Verified Calculation of Multiscale Combustion in Gaseous Mixtures

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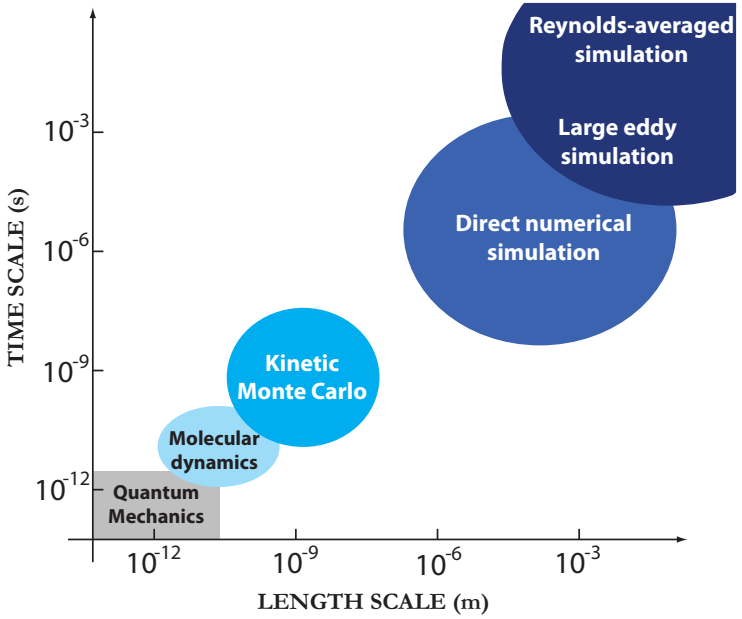
Outline

- Part I: Preliminaries
- Part II: Fundamental linear analysis of length scales of reacting flows with detailed chemistry and multicomponent transport. *(with al-Khateeb and Paolucci)*
- Part III: Direct Numerical Simulation (DNS) of complex reacting and inert flows with a) traditional methods, and b) a wavelet-based adaptive algorithm implemented in a massively parallel computing architecture. *(1D detonations with Romick and Aslam; 2D detonations of Zikoski and Paolucci, inert implosions with Voelkel and Romick using Zikoski's algorithm)*

Part I: Preliminaries

Some Semantics

- *Verification*: Solving the equations right—a math exercise.
- *Validation*: Solving the right equations—a physics exercise.
- *DNS*: a verified and validated computation that resolves *all* ranges of relevant continuum physical scales present.



"Research needs for future internal combustion engines," *Phys. Today, 2008.*

Hypothesis

DNS of fundamental compressible reactive flow fields (thus, detailed kinetics, viscous shocks, multi-component diffusion, etc. are represented, verified, and validated) is on a trajectory toward realization via advances in

- adaptive refinement algorithms, and
- massively parallel architectures.

Corollary I

A variety of modeling compromises, e.g.

- shock-capturing (FCT, PPM, ENO, WENO, etc.),
- implicit chemistry with operator splitting,
- low Mach number approximations,
- turbulence modeling (RANS, $k - \epsilon$, LES, etc.), or
- reduced/simplified kinetics, flamelet models,

need not be invoked *when and if* this difficult goal of DNS is realized; **simple low order explicit discretizations suffice if spatio-temporal grid resolution is achieved.**

Corollary II

Micro-device level DNS is feasible today; macro-device level DNS remains in the distant future.

Corollary III

A variety of challenging fundamental unsteady multi-dimensional compressible reacting flows are now becoming amenable to DNS, especially in the weakly unstable regime; **we would do well as a community to direct more of our efforts towards *unfiltered* simulations so as to more starkly expose the richness of unadulterated continuum scale physics.**

[Example (only briefly shown today): ordinary WENO shock-capturing applied to unstable detonations can dramatically corrupt the long time limit cycle behavior; retention of physical viscosity allows relaxation to a unique dissipative structure in the unstable regime.]

Part II: Fundamental Linear Analysis of Length Scales

Motivation

- To achieve DNS, the interplay between chemistry and transport needs to be captured.
- The interplay between reaction and diffusion length and time scales is well summarized by the classical formula (see Al-Khateeb, Powers, and Paoucci, *CTM*, 2012, to appear.)

$$\ell \sim \sqrt{D\,\tau}.$$

- Segregation of chemical dynamics from transport dynamics is a prevalent notion in reduced kinetics combustion modeling.
- But, can one rigorously mathematically verify a Navier-Stokes model without resolving the small length scale induced by fast reaction? *Answer: no.*
- Do micro-scales play a role in macro-scale non-linear dynamics? *Answer: in some cases, yes*; see Romick, Aslam, & Powers, 2012, *JFM*.

Illustrative Linear Model Problem

A linear one-species, one-dimensional unsteady model for reaction, advection, and diffusion:

$$\frac{\partial \psi}{\partial t} + u\frac{\partial \psi}{\partial x} = D\frac{\partial^2 \psi}{\partial x^2} - a\psi,$$

$$\psi(0,t) = \psi_u, \quad \left.\frac{\partial \psi}{\partial x}\right|_{x=\mathtt{L}} = 0, \qquad \psi(x,0) = \psi_u.$$

Time scale spectrum

For the spatially homogenous version: $\psi_h(t) = \psi_u \exp(-at)$,

reaction time constant: $\tau = \dfrac{1}{a} \implies \Delta t \ll \tau.$

Length Scale Spectrum

- The steady structure:

$$\psi_s(x) = \psi_u \left(\frac{\exp(\mu_1 x) - \exp(\mu_2 x)}{1 - \frac{\mu_1}{\mu_2} \exp(\mathrm{L}(\mu_1 - \mu_2))} + \exp(\mu_2 x) \right),$$

$$\mu_1 = \frac{u}{2D} \left(1 + \sqrt{1 + \frac{4aD}{u^2}} \right), \qquad \mu_2 = \frac{u}{2D} \left(1 - \sqrt{1 + \frac{4aD}{u^2}} \right),$$

$$\ell_i = \left| \frac{1}{\mu_i} \right|.$$

- For fast reaction ($a \gg u^2/D$):

$$\ell_1 = \ell_2 = \sqrt{\frac{D}{a}} = \sqrt{D\tau} \implies \Delta x \ll \sqrt{D\tau}.$$

Spatio-Temporal Spectrum

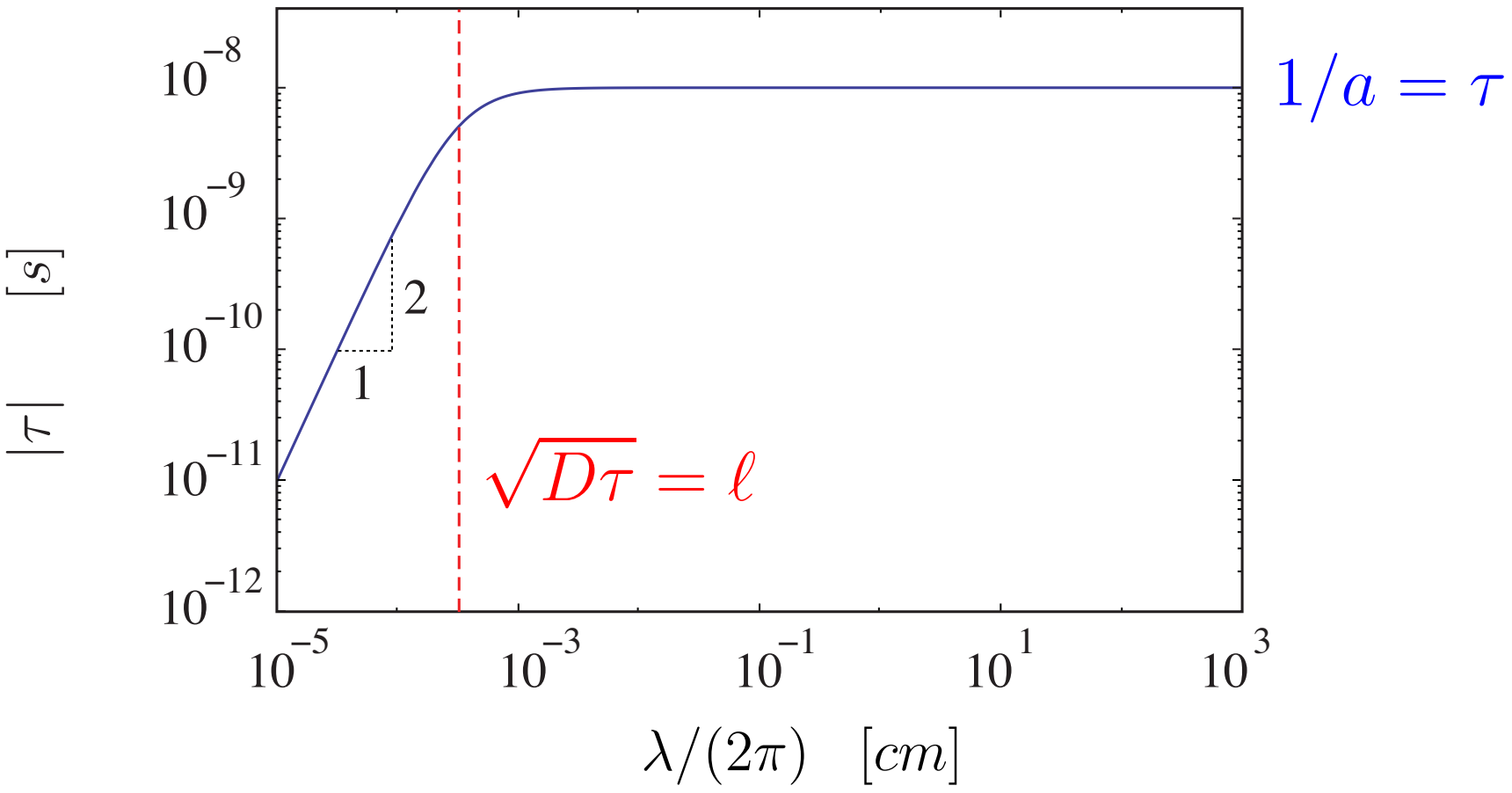
$$\psi(x,t) = \Psi(t) e^{\mathbf{i}kx} \quad \Rightarrow \quad \frac{d\Psi}{dt} = \left(-a \left(1 + \frac{\mathbf{i}ku}{a} + \frac{Dk^2}{a} \right) t \right) \Psi.$$

$$\Psi(t) = C \exp \left(-a \left(1 + \frac{\mathbf{i}ku}{a} + \frac{Dk^2}{a} \right) t \right).$$

- For long length scales: $\lim_{k \to 0} \tau = \lim_{\lambda \to \infty} \tau = \frac{1}{a},$
- For fine length scales: $\lim_{k \to \infty} \tau = \lim_{\lambda \to 0} \tau = \frac{\lambda^2}{4\pi^2} \frac{1}{D},$

$$\Bigg\} \quad \mathcal{S}_t = \left(\frac{2\pi}{\lambda} \sqrt{\frac{D}{a}} \right)^2 .$$

- Balance between reaction and diffusion at $k \equiv \frac{2\pi}{\lambda} = \sqrt{\frac{a}{D}} = 1/\ell,$



- Similar to $H_2 - air$: $\tau = 1/a = 10^{-8}\ s, D = 10\ cm^2/s,$
- $\ell = \sqrt{\frac{D}{a}} = \sqrt{D\tau} = 3.2 \times 10^{-4}\ cm.$

Laminar Premixed Flames

Adopted Assumptions:

- One-dimensional,
- Low Mach number,
- Neglect thermal diffusion effects and body forces.

