}{\rho_o},$$

$$p = \rho \Re T \sum_{i=1}^{N} \frac{Y_i}{M_i},$$

$$e = \sum_{i=1}^{N} Y_i \left(h_{i,f}^o + \int_{T_o}^{T} c_{pi}(\hat{T})\, d\hat{T} - \frac{\Re T}{M_i} \right),$$

$$\frac{dY_i}{dx} = \frac{M_i}{\rho_o D} \sum_{j=1}^{J} \nu_{ij} A_j T^{\beta_j} e^{\left(\frac{-E_j}{\Re T}\right)} \left(\underbrace{\prod_{k=1}^{N} \left(\frac{\rho Y_k}{M_k}\right)^{\nu'_{kj}}}_{\text{forward}} - \underbrace{\frac{1}{K_j^c} \prod_{k=1}^{N} \left(\frac{\rho Y_k}{M_k}\right)^{\nu''_{kj}}}_{\text{reverse}} \right)$$

Eigenvalue Analysis of Local Length Scales

Algebraic reduction yields

$$\frac{d\mathbf{Y}}{dx} = \mathbf{f}(\mathbf{Y}).$$

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: Steady Detonation

- 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 one minute on a $1\,GHz$ HP Linux machine.

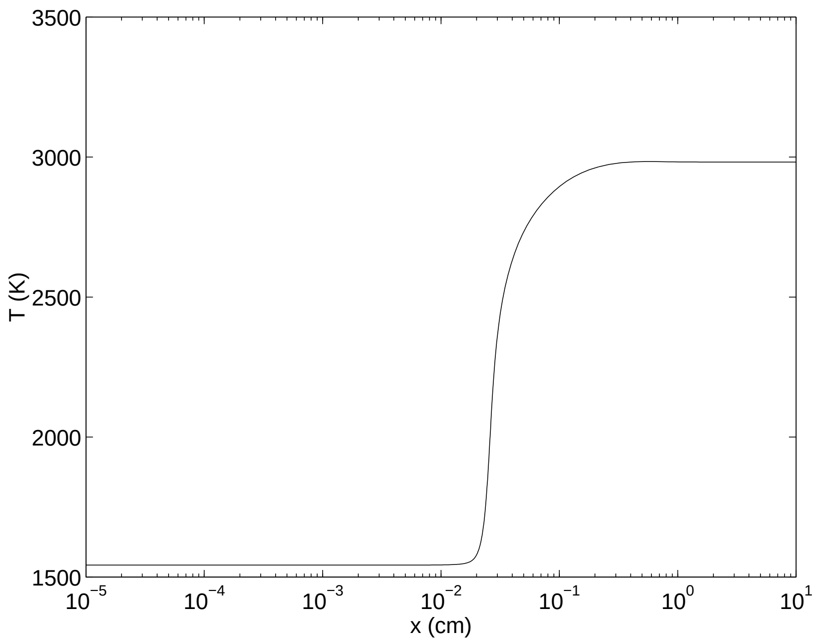
Physical System

- 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).

Detailed Kinetics Model

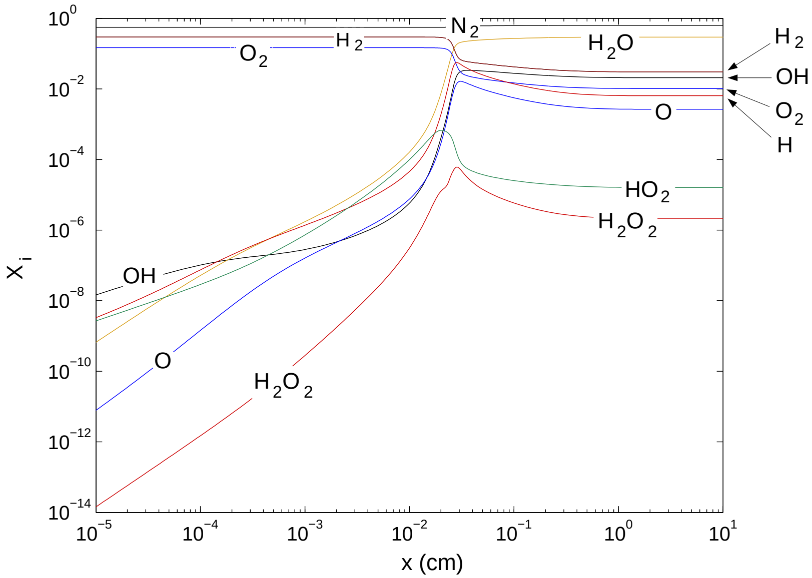
j	Reaction	A_j	β_j	E_j
1	$H_2 + O_2 \rightleftharpoons OH + OH$	1.70×10^{13}	0.00	47780
2	$OH + H_2 \rightleftharpoons H_2O + H$	1.17×10^{9}	1.30	3626
3	$H + O_2 \rightleftharpoons OH + O$	5.13×10^{16}	-0.82	16507
4	$O + H_2 \rightleftharpoons OH + H$	1.80×10^{10}	1.00	8826
5	$H + O_2 + M \rightleftharpoons HO_2 + M$	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

Temperature Profile



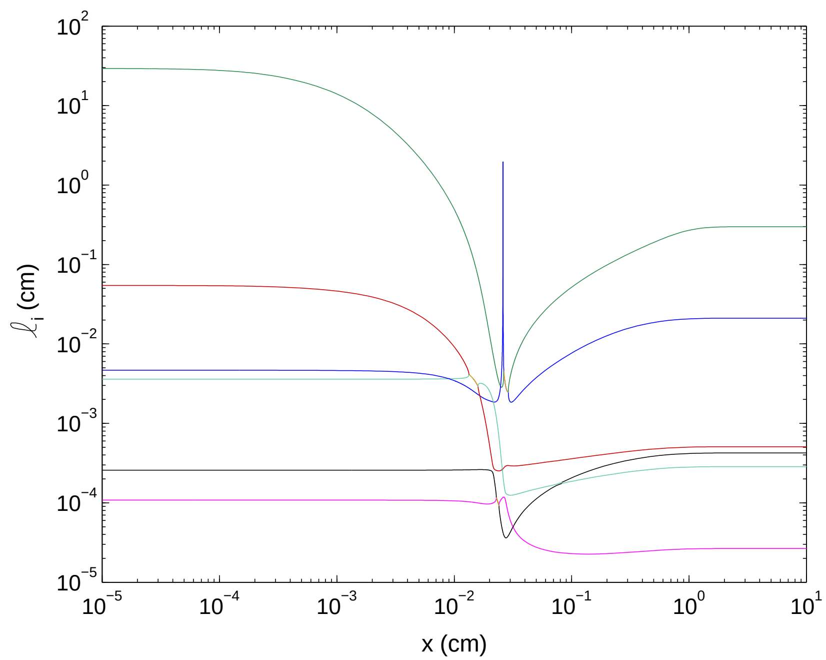
- Temperature flat in the post-shock induction zone $0 < x < 2.6 \times 10^{-2}\ cm$.
- Thermal explosion followed by relaxation to equilibrium at $x \sim 10^{0}\ cm$.

