Mathematical Verification of Simulations of Reactive Flows with Embedded Discontinuities

or "High Order" Shock-Capturing Methods Aren't Always What They're Cracked Up to Be!

Joseph M. Powers (powers@nd.edu)
University of Notre Dame

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Verification and Validation

- *Verification*: solving the equations right (mathematics)
- *Validation*: solving the right equations (physics)
- Verification must precede validation; both must be done for a *pre-dictive* scientific computation.
- Strong verification: a solution achieves a convergence rate consistent with its claimed order of accuracy.

Motivation

- Tuning computations to match experiments without harmonizing with underlying mathematics renders pre-dictions unreliable.
- Attempts to computationally *pre-dict*, not post-dict, results of a benchmark high speed combustion experiment generated "widely different outcomes," LeBlanc, et al., *J. Physique IV*, 2000.
- Mis-understanding of how to rigorously verify computations of flows with embedded shocks is widespread, *e.g.* the recent incorrect statement in *JCP*, 2006, "High-order accurate shock-capturing schemes are capable of properly resolving discontinu-ities...The convergence rate is correct."

Contradiction: “High Order” Shock-Capturing

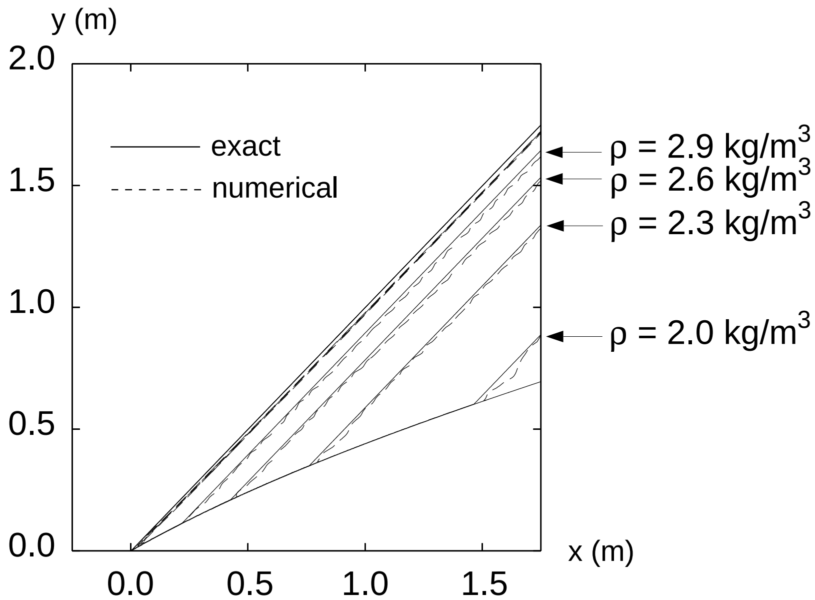
- High order shock-capturing methods only converge at high order on *smooth* problems.
- Even when smooth, Henrick, Aslam & Powers, *JCP*, 2005, show
  - The standard “fifth order” WENO5 method only converges at *third order*.
  - A modification (WENO5M) recovers fifth order.
  - However, both WENO5 and WENO5M converge *at no more than first order* for captured shocks.