Governing Equations:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) = 0,$$

$$\rho \frac{\partial h}{\partial t} + \rho u \frac{\partial h}{\partial x} + \frac{\partial j^q}{\partial x} = 0,$$

$$\rho \frac{\partial y_l}{\partial t} + \rho u \frac{\partial y_l}{\partial x} + \frac{\partial j_l^m}{\partial x} = 0, \quad l = 1, \ldots, L-1,$$

$$\rho \frac{\partial Y_i}{\partial t} + \rho u \frac{\partial Y_i}{\partial x} + \frac{\partial j_i^m}{\partial x} = \dot{\omega}_i \bar{m}_i, \quad i = 1, \ldots, N-L.$$

- Unsteady spatially homogeneous reactive system:

$$\frac{d\mathbf{z}(t)}{dt} = \mathbf{f}\left(\mathbf{z}(t)\right), \qquad \mathbf{z}(t) \in \mathbb{R}^N, \quad \mathbf{f} : \mathbb{R}^N \rightarrow \mathbb{R}^N.$$

$$\mathbf{0} = (\mathbf{J} - \lambda \mathbf{I}) \cdot \boldsymbol{v}.$$

$$\mathcal{S}_t = \frac{\tau_{slowest}}{\tau_{fastest}}, \quad \tau_i = \frac{1}{|Re(\lambda_i)|}, \qquad i = 1, \ldots, R \leq N - L.$$

- Steady spatially inhomogeneous reactive system:

$$\tilde{\mathbf{B}}\left(\tilde{\mathbf{z}}(x)\right) \cdot \frac{d\tilde{\mathbf{z}}(x)}{dx} = \tilde{\mathbf{f}}\left(\tilde{\mathbf{z}}(x)\right), \qquad \tilde{\mathbf{z}}(x) \in \mathbb{R}^{2N+2}, \quad \tilde{\mathbf{f}} : \mathbb{R}^{2N+2} \rightarrow \mathbb{R}^{2N+2}.$$

$$\tilde{\lambda}\tilde{\mathbf{B}} \cdot \tilde{\boldsymbol{v}} = \tilde{\mathbf{J}} \cdot \tilde{\boldsymbol{v}}.$$

$$\mathcal{S}_x = \frac{\ell_{coarsest}}{\ell_{finest}}, \quad \ell_i = \frac{1}{|Re(\tilde{\lambda}_i)|}, \qquad i = 1, \ldots, 2N - L.$$

Laminar Premixed Hydrogen–Air Flame

- Standard detailed mechanism[a]; $N = 9$ species, $L = 3$ atomic elements, and $J = 19$ reversible reactions,
- stoichiometric hydrogen-air: $2H_2 + (O_2 + 3.76N_2)$,
- adiabatic and isobaric: $T_u = 800\ K,\ p = 1\ atm$,
- calorically imperfect ideal gases mixture,
- neglect Soret effect, Dufour effect, and body forces,
- CHEMKIN and IMSL are employed.

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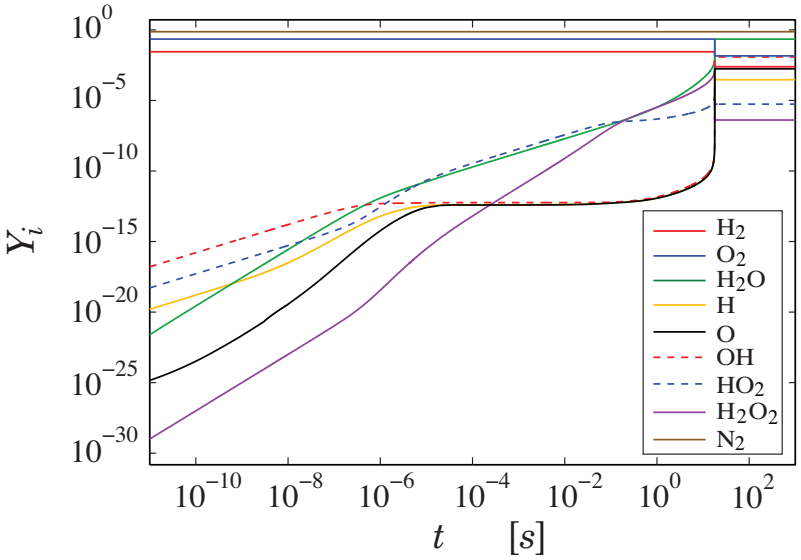
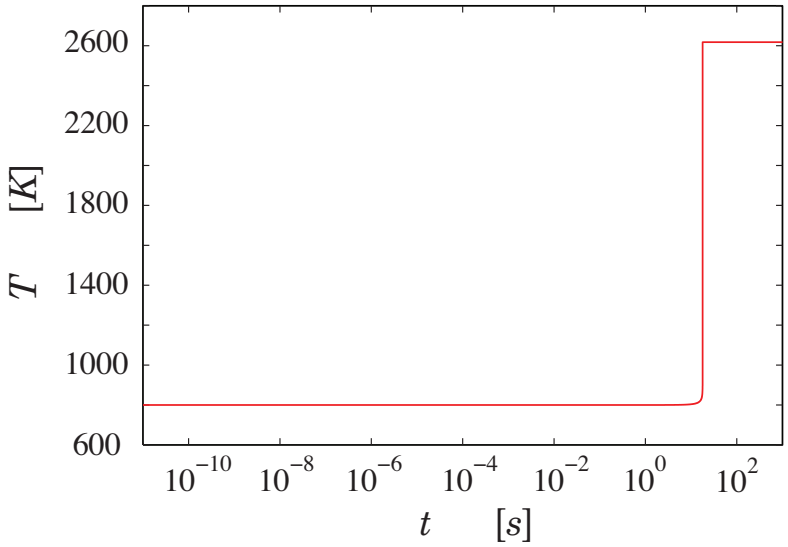
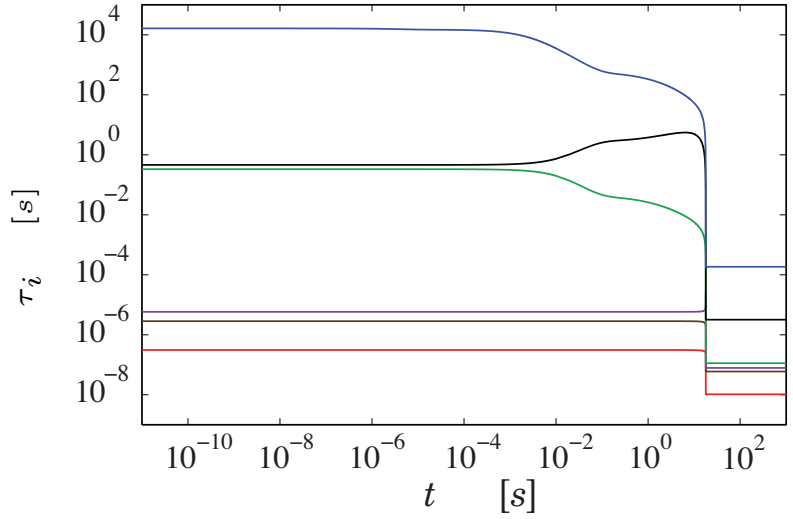
[a] J. A. Miller, R. E. Mitchell, M. D. Smooke, and R. J. Kee, *Proc. Combust. Ins.* **19**, p. 181, 1982.

- Unsteady spatially homogeneous reactive system:





