Shock-Fitted Calculation of Unsteady Detonation in Ozone

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Motivation

- Computational tools are critical in design of aerospace vehicles which employ high speed reactive flow.
- Steady wave calculations reveal sub-micron scale structures in detonations with detailed kinetics (Powers and Paolucci, *AIAA J.*, 2005).
- Small structures are continuum manifestation of molecular collisions.
- We explore, for the first time, 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: Reactive Euler Equations

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

Model: Reactive Euler PDEs

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

Computational Methods

- Steady wave structure:
  - LSODE solver with IMSL DNEQNF for root finding,
  - Ten second run time on single processor machine,
  - see Powers and Paolucci, *AIAA J.*, 2005.
- Unsteady wave structure:
  - Shock fitting coupled with a high order method for continuous regions,
  - 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.
  - example: mass equation becomes

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

- In interior, approximate spatial derivatives with fifth order Lax-Friedrichs discretization.
- At shock boundary, one-sided high order differences are utilized.

Outline of Shock Fitting Method

- 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.
- Fifth order Runge-Kutta time integration is employed via the Butcher formulation.

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

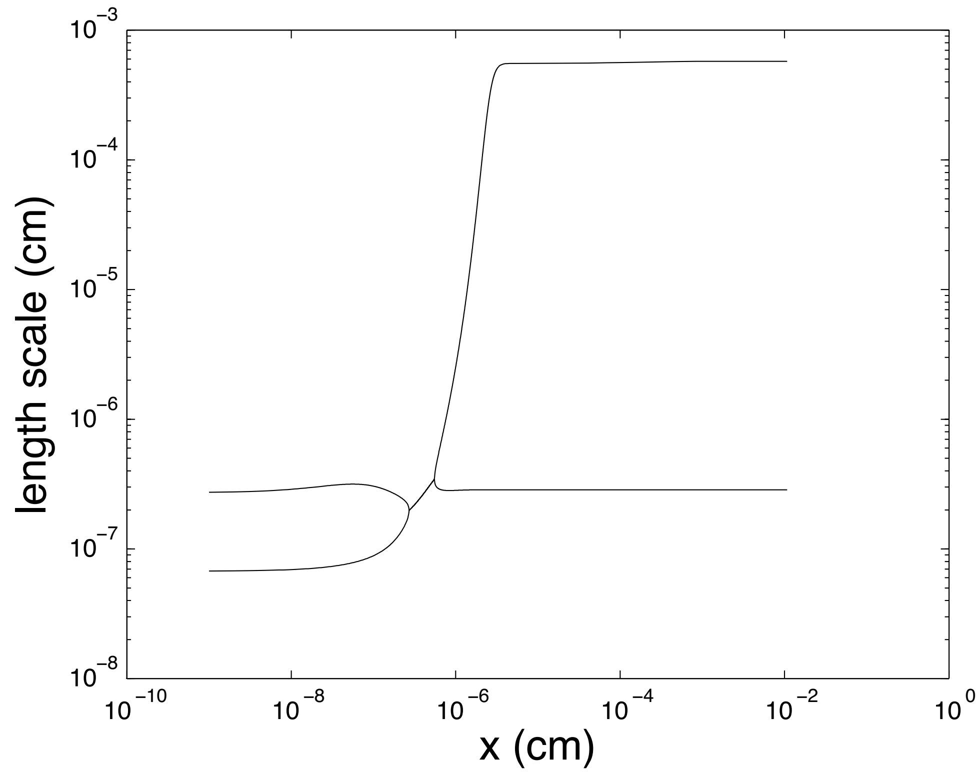
- Streng, *et al.*, *J. Chem. Phys.*, 1958.
- $p_o = 1.01325 \times 10^6\ dyne/cm^2$, $T_o = 298.15\ K$, $Y_{O_3} = 1, Y_{O_2} = 0, Y_O = 0$.

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 from Spatial Eigenvalue Analysis.