Model: Reactive Euler Equations

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

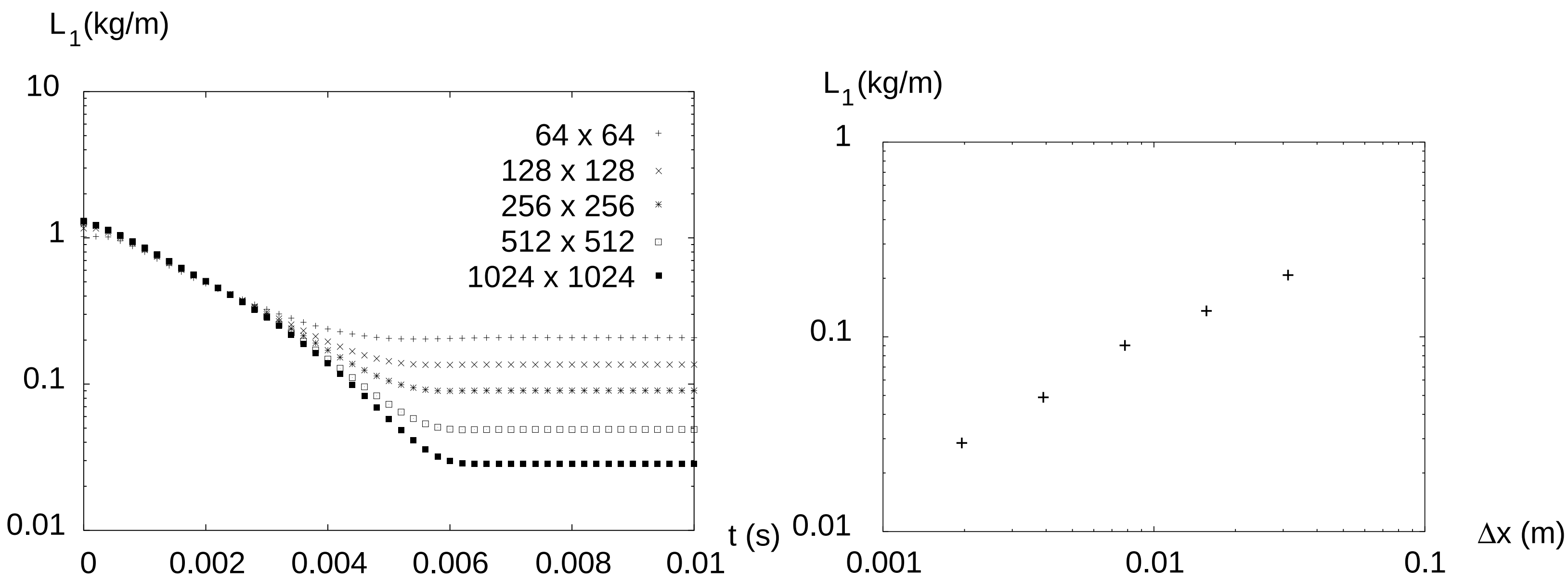
Here: mainly one-step, some detailed kinetics.

Two-Dimensional Oblique Detonation via "High Order" Shock-Capturing



- Powers & Aslam, *AIAA J.*, 2006,
- one-step kinetics,
- closed form exact solution available.

Convergence Rate of “High Order” Shock-Capturing Method $= 0.779$



$L_1 = \int\int |\rho_n - \rho_e|\, dA$, the density error.

Shock-Fitting for True High Order Convergence

- Enforce unsteady Rankine-Hugoniot jump conditions,
- Transform to shock-attached frame via

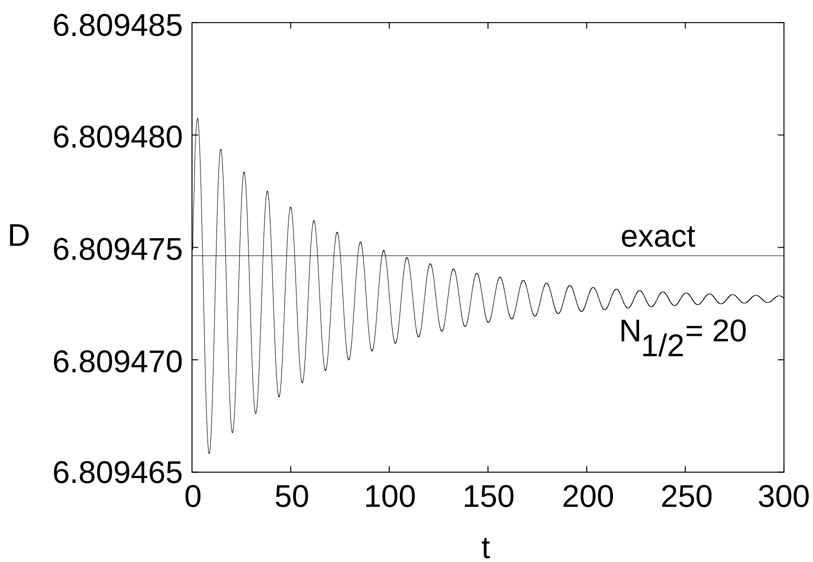
$$x = \xi - \int_0^t D(\tau) d\tau,$$

- Shock-change equation for shock acceleration:

$$\frac{dD}{dt} = -\left(\frac{d(\rho_s u_s)}{dD}\right)^{-1} \left(\frac{\partial}{\partial x}\left(\rho u(u-D)+p\right)\right).$$