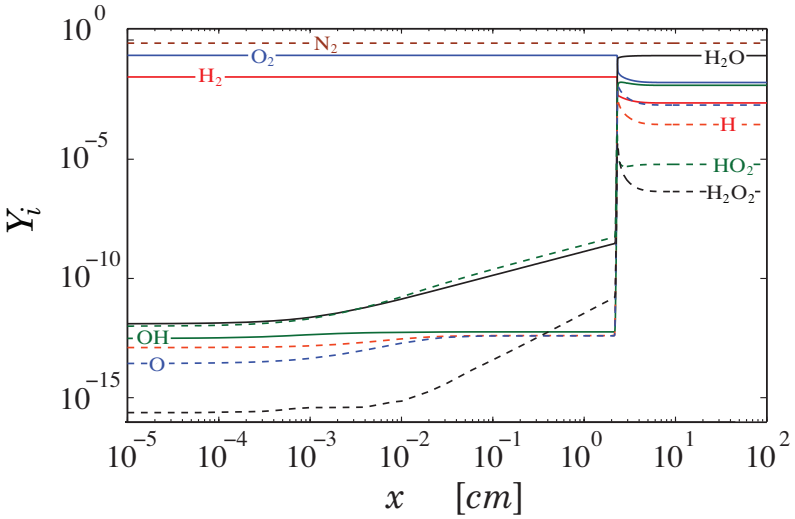


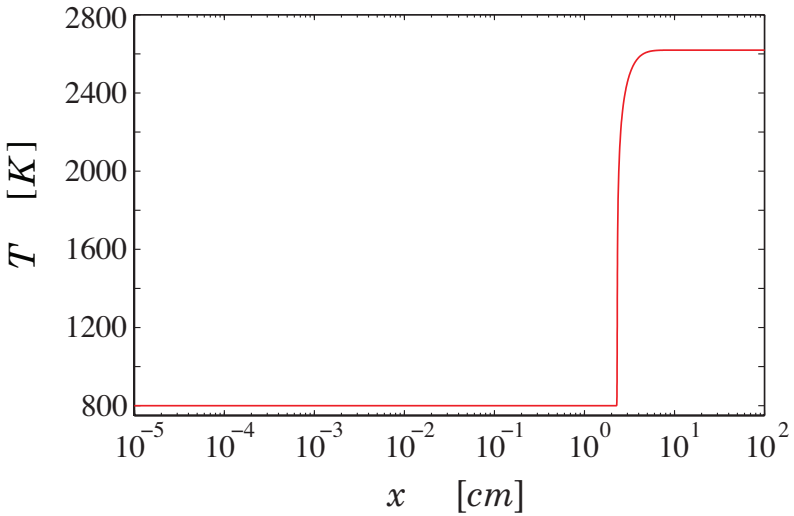
$\tau_{slowest} = 1.8\times10^{-2}\ s$

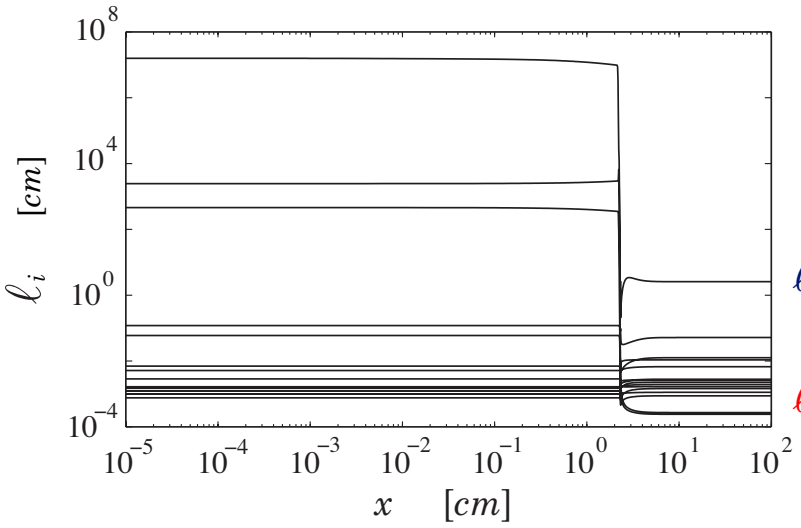
$\tau_{fastest} = 1.0\times10^{-8}\ s$

$\mathcal{S}_t \sim \mathcal{O}\left(10^4\right).$

- Steady spatially inhomogeneous reactive system:[a]







$\ell_{coarsest} = 2.6\times10^{0}\ cm$

$\ell_{finest} = 2.4\times10^{-4}\ cm$

$\mathcal{S}_x \sim \mathcal{O}\left(10^4\right).$

[a] A. N. Al-Khateeb, J. M. Powers, and S. Paolucci, *Comm. Comp. Phys.* 8(2): 304, 2010.

Spatio-Temporal Spectrum

- PDEs $\longrightarrow$ $2N+2$ PDAEs,

$$\mathbf{A}(\mathbf{z}) \cdot \frac{\partial \mathbf{z}}{\partial t} + \mathbf{B}(\mathbf{z}) \cdot \frac{\partial \mathbf{z}}{\partial x} = \mathbf{f}(\mathbf{z}).$$

- Spatially homogeneous system at chemical equilibrium subjected to a spatially inhomogeneous perturbation, $\mathbf{z}' = \mathbf{z} - \mathbf{z}^e$,

$$\mathbf{A}^e \cdot \frac{\partial \mathbf{z}'}{\partial t} + \mathbf{B}^e \cdot \frac{\partial \mathbf{z}'}{\partial x} = \mathbf{J}^e \cdot \mathbf{z}'.$$

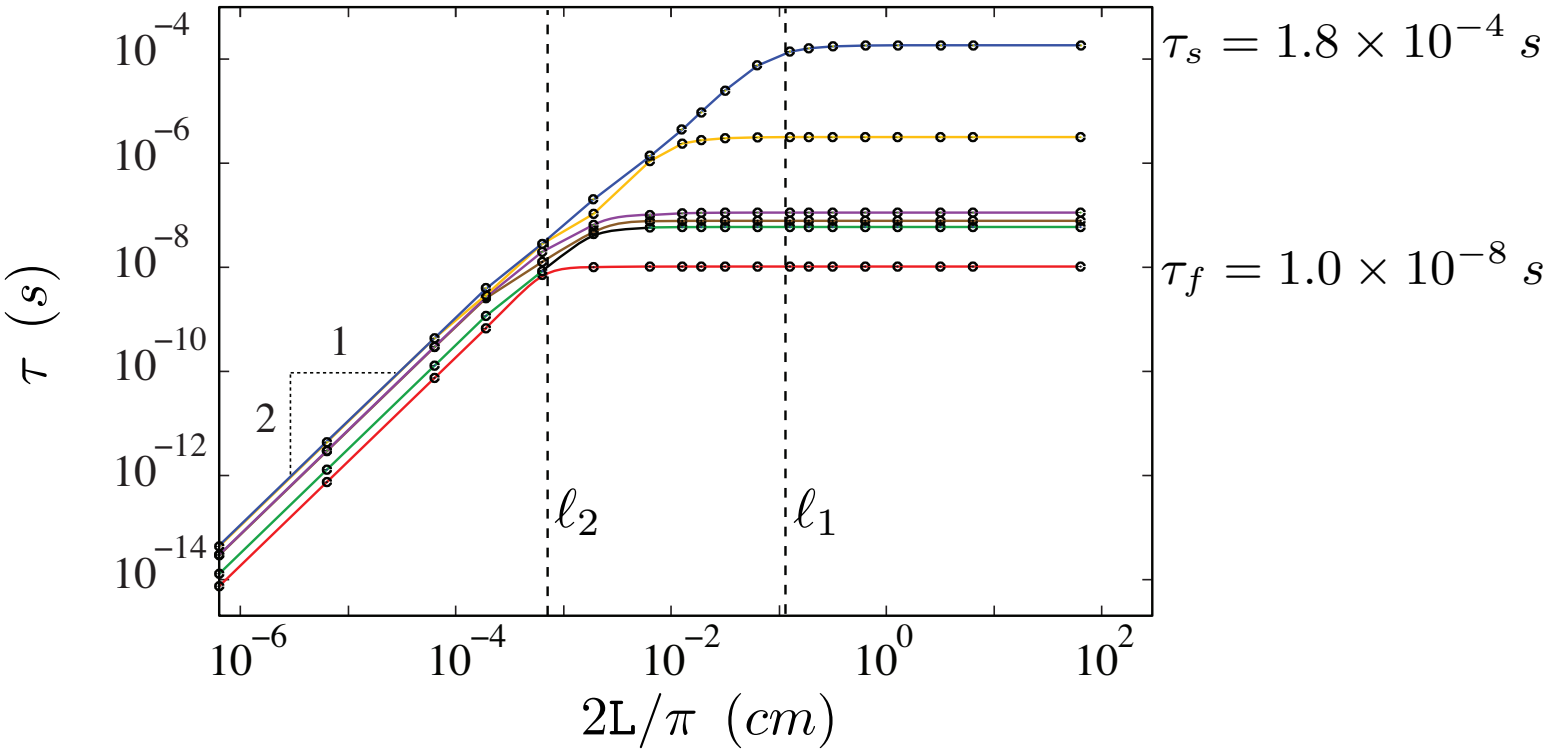
- Spatially discretized spectrum,

$$\boldsymbol{\mathcal{A}}^e \cdot \frac{d\boldsymbol{\mathcal{Z}}}{dt} = (\boldsymbol{\mathcal{J}}^e - \boldsymbol{\mathcal{B}}^e) \cdot \boldsymbol{\mathcal{Z}}, \qquad \boldsymbol{\mathcal{Z}} \in \mathbb{R}^{2\mathcal{N}(N+1)}.$$

- The time scales of the generalized eigenvalue problem,

$$\tau_i = \frac{1}{|Re\,(\lambda_i)|}, \quad i = 1, \ldots, (\mathcal{N}-1)(N-1).$$

- $D_{mix} = \frac{1}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} \mathfrak{D}_{ij}$,
- $\ell_1 = \sqrt{D_{mix} \tau_s} = 1.1 \times 10^{-1}\ cm$,
- $\ell_2 = \sqrt{D_{mix} \tau_f} = 8.0 \times 10^{-4}\ cm \approx \ell_{finest} = 2.4 \times 10^{-4}\ cm$.

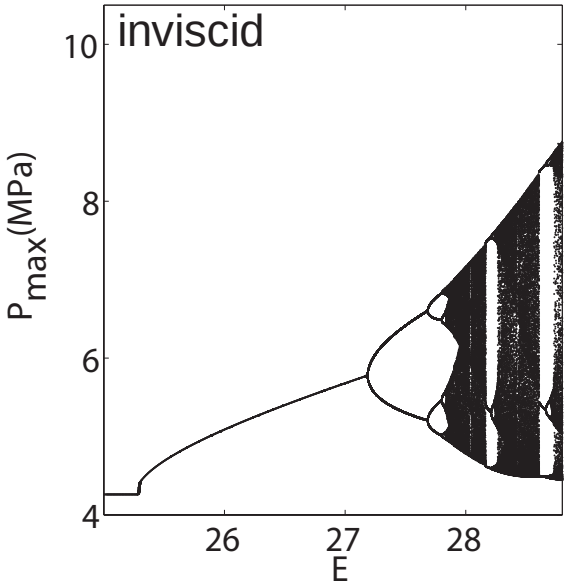


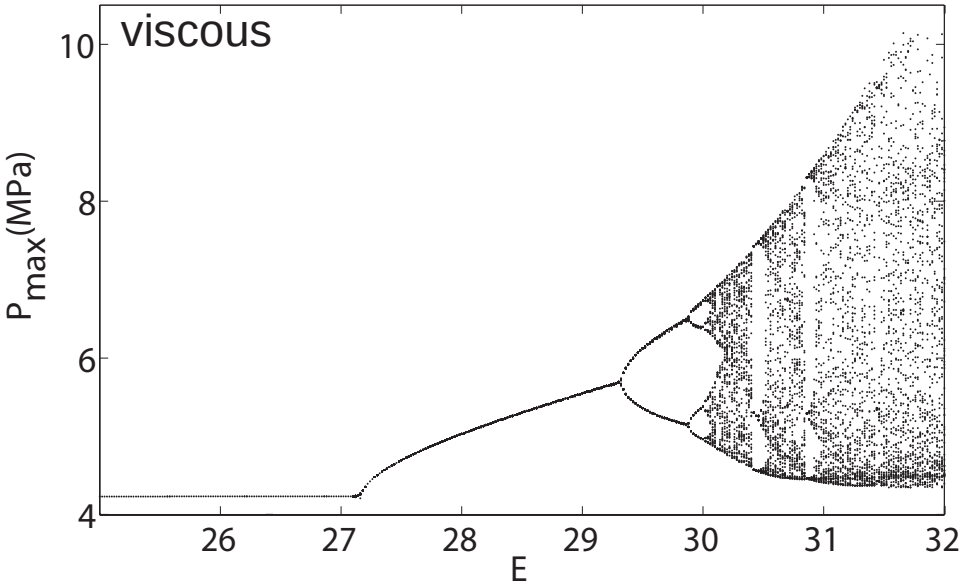
Conclusions: Part II

- Time and length scales are coupled.
- Coarse wavelength modes have time scales dominated by reaction.
- Short wavelength modes have time scales dominated by diffusion.
- Fourier modal analysis reveals a cutoff length scale for which time scales are dictated by a balance between transport and chemistry.
- Fine scales, temporal and spatial, are essential to resolve reacting systems; the finest length scale is related to the finest time scale by $\ell \sim \sqrt{D\tau}$.
- For a $p = 1\ atm, H_2 + air$ laminar flame, the length scale where fast reaction balances diffusion is $\sim 2\ \mu m$, the necessary scale for a DNS.