Mole Fractions versus Distance



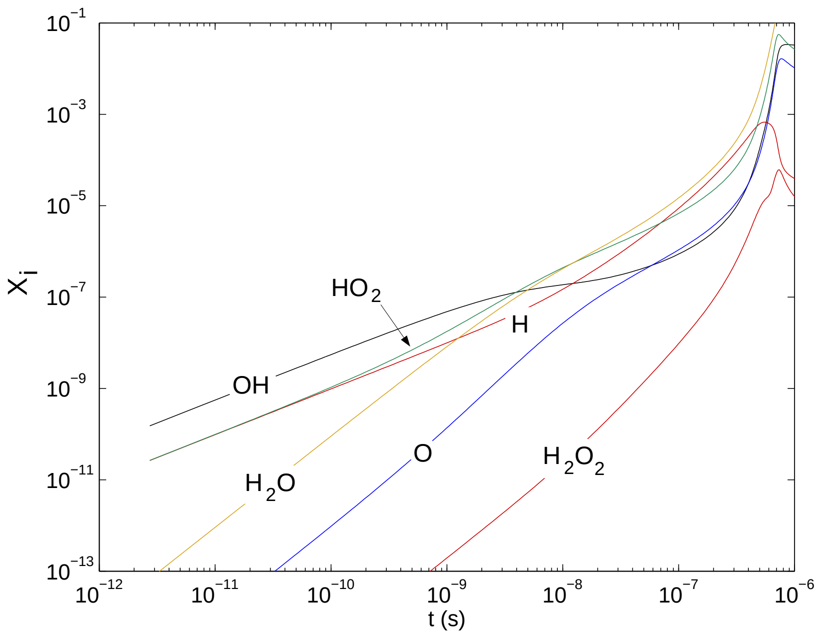
- significant evolution at fine length scales $x < 10^{-3}\ cm$.
- results agree with those of Shepherd.

Eigenvalue Analysis: Length Scale Evolution



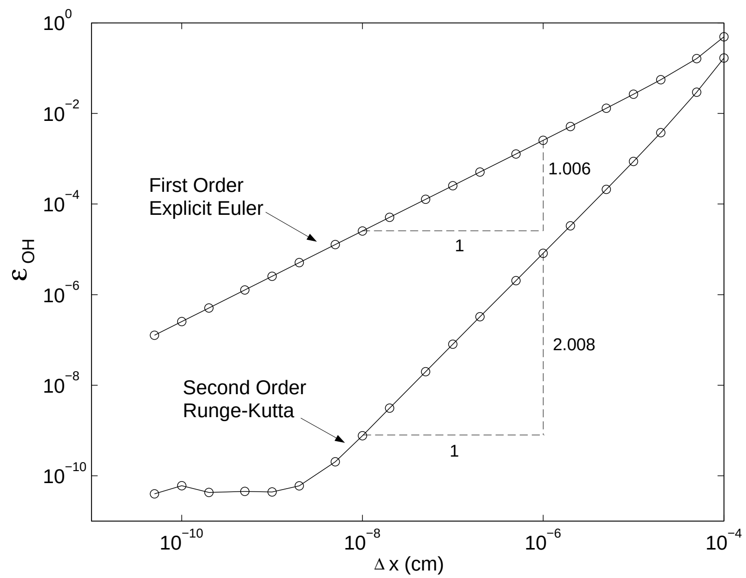
- Finest length scale: $2.3 \times 10^{-5}\ cm$.
- Coarsest length scale $3.0 \times 10^{1}\ cm$.
- Finest length scale similar to that necessary for numerical stability of ODE solver.

Verification: Comparison with Mikolaitis



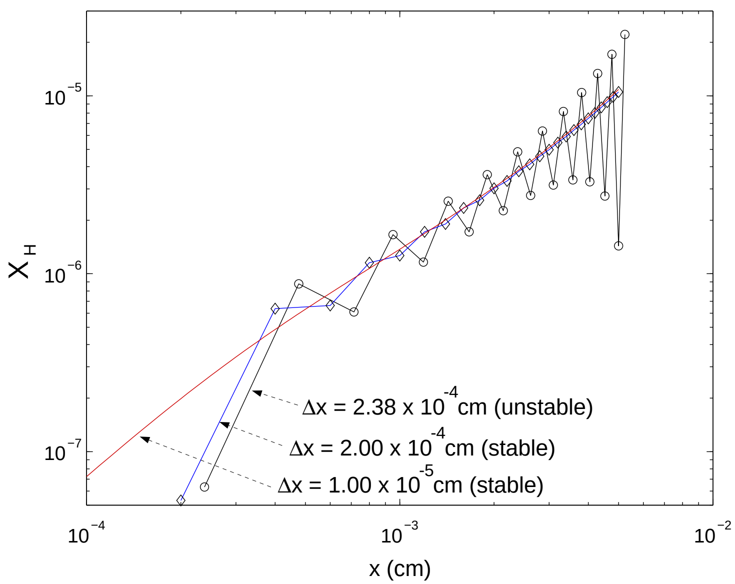
- Lagrangian calculation allows direct comparison with Mikolaitis' results.
- agreement very good.

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.

Unsteady Model: Reactive Euler Equations

- one-dimensional,
- inviscid,
- detailed mass action kinetics with Arrhenius temperature dependency,
- ideal mixture of calorically imperfect ideal gases

Model: Unsteady Reactive Euler PDEs

$$
\begin{aligned}
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}\left(\rho u\right) &= 0, \\
\frac{\partial}{\partial t}\left(\rho u\right) + \frac{\partial}{\partial x}\left(\rho u^2 + p\right) &= 0, \\
\frac{\partial}{\partial t}\left(\rho\left(e + \frac{u^2}{2}\right)\right) + \frac{\partial}{\partial x}\left(\rho u\left(e + \frac{u^2}{2} + \frac{p}{\rho}\right)\right) &= 0, \\
\frac{\partial}{\partial t}\left(\rho Y_i\right) + \frac{\partial}{\partial x}\left(\rho u Y_i\right) &= M_i \dot{\omega}_i, \\
p &= \rho \Re T \sum_{i=1}^{N} \frac{Y_i}{M_i}, \\
e &= e(T, Y_i), \\
\dot{\omega}_i &= \dot{\omega}_i(T, Y_i).
\end{aligned}
$$