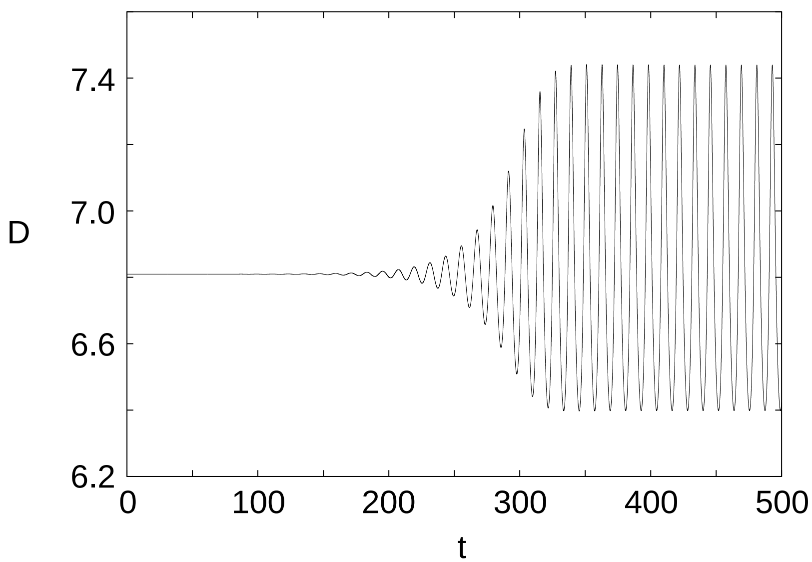
- point-wise method of lines on uniform spatial grid,
- fifth order spatial discretization: PDEs$\longrightarrow$ ODEs in time,
- fifth order temporal discretization to solve ODEs.
- Vary activation energy, $25 \leq E \leq 28.4$.

Stable Case, $E = 25$, with Shock-Fitting



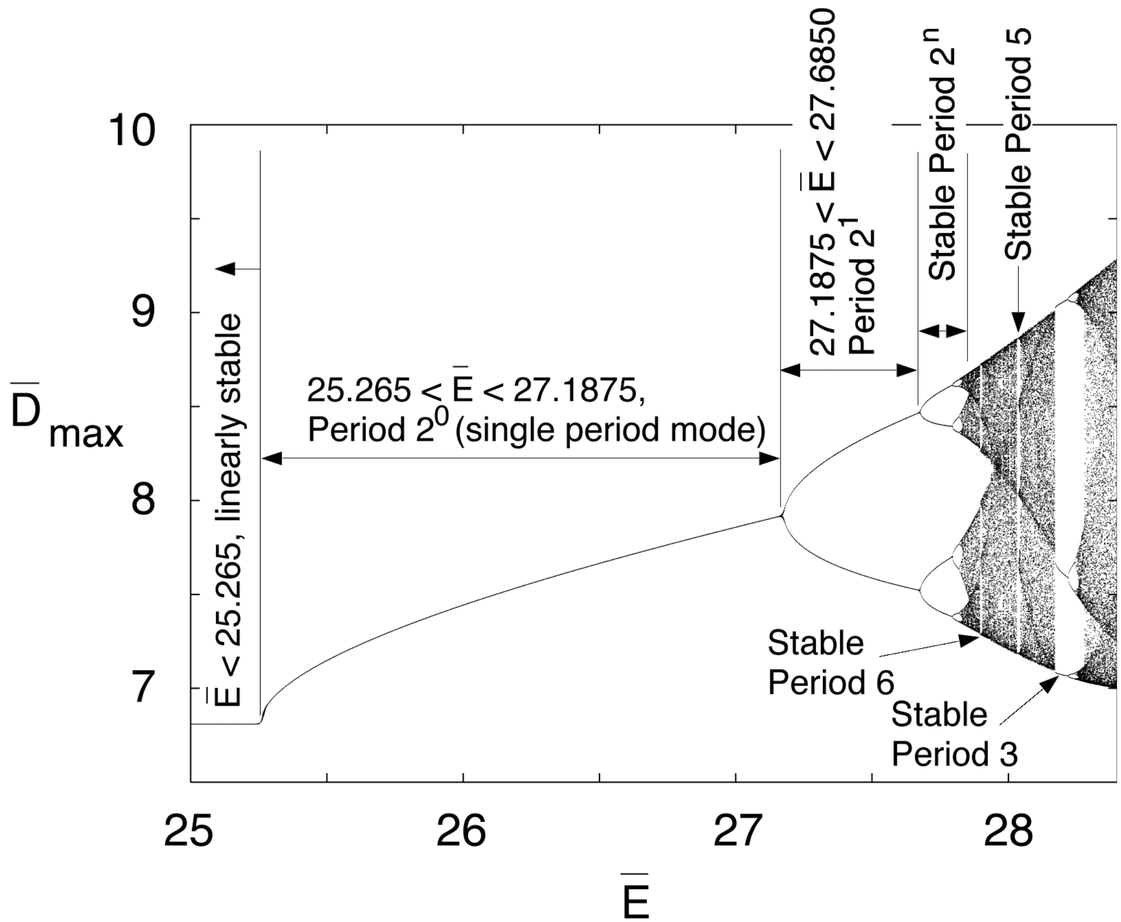
- one-step kinetics,
- closed form, exact solution for D available, $D = \sqrt{11} + \sqrt{\frac{61}{5}}$,
- error in D converges at $O(\Delta x^{5.01})$.