Part III: DNS of Complex Reacting and Inert Flows

Effect of Diffusion on Detonation Dynamics: 1D, 1-Step





- Small physical diffusion significantly delays transition to instability.
- In the unstable regime, small diffusion has a large role in determining role for the long time dynamics.
- Romick, Aslam, Powers, *JFM*, 2012.

Effect of Diffusion on Detonation Dynamics: 1D, N-Step

Case Examined

- Romick, Aslam, Powers, AIAA ASM, 2012
- Overdriven detonations with ambient conditions of $0.421\ atm$ and $293.15\ K$
- Initial stoichiometric mixture of $2H_2 + O_2 + 3.76N_2$
- Detailed kinetics: 9 species, 19 reversible reactions
- a) Inviscid via shock-fitting, and b) viscous (multicomponent diffusion of a viscous, heat conducting fluids) via WAMR studied
- $D_{CJ} \sim 1961\ m/s$
- Overdrive is defined as $f = D_o^2/D_{CJ}^2$
- Overdrives of $1.025 < f < 1.150$ were examined

Continuum Scales

- The mean-free path scale is the cut-off minimum length scale associated with continuum theories.
- A simple estimate for this scale is given by Vincenti and Kruger (1967):

$$\lambda = \frac{\overline{M}}{\sqrt{2}\pi \mathcal{N}_A \rho d^2} \sim \mathcal{O}\left(10^{-6}\ cm\right). \tag{1}$$

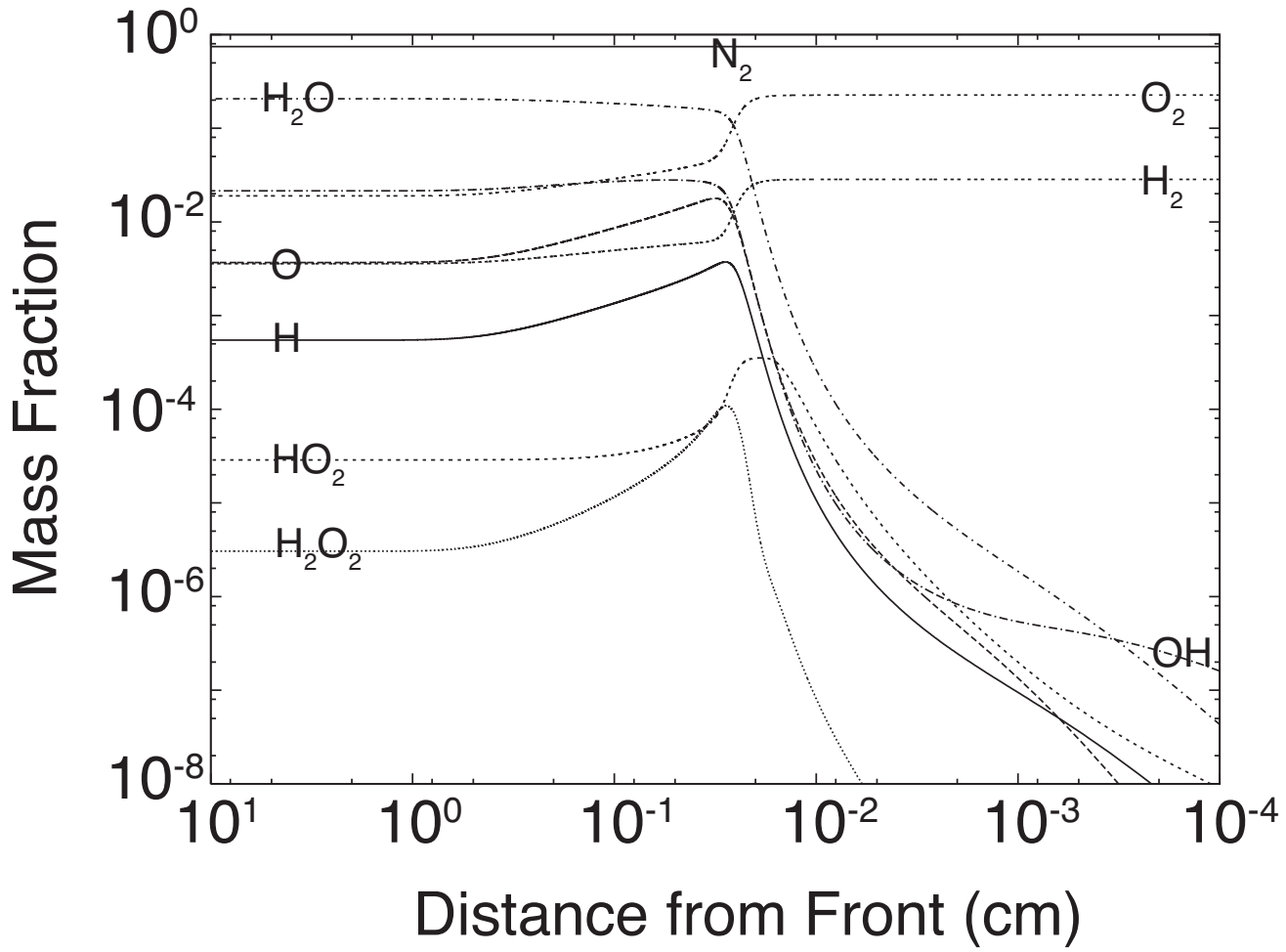
- The finest reaction length scale is $L_r \sim \mathcal{O}\left(10^{-4}\ cm\right)$.
- A simple estimate of a viscous length scale is:

$$L_\mu = \frac{\nu}{c} = \frac{6 \times 10^{-1}\ cm^2/s}{9 \times 10^4\ cm/s} \sim \mathcal{O}\left(10^{-5}\ cm\right). \tag{2}$$