Computational Method

- Shock fitting coupled with a fifth order method for continuous regions
  - Fifth order WENO5M for spatial discretization
  - Fifth order Runge-Kutta for temporal discretization
- see Henrick, Aslam, Powers, *J. Comp. Phys.*, 2006, for full details on shock fitting

Outline of Shock Fitting Method

- Transform from lab frame to shock-attached frame, $(x, t) \rightarrow (\xi, \tau)$
  - example mass equation becomes

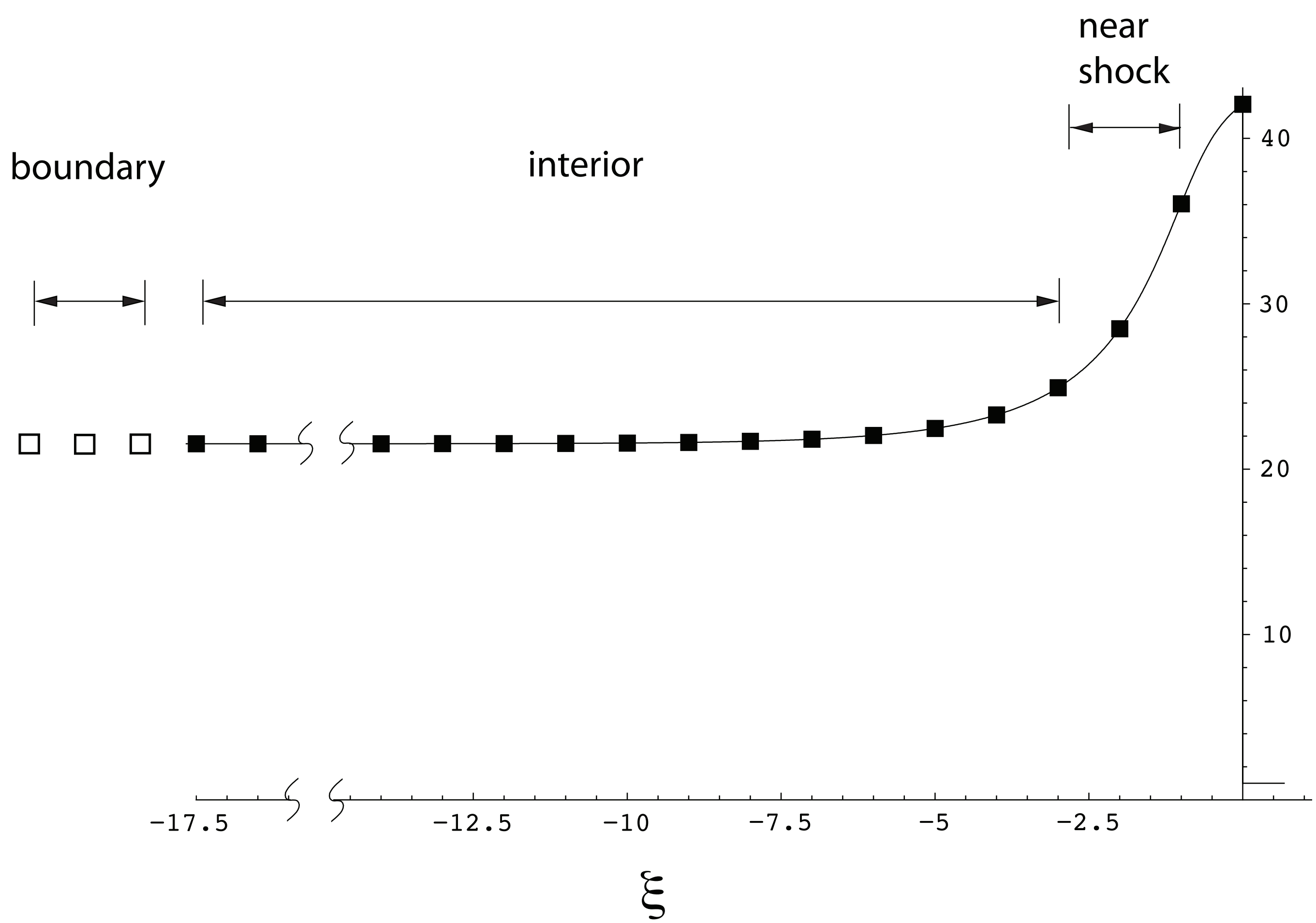
$$\frac{\partial \rho}{\partial \tau} + \frac{\partial}{\partial \xi}\left(\rho\left(u - D\right)\right) = 0$$

- In interior
  - fifth order WENO5M for spatial discretization
  - fifth order Runge-Kutta for temporal discretization

Outline of Shock Fitting Method, cont.

- At shock boundary, one-sided high order differences are utilized
- Note that some form of an approximate Riemann solver must be used to determine the shock speed, D, and thus set a valid shock state
- At downstream boundary, a zero gradient (constant extrapolation) approximation is utilized

Summary of Shock-Fitting Method



Difficulties in Unsteady Calculations

- Note that H_2-air steady detonation had length scales spanning six orders of magnitude
- This is feasible for steady calculations but extremely challenging in a transient calculation.
- To cleanly illustrate the challenges of coupled length and time scales, we choose a realistic problem with less stiffness that we can verify and validate: ozone detonation.

Ozone Reaction Kinetics

Reaction	A_j^f, A_j^r	β_j^f, β_j^r	E_j^f, E_j^r
$O_3 + M \leftrightarrows O_2 + O + M$	6.76×10^6	2.50	1.01×10^{12}
	1.18×10^2	3.50	0.00
$O + O_3 \leftrightarrows 2O_2$	4.58×10^6	2.50	2.51×10^{11}
	1.18×10^6	2.50	4.15×10^{12}
$O_2 + M \leftrightarrows 2O + M$	5.71×10^6	2.50	4.91×10^{12}
	2.47×10^2	3.50	0.00

see Margolis, *J. Comp. Phys.*, 1978, or Hirschfelder, *et al.*, *J. Chem. Phys.*, 1953.