Linearly Unstable, Non-linearly Stable Case: $E = 26$



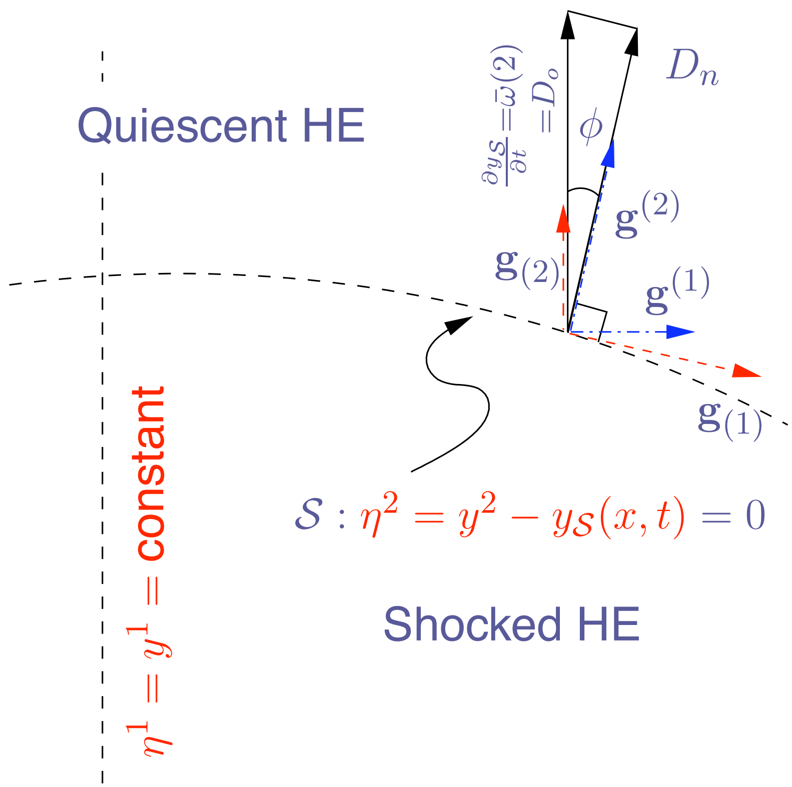
- One linearly unstable mode, stabilized by non-linear effects,
- Growth rate and frequency match linear theory to five decimal places.