$D = 2.5 \times 10^5\ cm/s$. Smallest Scale $\approx 10^{-7} cm$.



Mean-Free-Path Estimate

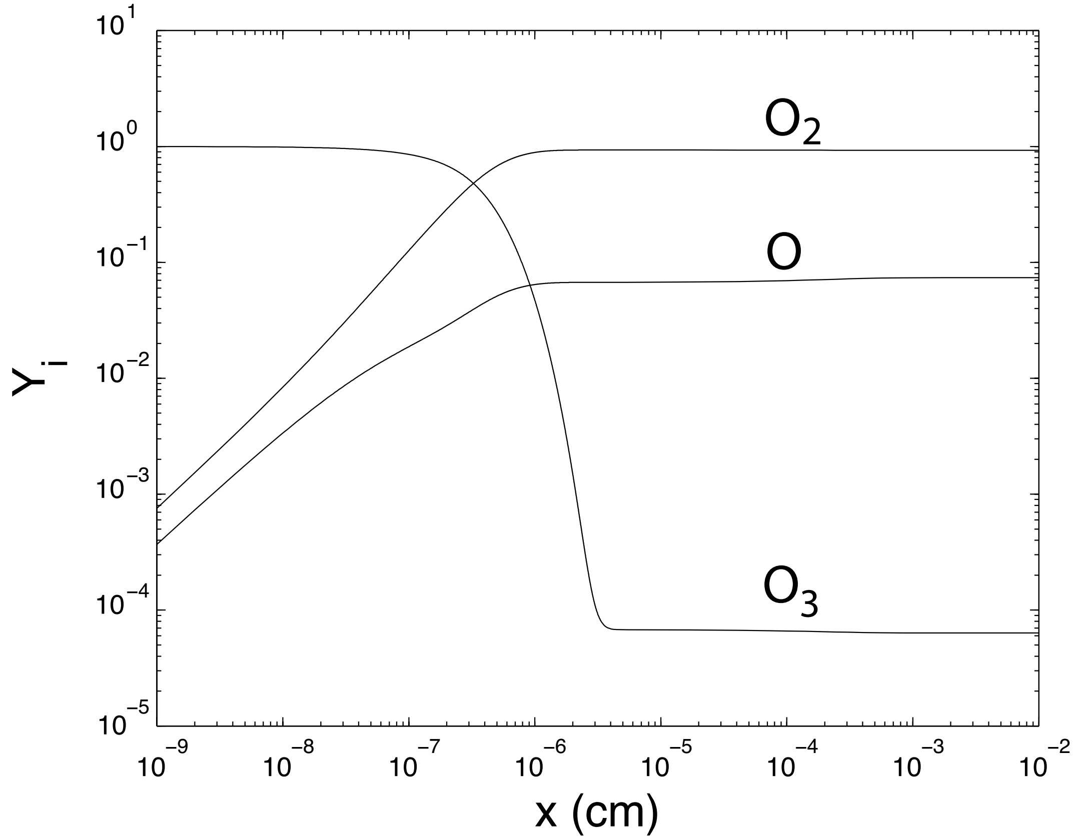
- The mixture mean-free-path scale is the cutoff *minimum* length scale associated with continuum theories.