- $\lambda < L_\mu < L_r$

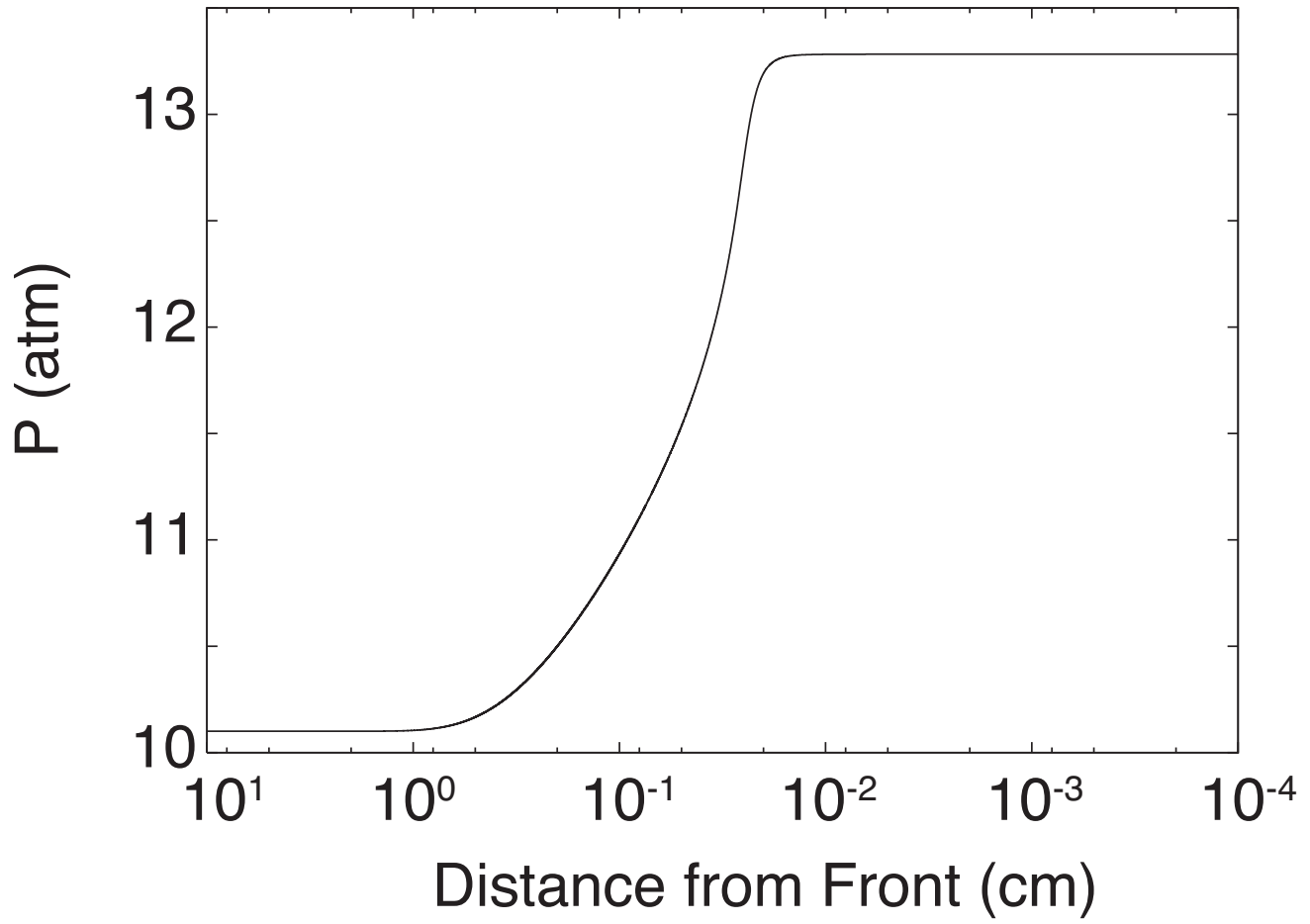
Inviscid Steady-State: Mass Fractions

$f = 1.15$



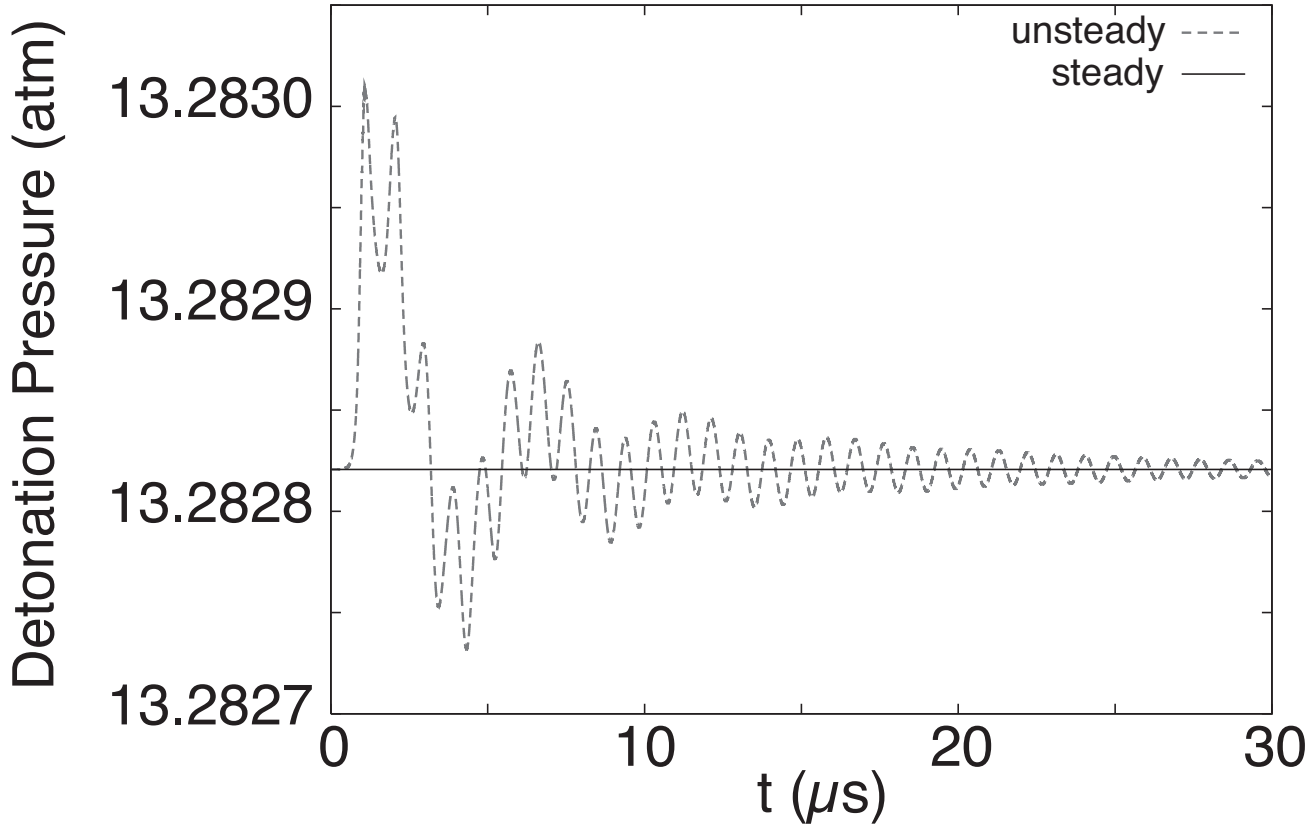
Inviscid Steady-State: Pressure

$f = 1.15$

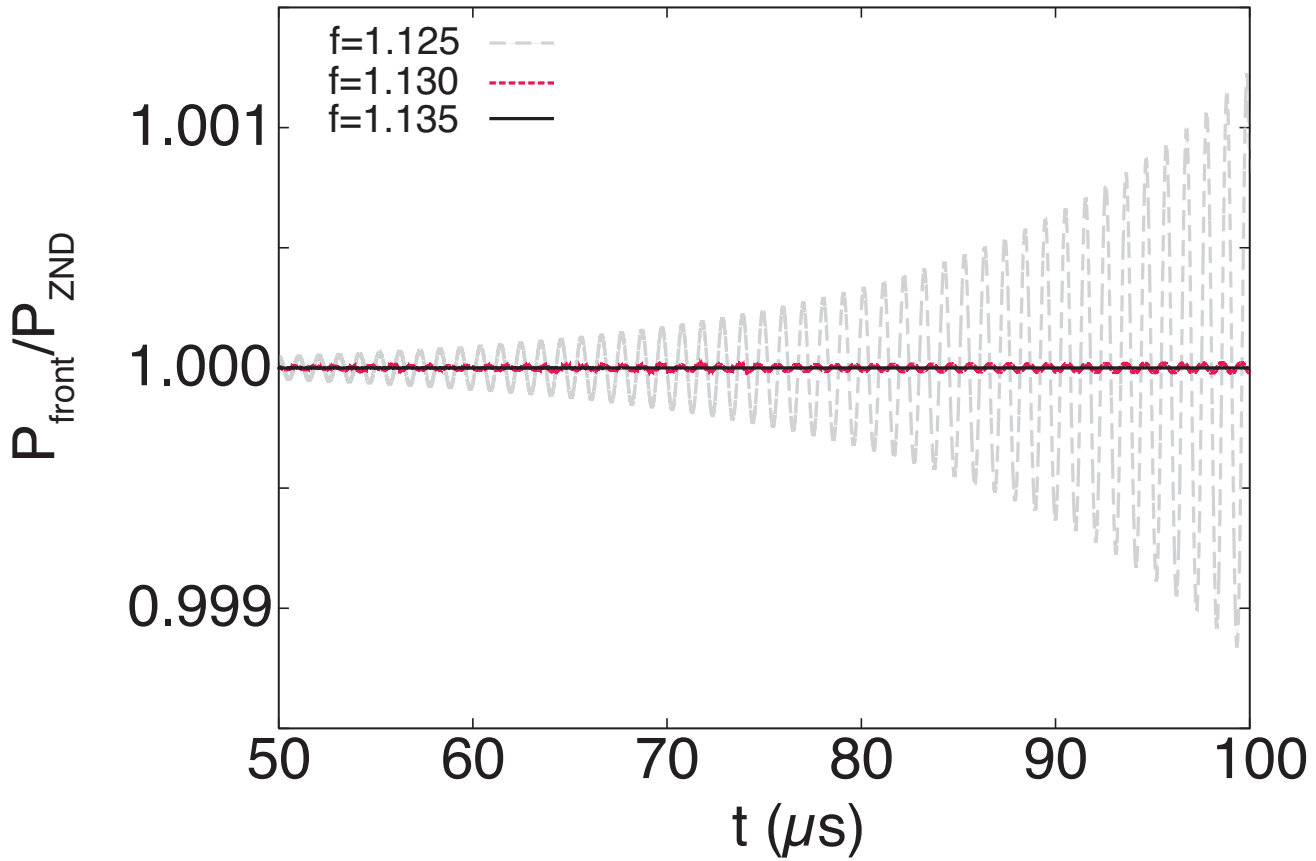


Inviscid Transient Behavior: Stable Detonation

$f = 1.15$

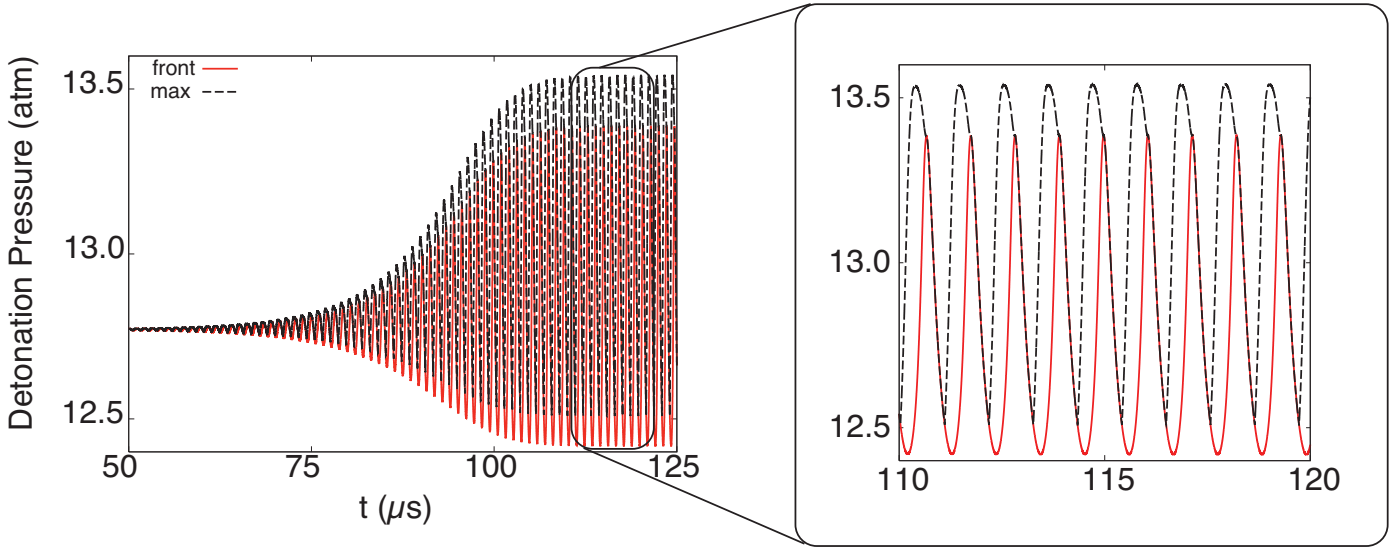


Near Neutral Stability



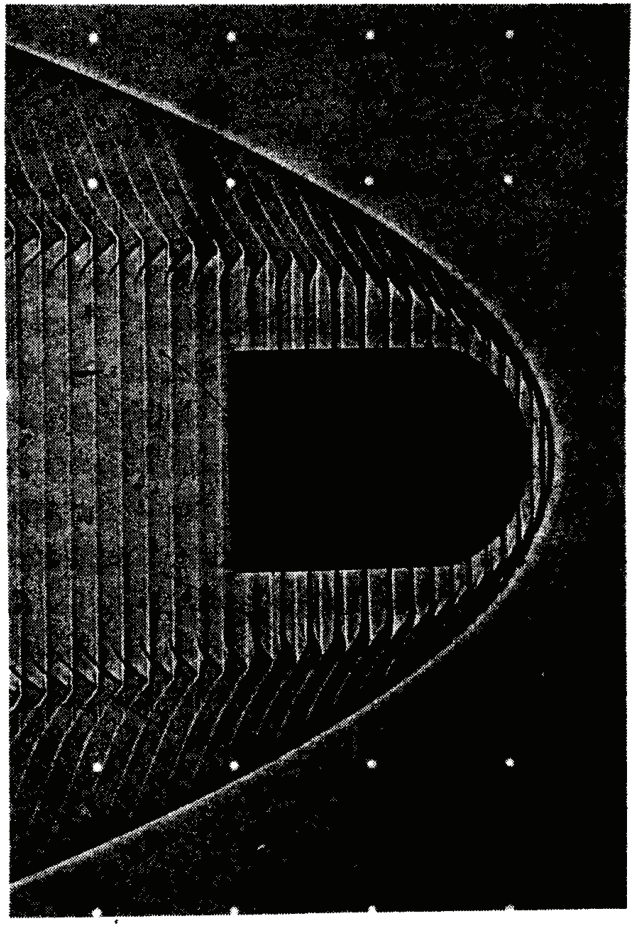
Inviscid Transient Behavior: Unstable Detonation

$f = 1.10$



- Frequency of $0.97\ MHz$ agrees well with both the frequency, $1.04\ MHz$, observed by Lehr (*Astro. Acta*, 1972) in experiments and the frequency, $1.06\ MHz$, predicted by Yungster and Radhakrishan.
- The maximum detonation front pressure predicted, $13.5\ atm$, is similar to the value of $14.0\ atm$ found by Daimon and Matsuo.