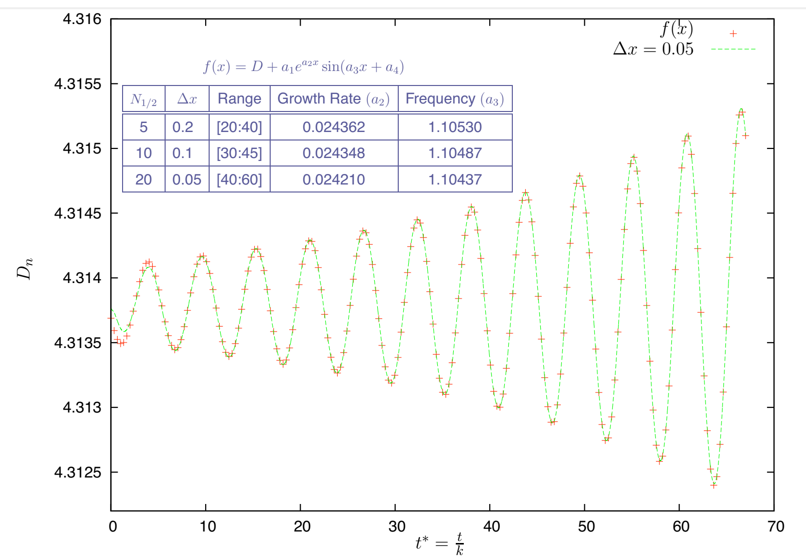
Bifurcation Diagram and Transition to Chaos



Feigenbaum's number, $4.669201...$, captured as 4.66 ± 0.09.

Two-Dimensional Unsteady Reactive Euler Equations with One-Step Kinetics and Shock-Fitting

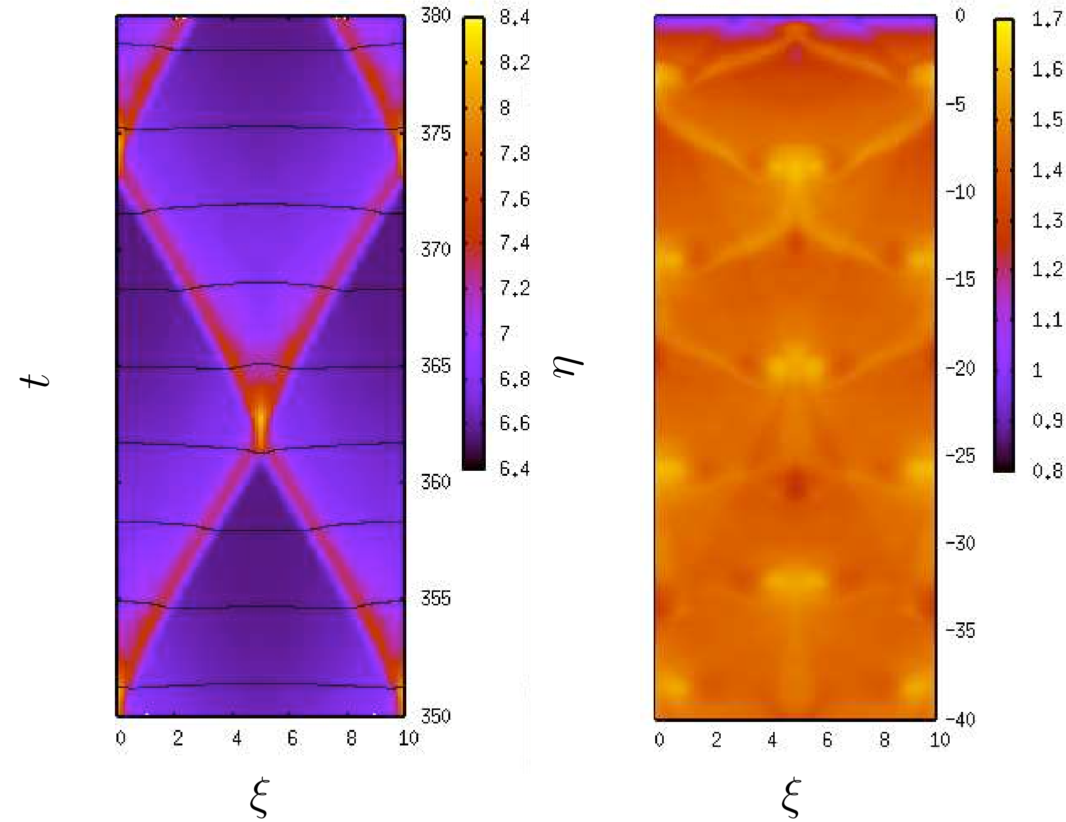




$N_{1/2}$	Δx	Range	Growth Rate (a_2)	Frequency (a_3)
5	0.2	[20:40]	0.024362	1.10530
10	0.1	[30:45]	0.024348	1.10487
20	0.05	[40:60]	0.024210	1.10437

Henrick, Aslam & Powers, 2006; 5th order convergence.