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

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

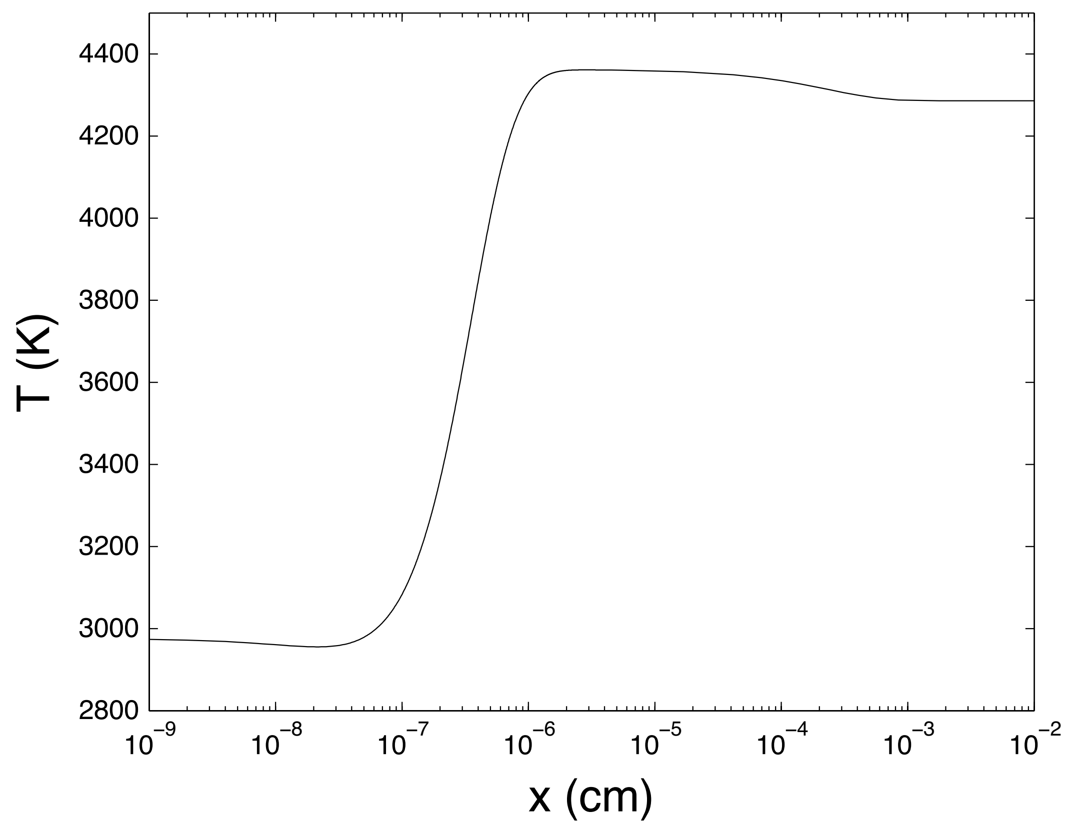
Stable Strongly Overdriven Case: Mass Fractions

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



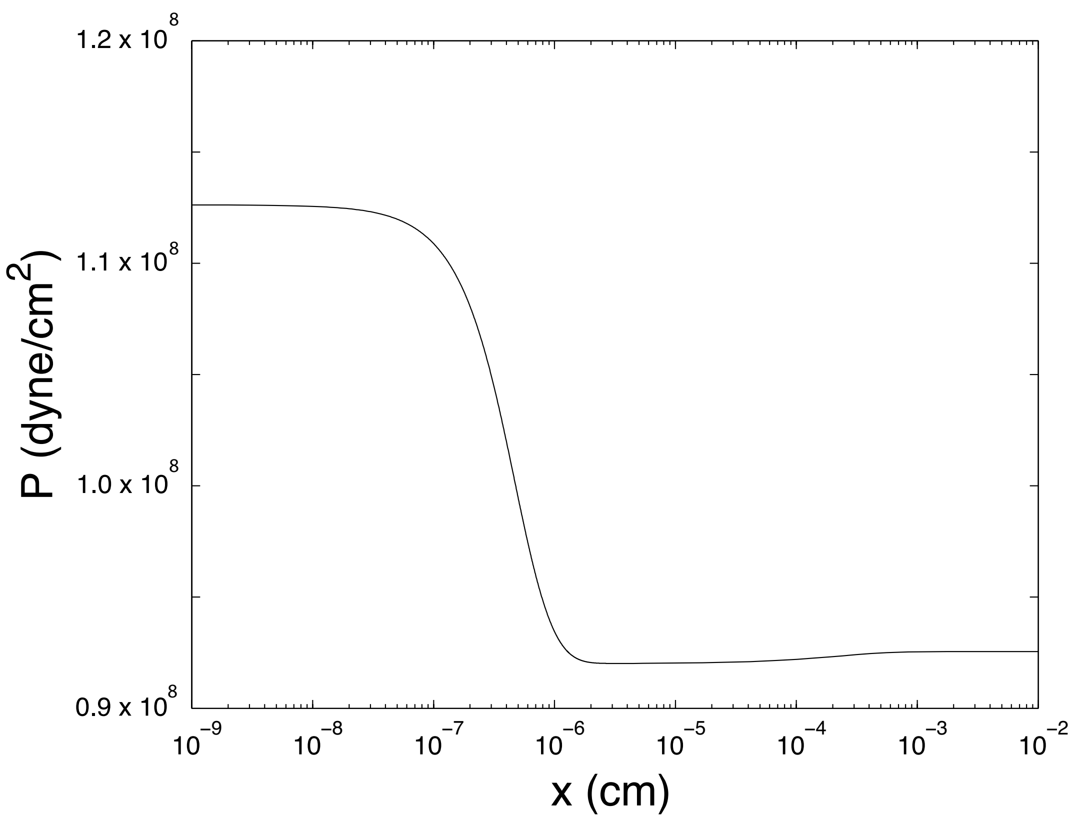
Stable Strongly Overdriven Case: Temperature