Validation: Recovering Lehr's High Frequency Instability

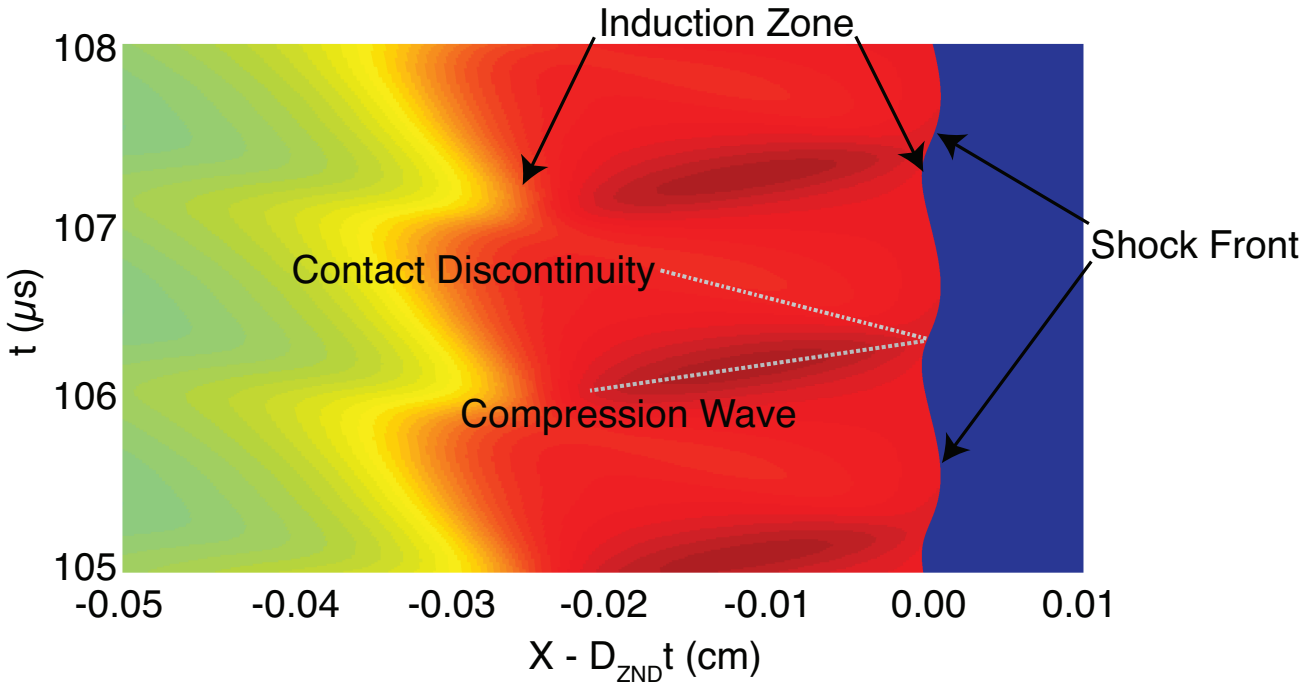


Lehr, *Astro. Acta*, 1972

- Experiment of shock-induced combustion in flow around a projectile in an ambient stoichiometric mixture of $2H_2 + O_2 + 3.76N_2$ at $0.421\ atm.$
- Projectile velocity yields an equivalent overdrive of $f \approx 1.1$
- The observed frequency was approximately $1.04\ MHz$
- Compare to 1D computation' prediction: $0.97\ MHz$

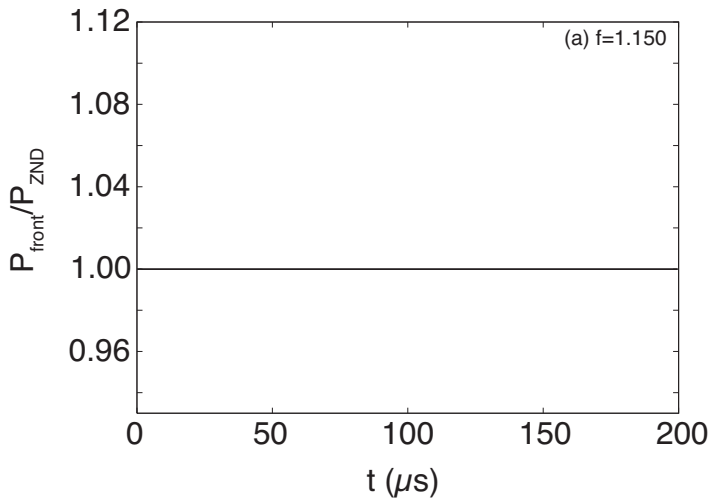
Unstable, Inviscid Detonation: x-t Diagram

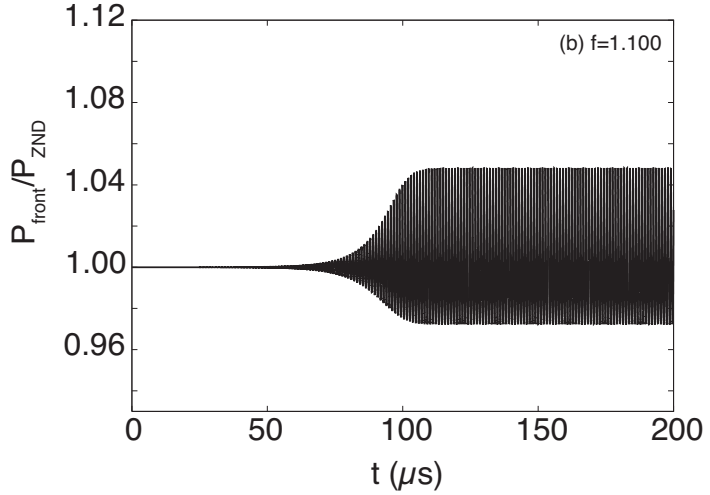
$f = 1.10$

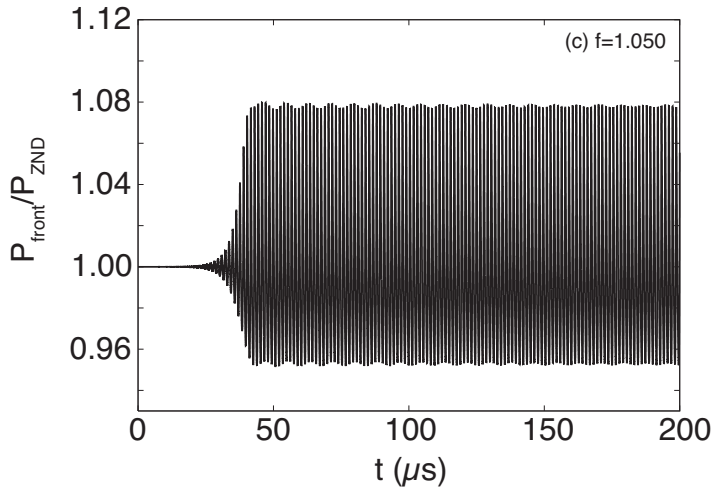


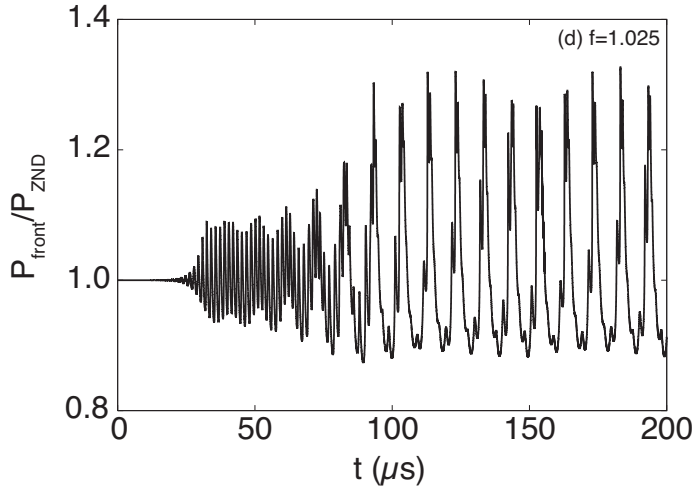
A x-t diagram of density in a Galilean reference frame traveling at $2057\ m/s$.