Validation: Comparison with Observation

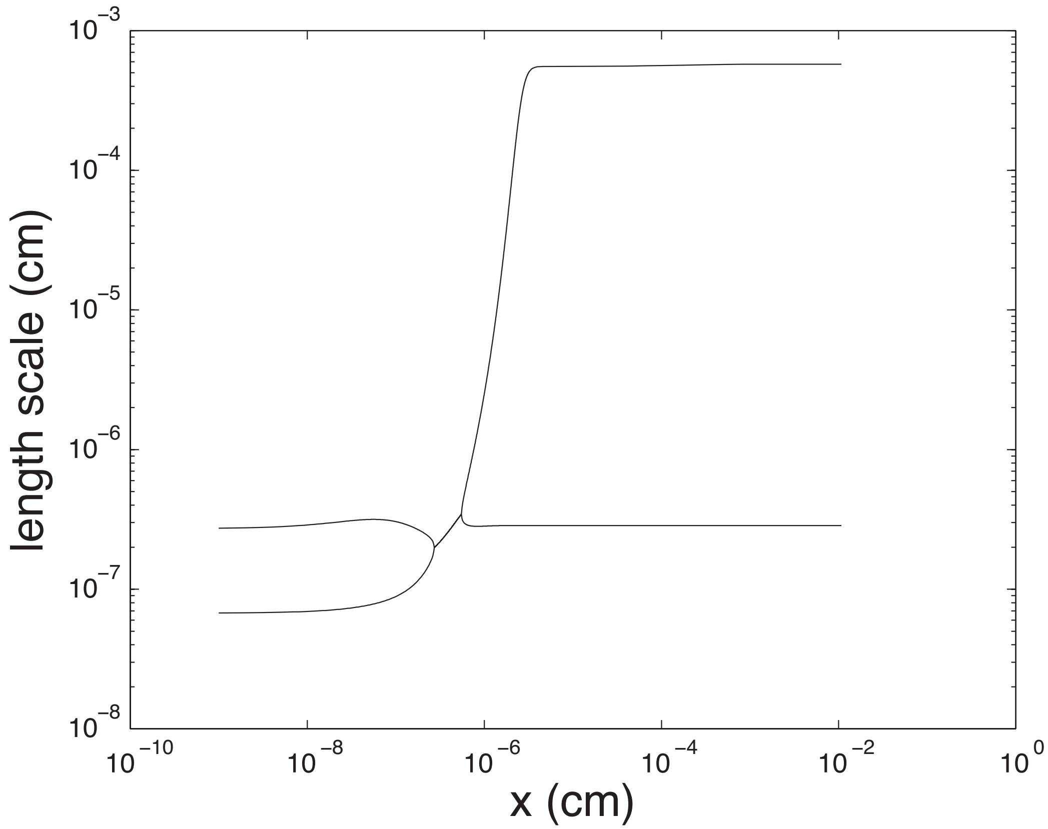
- Streng, *et al.*, *J. Chem. Phys.*, 1958.
- $p_o = 1.01325 \times 10^6\ dyne/cm^2$, $T_o = 298.15\ K$, $Y_{O_3} = 1, Y_{O_2} = 0, Y_O = 0$.

Value	Streng, *et al.*	this study
D_{CJ}	$1.863 \times 10^5\ cm/s$	$1.936555 \times 10^5\ cm/s$
T_{CJ}	$3340\ K$	$3571.4\ K$
p_{CJ}	$3.1188 \times 10^7\ dyne/cm^2$	$3.4111 \times 10^7\ dyne/cm^2$

Slight overdrive to preclude interior sonic points.

Stable Strongly Overdriven Case: Length Scales

$D_o = 2.5 \times 10^5 \; cm/s.$



Mean-Free-Path Estimate

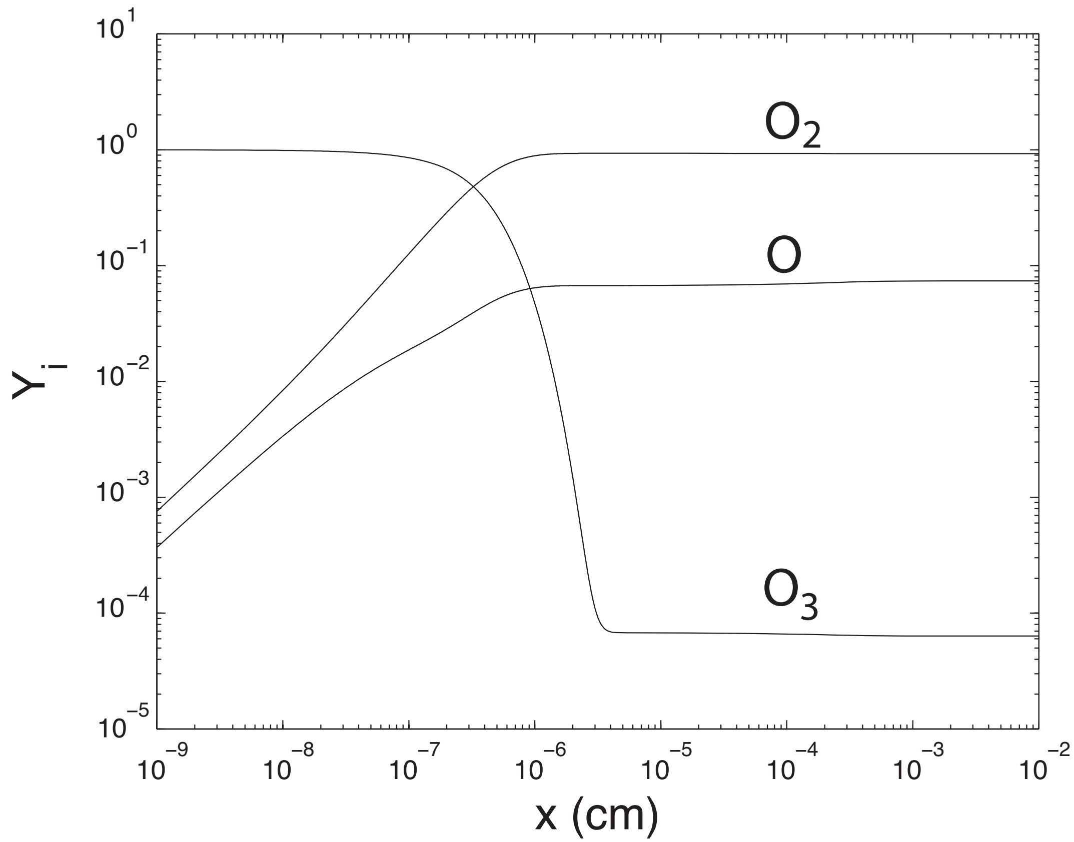
- The mixture mean-free-path scale is the cutoff *minimum* length scale associated with continuum theories.