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



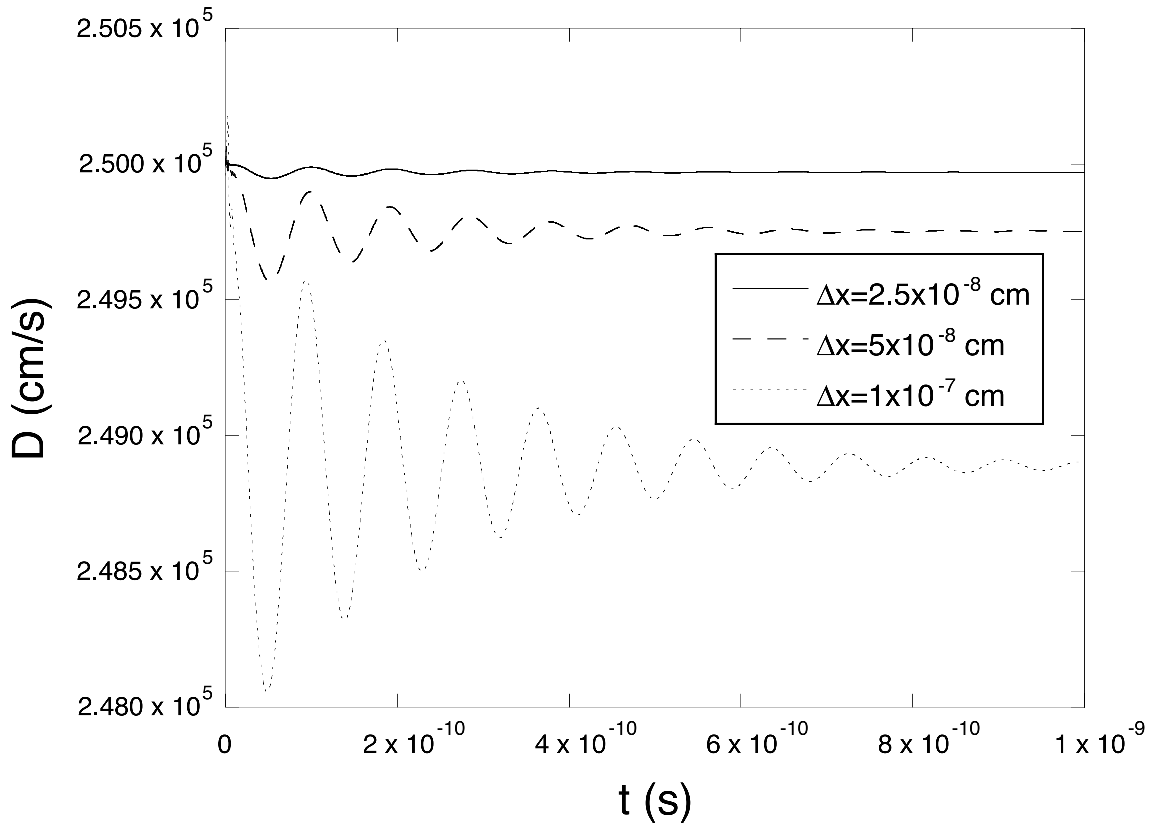
Stable Strongly Overdriven Case: Pressure