Two-Dimensional Detonation Cells



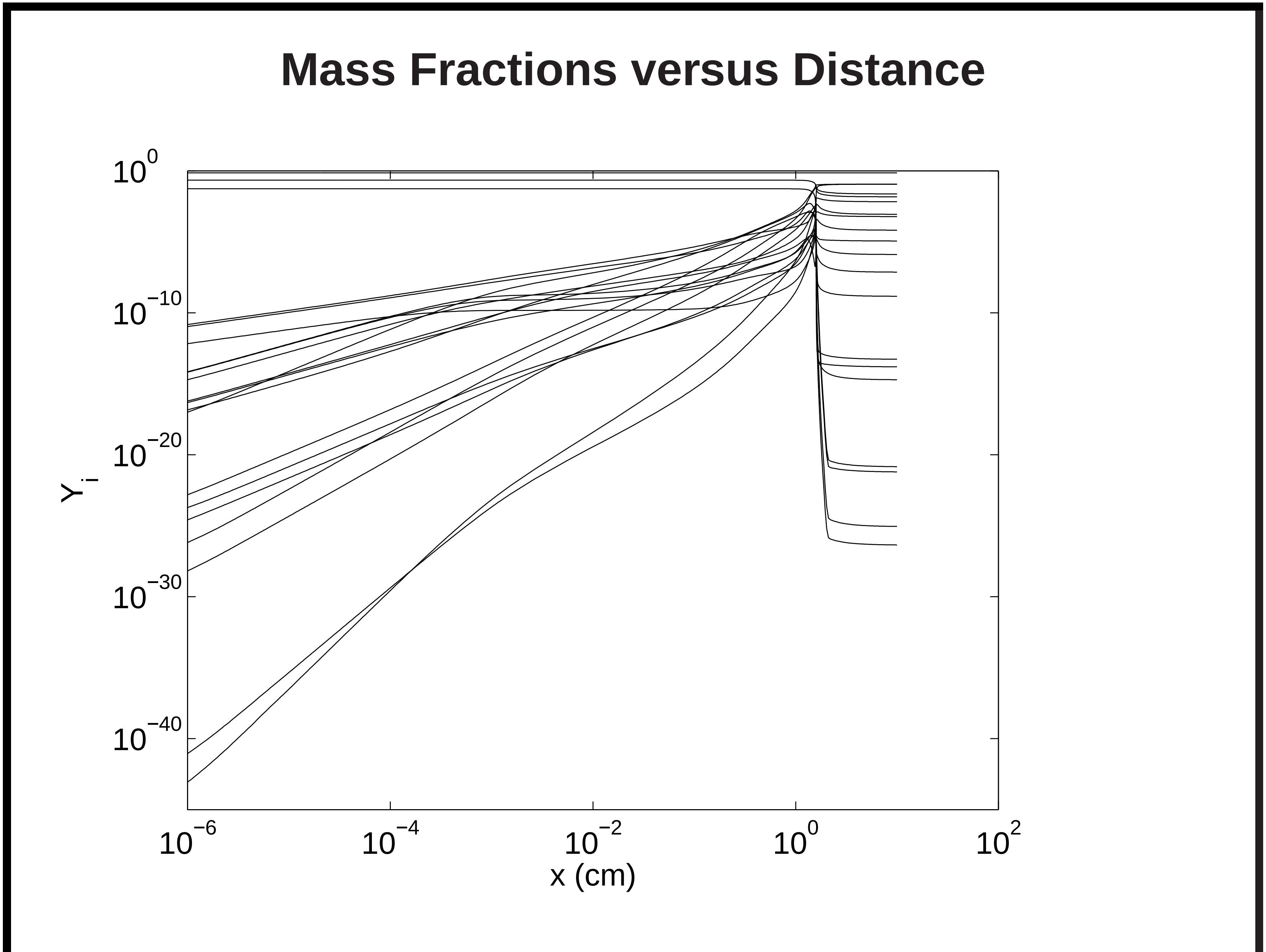
Complex shock topology reduces convergence rate to less than first order.