- A simple estimate for this scale is given by *Vincenti and Kruger, '65*:

$$\ell_{mfp} = \frac{M}{\sqrt{2}\mathcal{N}\pi d^2\rho} \sim 10^{-7}\, cm.$$

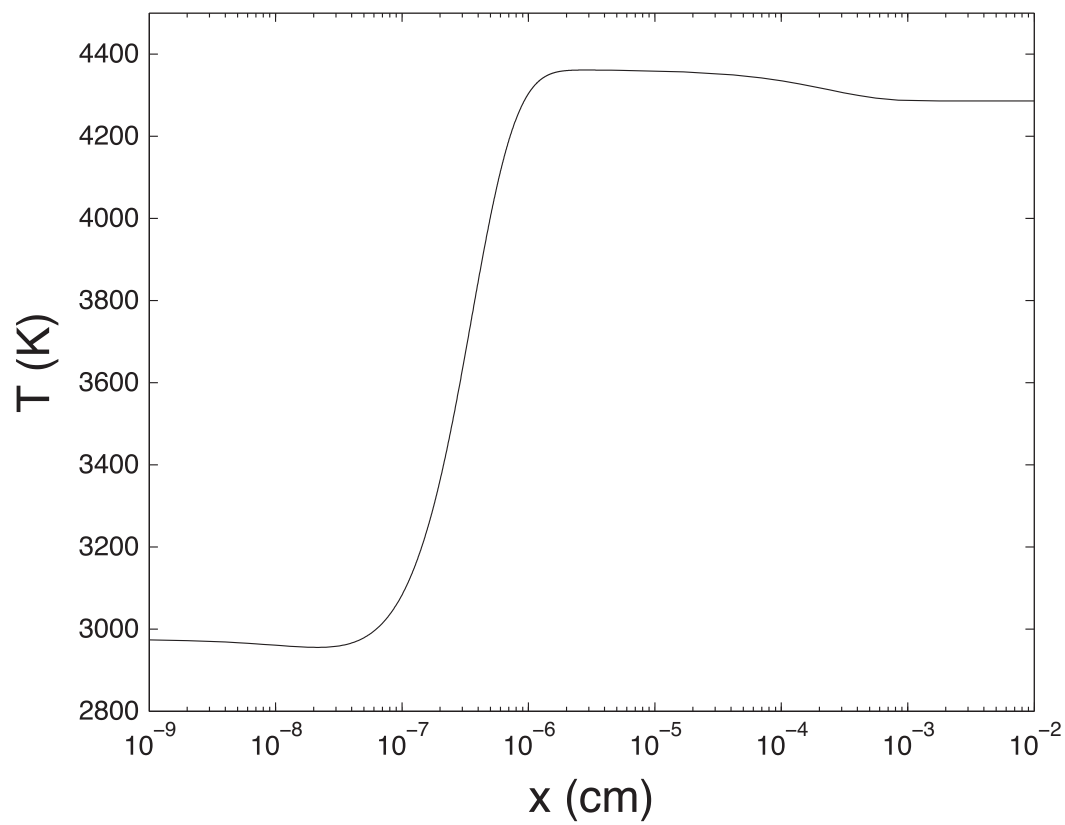
Stable Strongly Overdriven Case: Mass Fractions

$$D_o = 2.5 \times 10^5 \; cm/s.$$



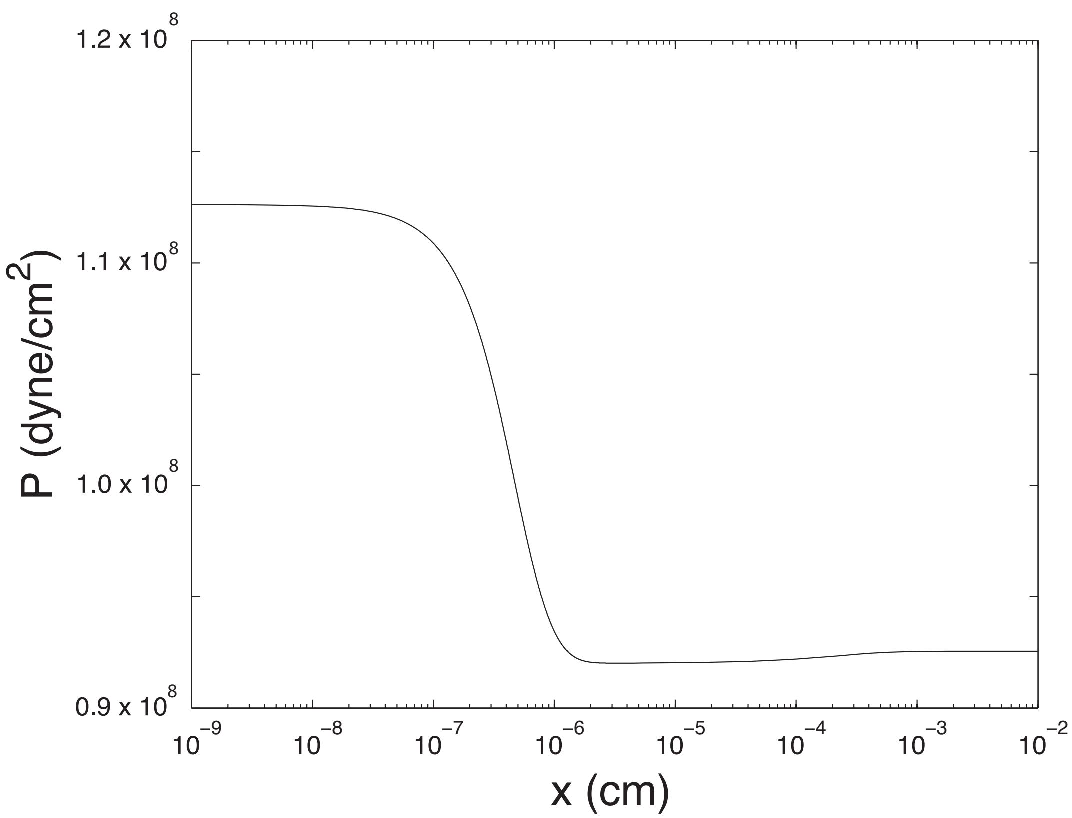
Stable Strongly Overdriven Case: Temperature