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



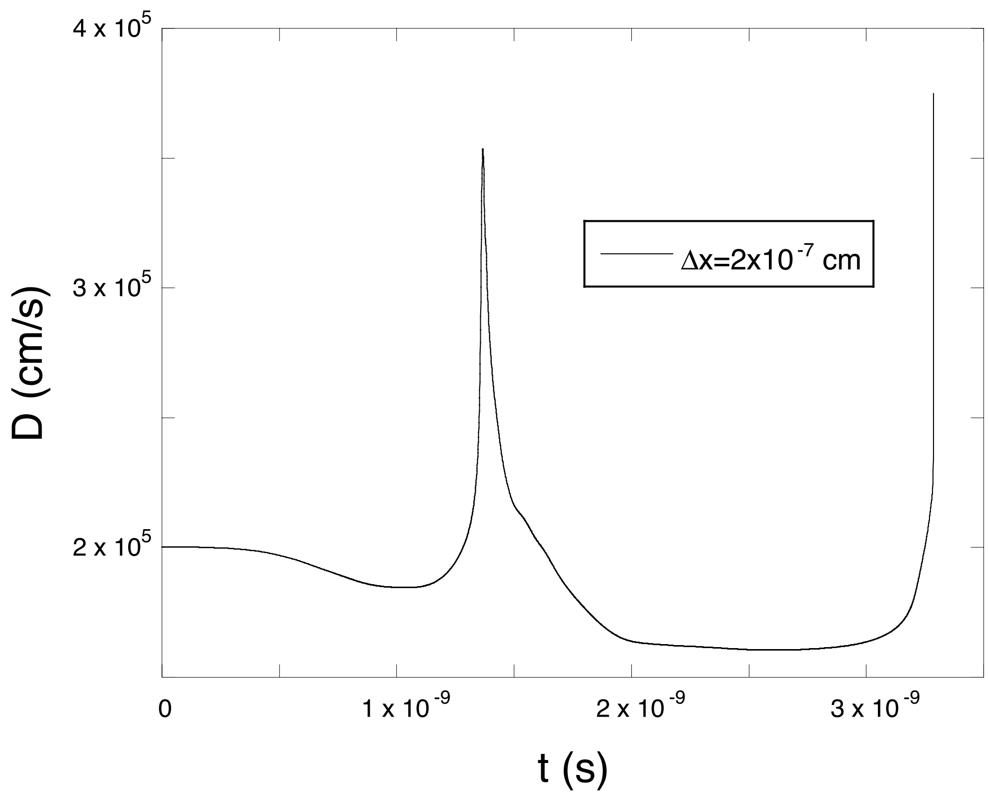
Stable Strongly Overdriven Case: Transient Behavior for various resolutions

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



Unstable Moderately Overdriven Case: Transient Behavior

Initialize with steady structure of $D = 2 \times 10^5\ cm/s$.



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.

Implications for Operator Splitting for Implicit Time Integration of Chemistry

- This popular method, while numerically stable, misses fine scale dynamics entirely.
- This method would capture the dynamics if $\Delta x = 10^{-7} cm$, in which case there would be no need for implicit time integration.

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 is consistent with results from one-step kinetic models.
- At these length scales, diffusion will play a role and should be included in future work.