Inviscid Transient Behavior: Various Overdrives

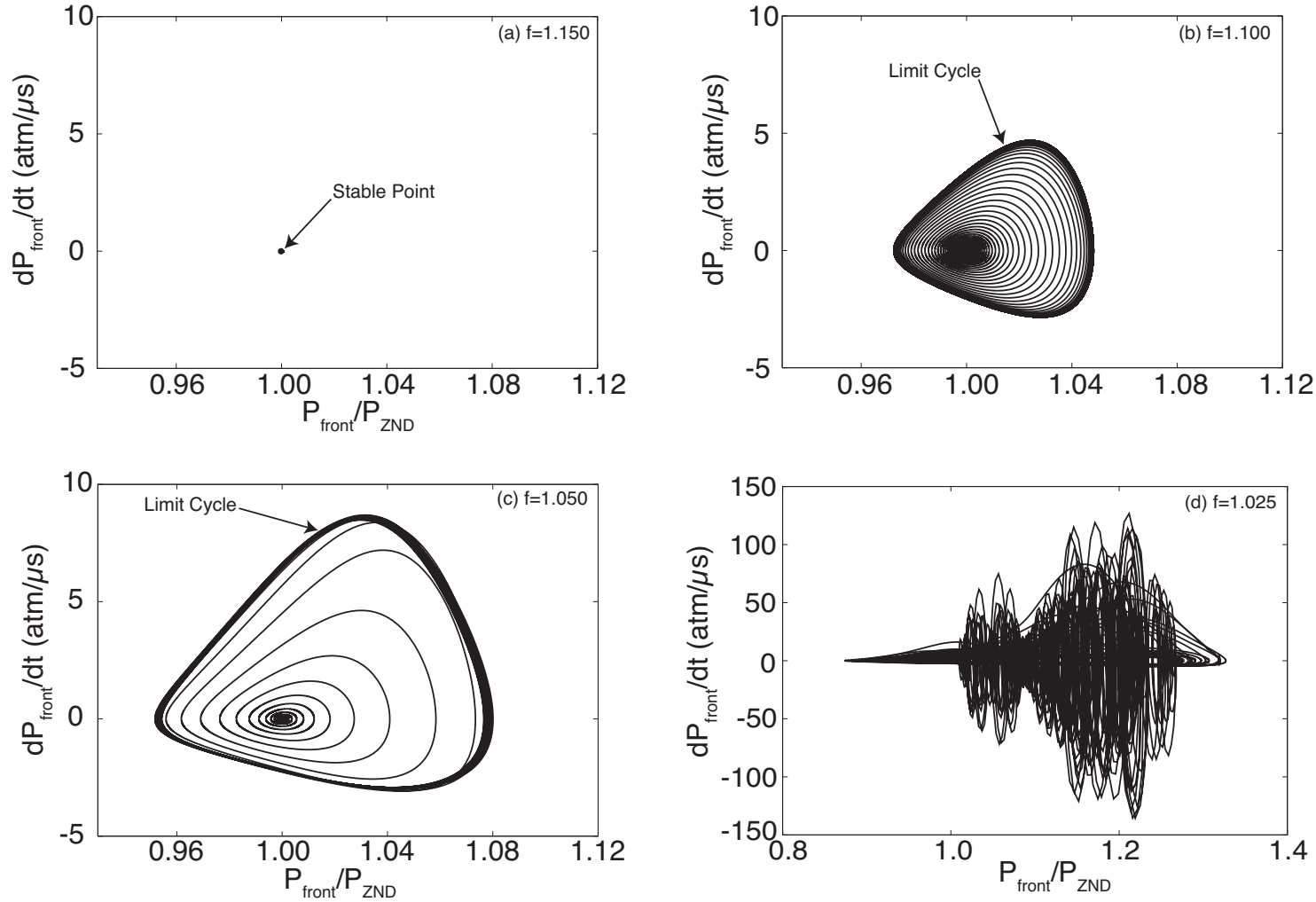






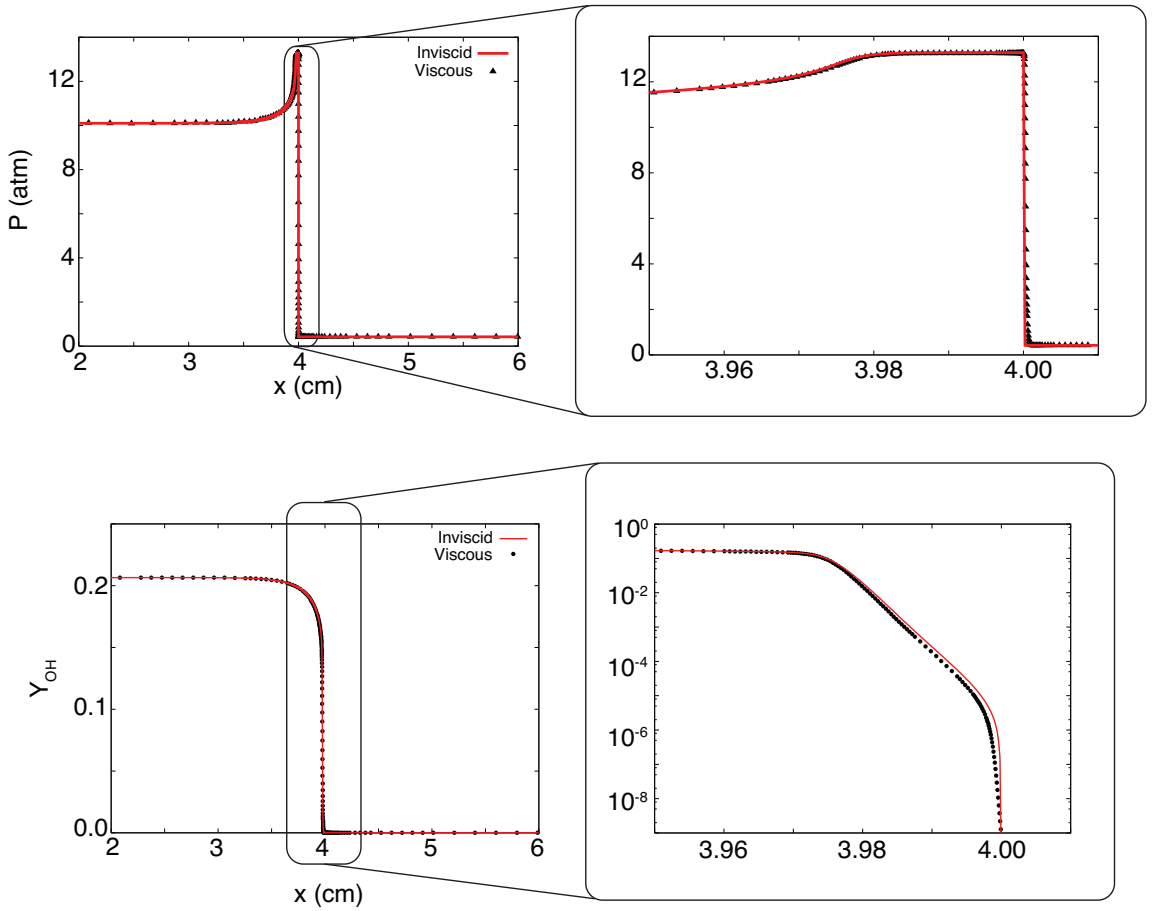


Inviscid Phase Portraits: Various Overdrives



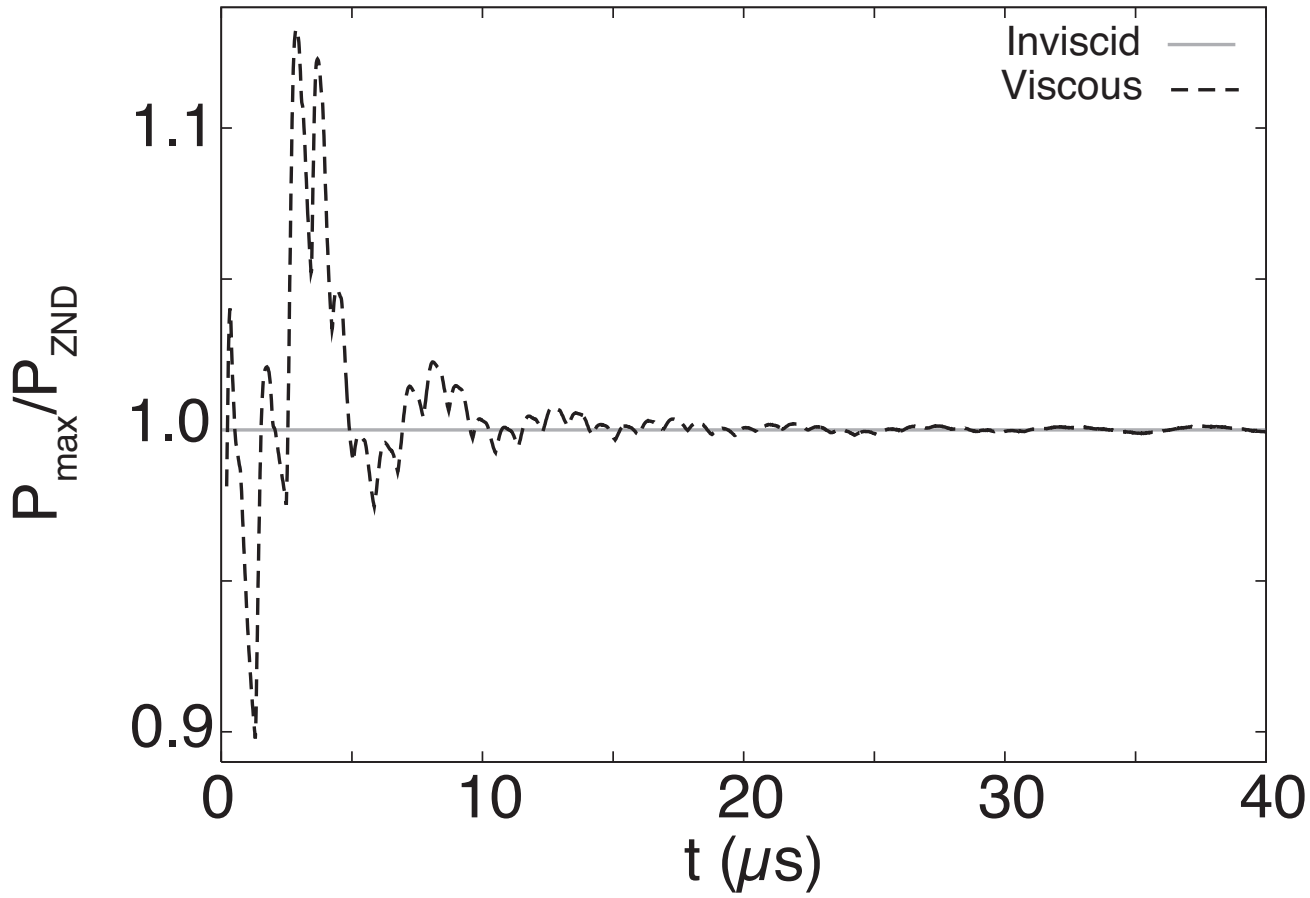
Stable, Viscous Detonation: Long Time Structure