$$D_o = 2.5 \times 10^5 \ cm/s.$$



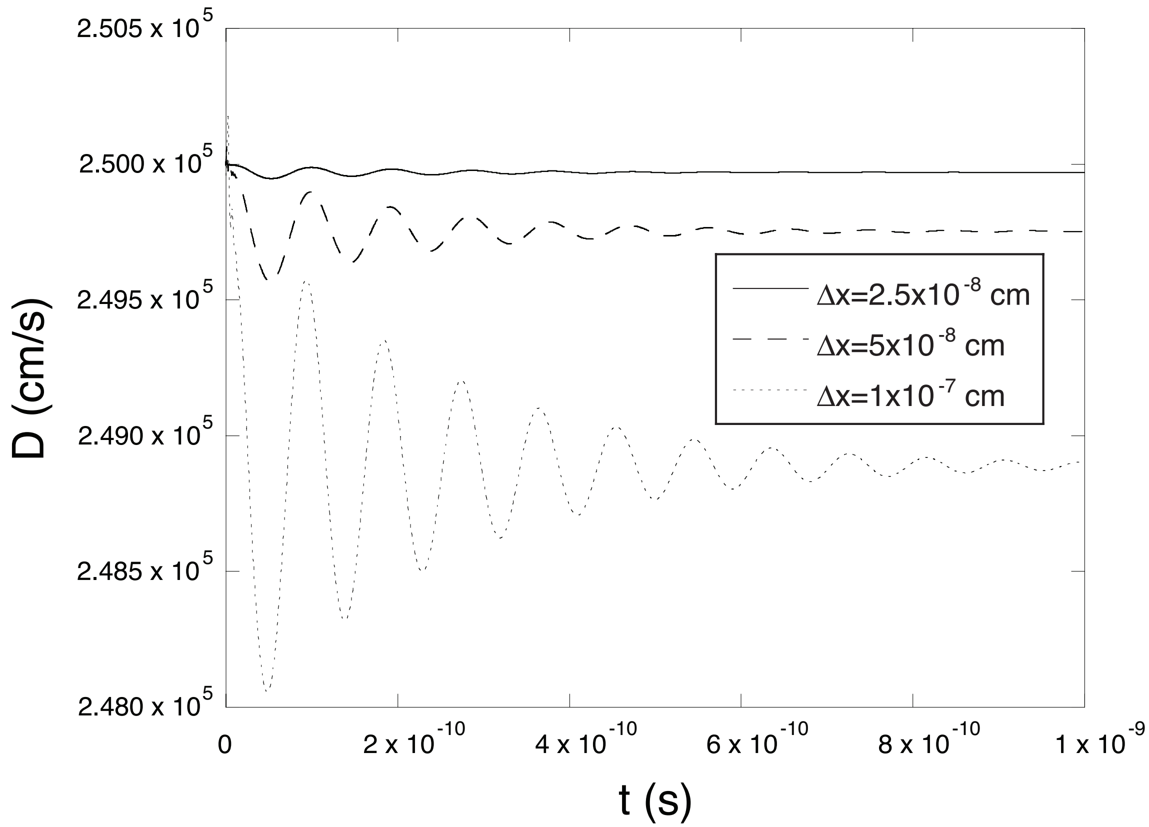
Stable Strongly Overdriven Case: Pressure

$D_o = 2.5 \times 10^5\ cm/s.$

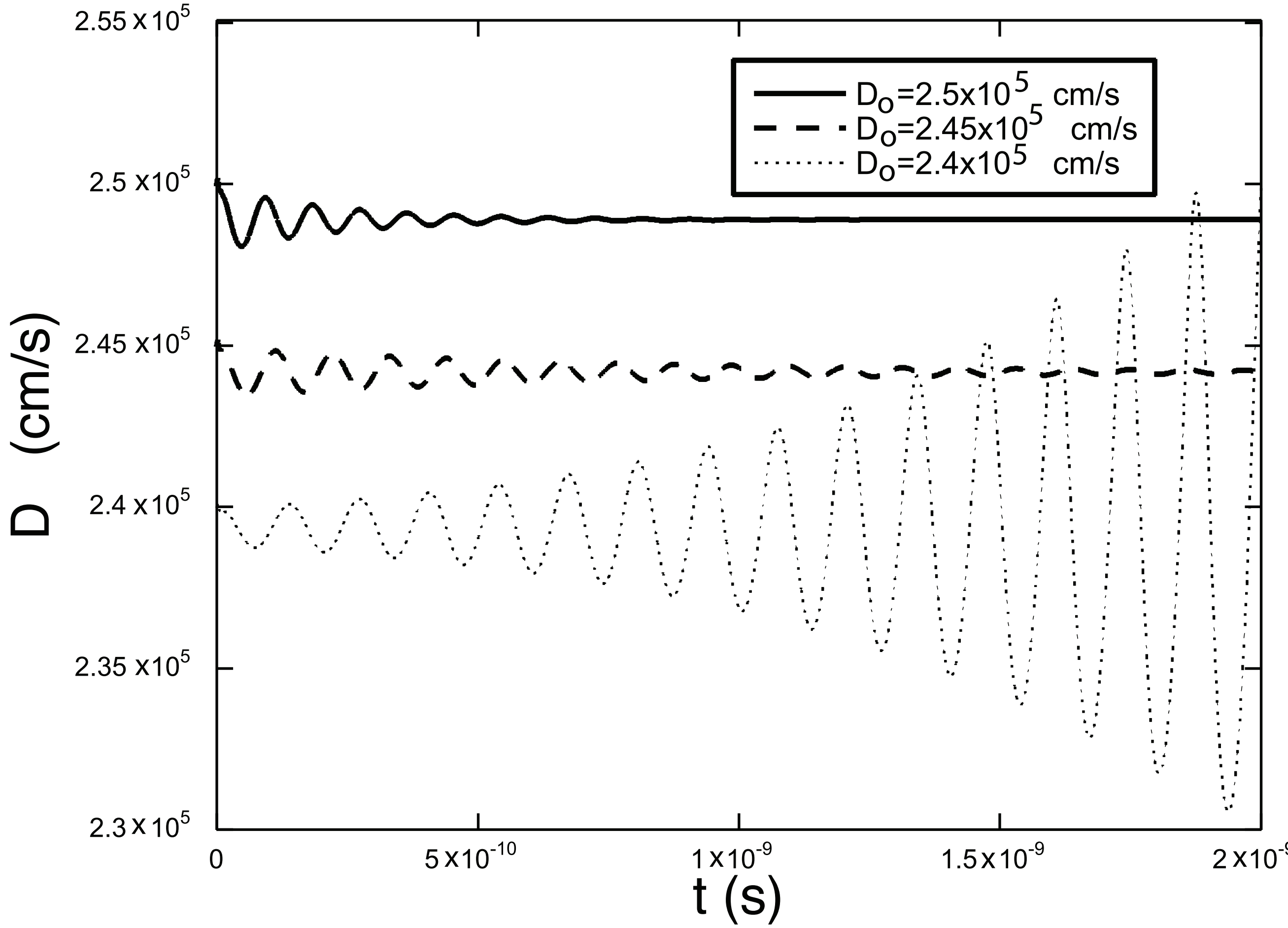


Stable Strongly Overdriven Case: Transient Behavior for Various Resolutions

Initialize with steady structure of $D_o = 2.5 \times 10^5 \ cm/s$.