One-Dimensional Steady Reactive Euler Equations with Detailed Kinetics and Shock-Fitting

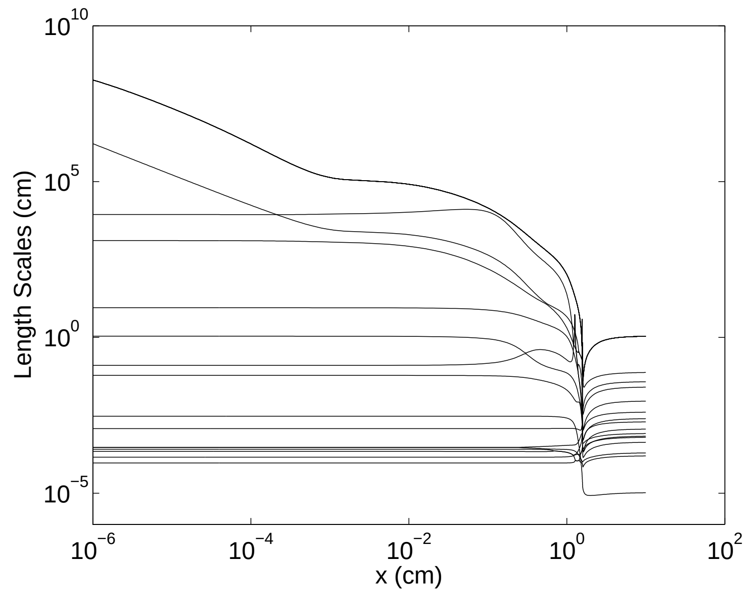
- see Powers & Paolucci, *AIAA J.*, 2005.
- CJ methane-air detonation: $CH_4 + 2O_2 + 7.52N_2$.
- $N = 21$ species, $J = 52$ reversible reactions.
- $p_o = 1\,atm, T_o = 298\,K$, $M_{CJ} = 5.13$.
- Rigorous spatial eigenvalue analysis gives precise estimates of advection/reaction length scales.

Verification and Validation of Detailed Kinetics Model

- Model exercised under isobaric, spatially homogeneous conditions to estimate ignition delay time.
- *Mathematical verification*: predicts similar ignition delay time as calculations of Petersen and Hanson: $30\ \mu s$ vs. $25\ \mu s$ at $T_o = 1500\ K$, $p_o = 150\ atm$.
- *Experimental validation*: predicts ignition delay time observations of Spadaccini and Colket: $115\ \mu s$ vs. $139\ \mu s$ at $T_o = 1705\ K$, $p_o = 6.6\ atm$.


Mass Fractions versus Distance
10^{0}
10^{-10}
10^{-20}
10^{-30}
10^{-40}
Y_i
10^{-6}
10^{-4}
10^{-2}
10^{0}
10^{2}
x (cm)

Eigenvalue Analysis: Length Scale Evolution



The finest length scale is $10^{-5}\ cm$. This scale arises from collision-based reaction constitutive models and suggests that a fully validated reactive flow model with detailed kinetics is obliged to include diffusive transport, which evolves on the same scales.

Discussion

- Verification of flow computations with embedded discontinuities exhibits less than first order convergence for shock-capturing and true high order convergence for shock-fitting of simple topologies.
- A physically rational model with detailed kinetics needs to be Navier-Stokes for validation; detailed kinetics with Euler can be useful, but is formally physically inconsistent.
- Algorithm craftsmanship can trump hardware improvements on certain problems.
- Reliance on hardware alone to achieve the gains described here would require many decades, even assuming the empirical Moore's Law continues to hold.

Discussion

"Fast computers help but it is the fast algorithms that make a big difference in our ability to simulate physical processes,"

P. Fast and M. J. Shelly, "Moore's Law and the Saffman-Taylor Instability," *JCP*, 2006.

Discussion

"If computational scientists and engineers are genuinely serious about these quality issues, they will take the responsibility and the relatively little extra effort to design their codes (or modify old ones) so that V2V can be confirmed by independent users."

P. J. Roache, "Building PDE Codes to be Verifiable and Validatable," *Comput. Sci. Eng.*, 2004.