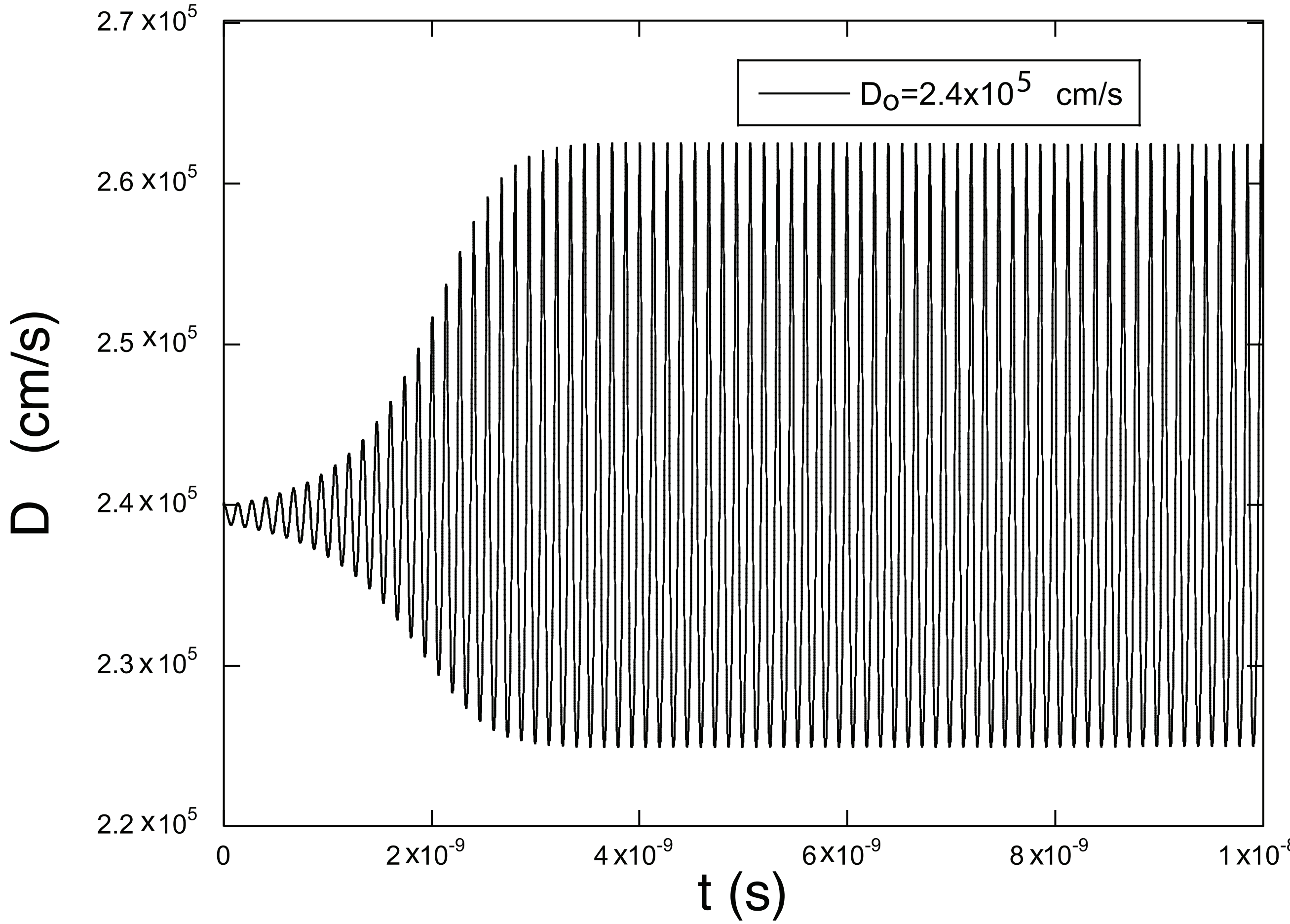


3 Cases Near Neutral Stability: Transient Behavior



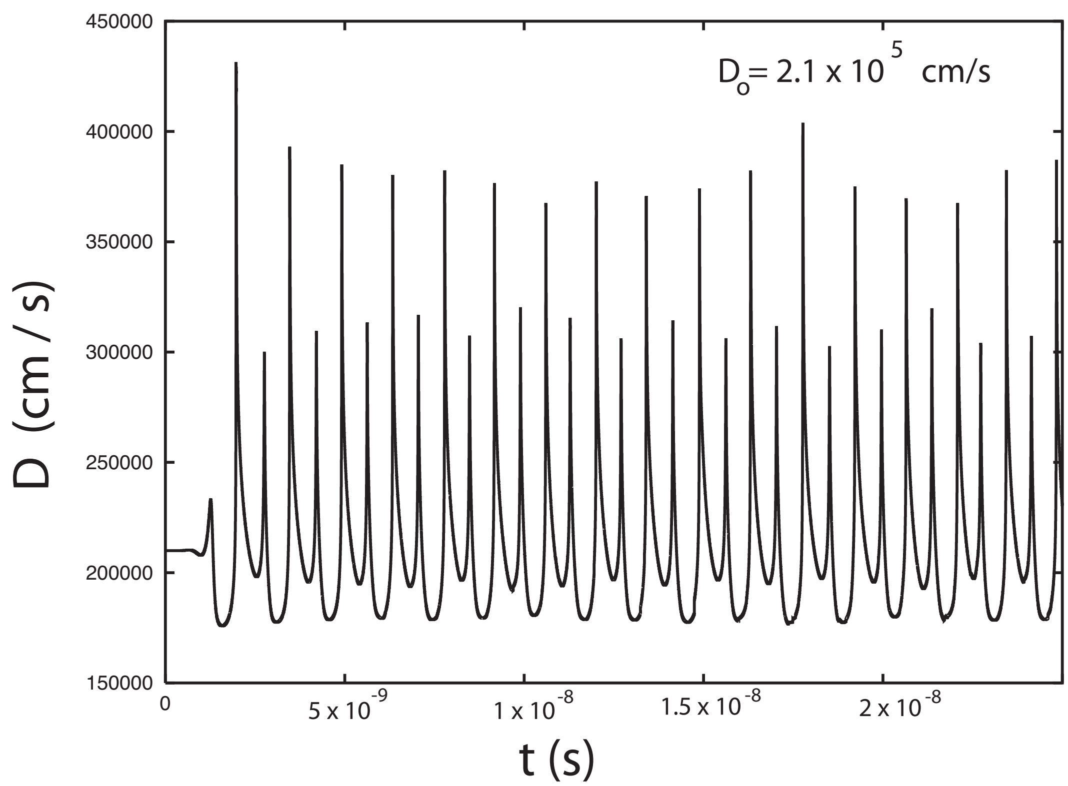
Slightly Unstable Case: Transient Behavior

Initialized with steady structure, $D_o = 2.4 \times 10^5\ cm/s$.

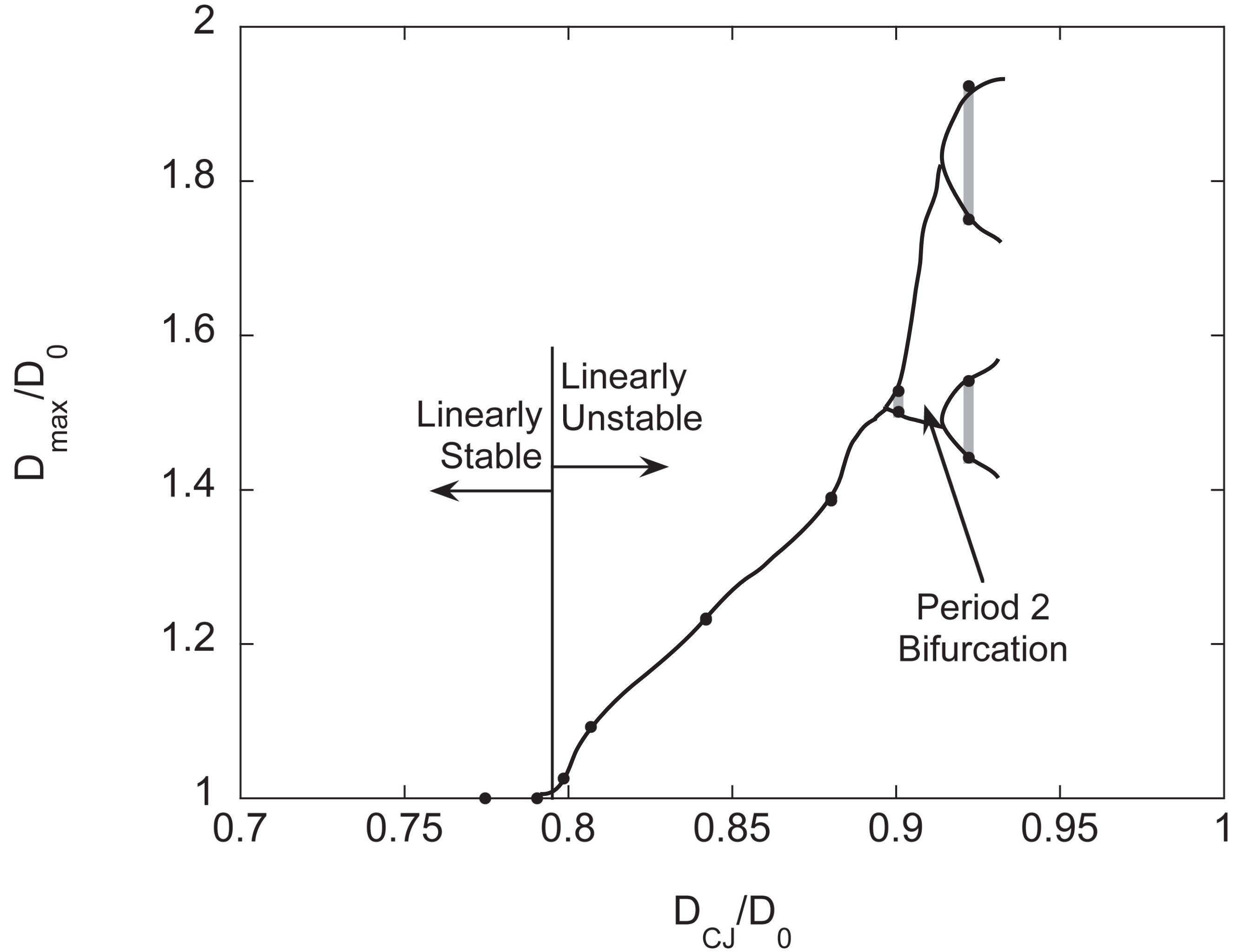


Case After Bifurcation: Transient Behavior

Initialized with steady structure of $D_o = 2.1 \times 10^5 \, cm/s$.



Long Time D_{max}/D_0 versus D_{CJ}/D_0



Effect of Resolution on Unstable Moderately Overdriven Case

Δx	Numerical Result
$1 \times 10^{-7}\ cm$	Unstable Pulsation
$2 \times 10^{-7}\ cm$	Unstable Pulsation
$4 \times 10^{-7}\ cm$	Unstable Pulsation
$8 \times 10^{-7}\ cm$	O_2 mass fraction > 1
$1.6 \times 10^{-6}\ cm$	O_2 mass fraction > 1

- Algorithm failure for insufficient resolution
- At low resolution, one misses critical dynamics

Examination of H_2-Air Results

Reference	ℓ_{ind} (cm)	ℓ_f (cm)	Δx (cm)	Under-resolution
Oran, *et al.*, 1998	2×10^{-1}	2×10^{-4}	4×10^{-3}	2×10^{1}
Jameson, *et al.*, 1998	2×10^{-2}	5×10^{-5}	3×10^{-3}	6×10^{1}
Hayashi, *et al.*, 2002	2×10^{-2}	1×10^{-5}	5×10^{-4}	5×10^{1}
Hu, *et al.*, 2004	2×10^{-1}	2×10^{-4}	3×10^{-3}	2×10^{1}
Powers, *et al.*, 2001	2×10^{-2}	3×10^{-5}	8×10^{-5}	3×10^{0}
Osher, *et al.*, 1997	2×10^{-2}	3×10^{-5}	3×10^{-2}	1×10^{3}
Merkle, *et al.*, 2002	5×10^{-3}	8×10^{-6}	1×10^{-2}	1×10^{3}
Sislian, *et al.*, 1998	1×10^{-1}	2×10^{-4}	1×10^{0}	5×10^{3}
Jeung, *et al.*, 1998	2×10^{-2}	6×10^{-7}	6×10^{-2}	1×10^{5}

All are under-resolved, some severely.

Conclusions

- Unsteady detonation dynamics can be accurately simulated when sub-micron scale structures admitted by detailed kinetics are captured with ultra-fine grids.
- Shock fitting coupled with high order spatial discretization assures numerical corruption is minimal.
- Predicted detonation dynamics consistent with results from one-step kinetic models.
- At these length scales, diffusion will play a role and should be included in future work.

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!