$f = 1.15$



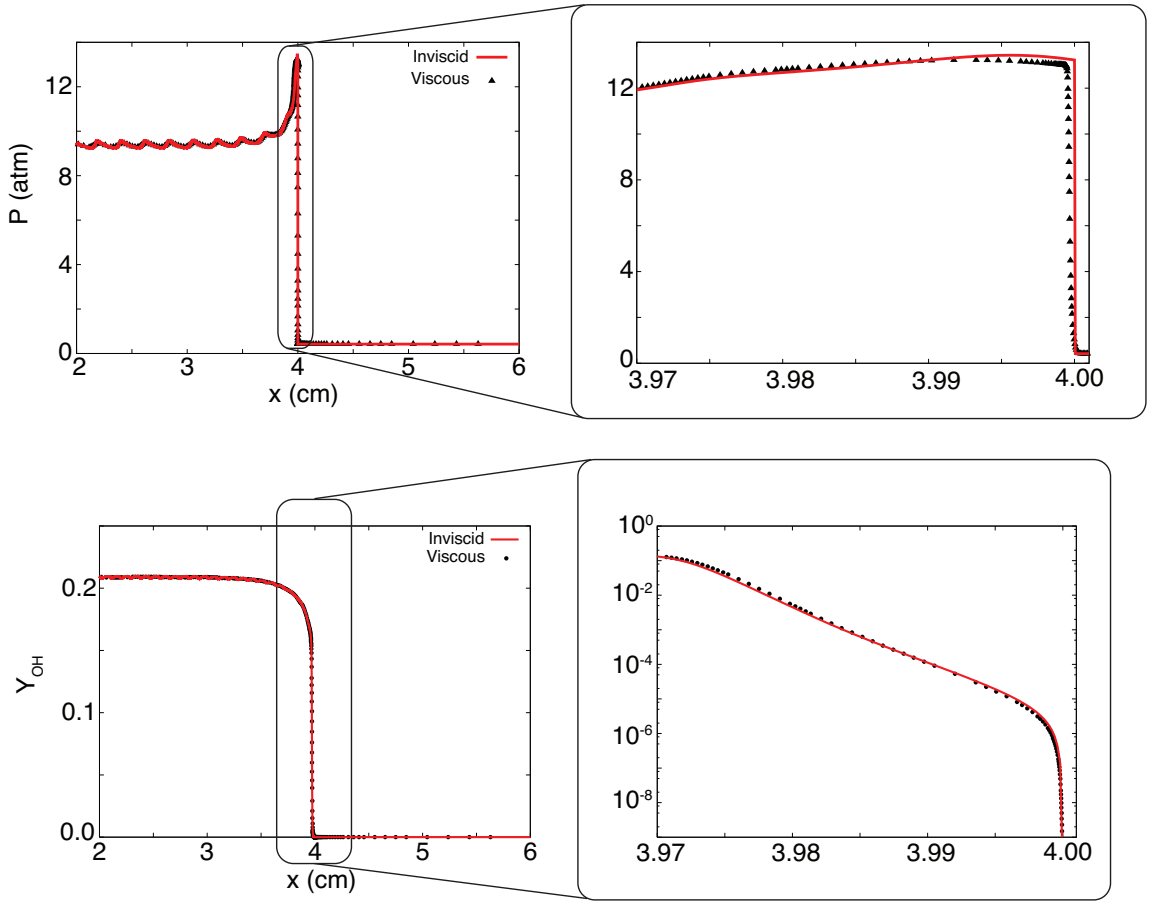
Stable, Viscous Detonation: Transient Behavior

$f = 1.15$



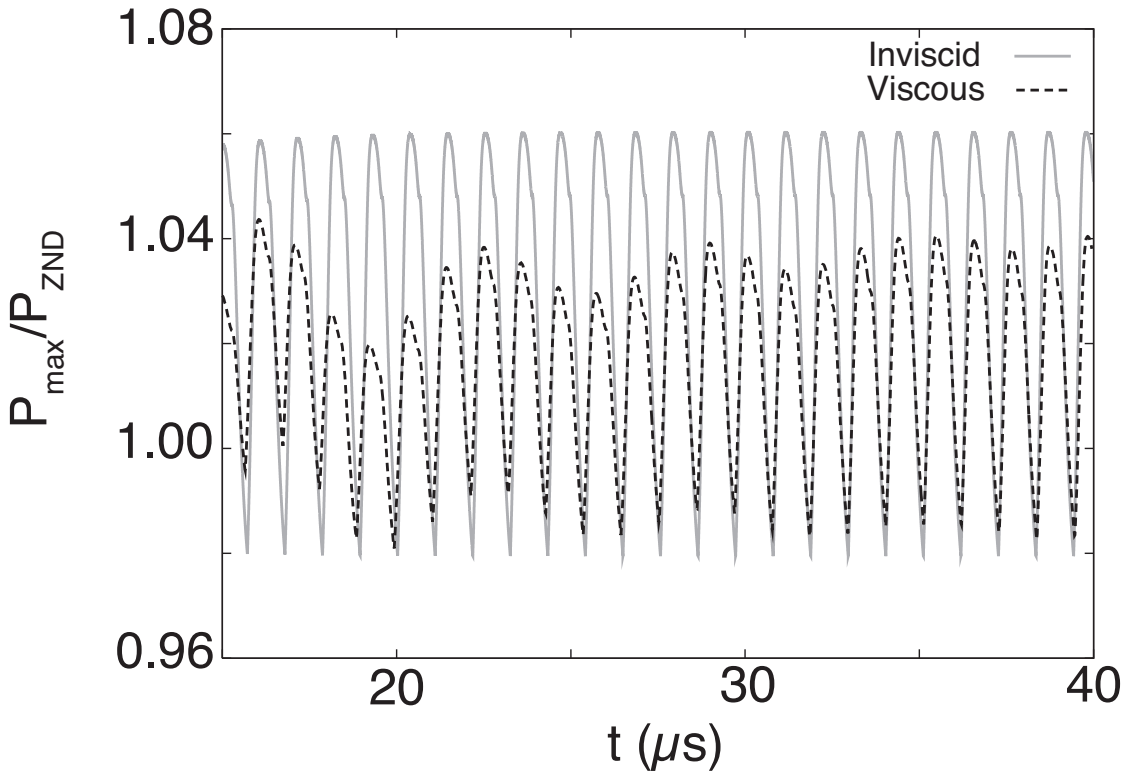
Unstable, Viscous Detonation: Long Time Structure

$f = 1.10$



Unstable, Viscous Detonation: Transient Behavior

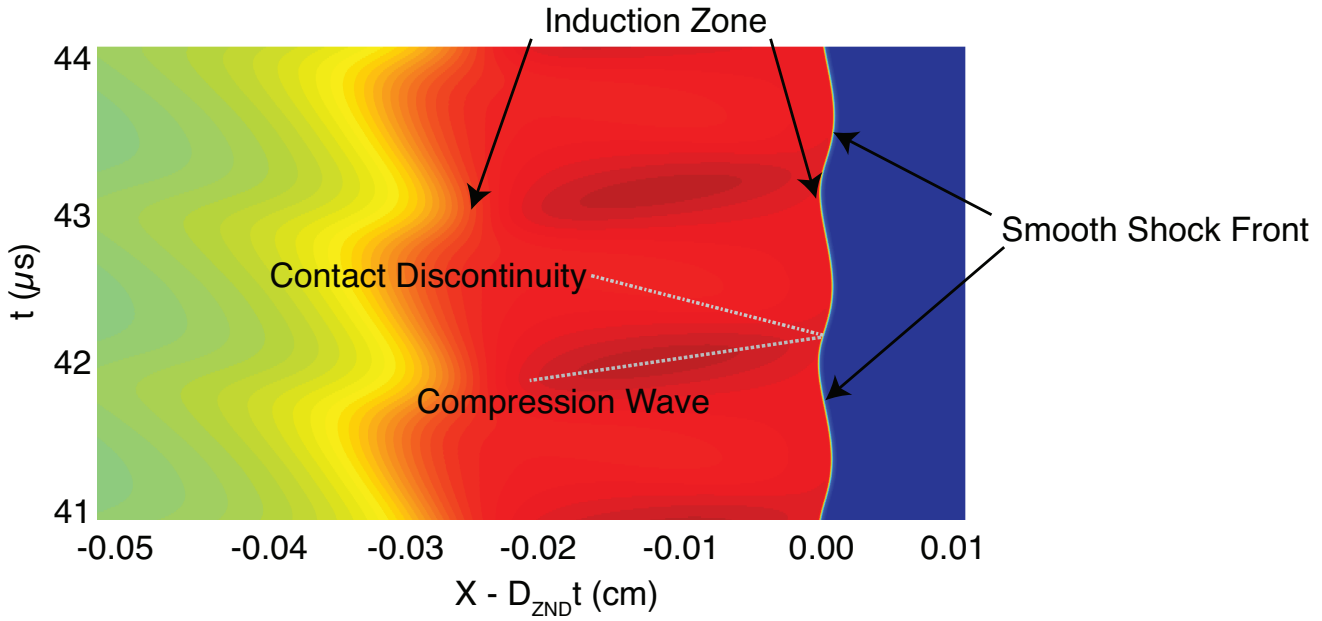
$f = 1.10$



The addition of viscous effects have a stabilizing effect, decreasing the amplitude of the oscillations by $\sim 25\%$.

Unstable, Viscous Detonation: x-t Diagram

$f = 1.10$



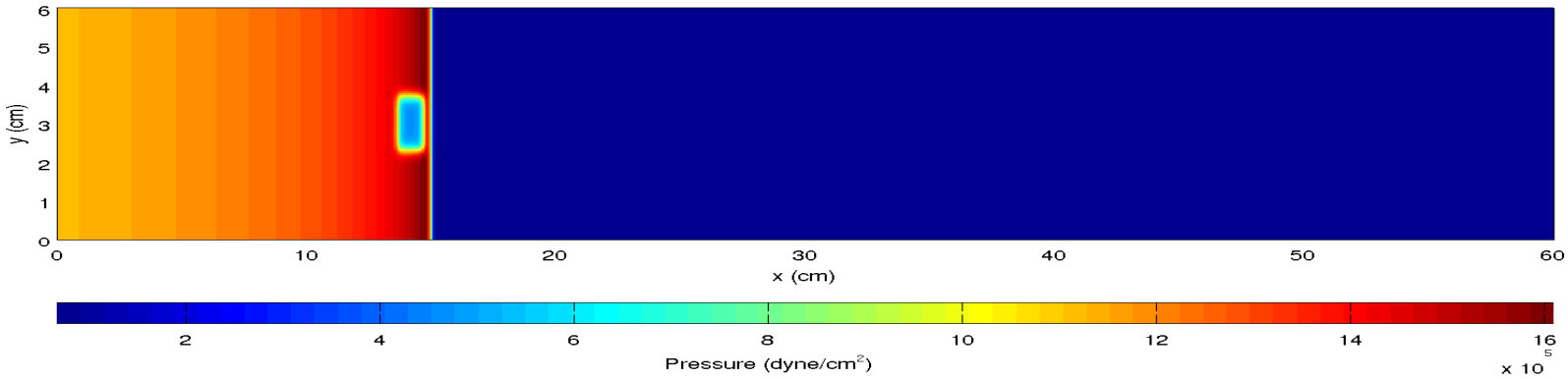
A x-t diagram of density in a Galilean reference frame traveling at $2057\ m/s$.

2D Viscous Detonation in Hydrogen-Air

- Wavelet Adaptive Multilevel Representation (WAMR, Zikoski and Paolucci), resolves multi-scale solutions in an adaptive fashion.
- User-defined error control guarantees a verified solution.
- The algorithm has been implemented with an MPI-based domain decomposition in a massively parallel computational architecture with linear scaling to at least 10^3 processors.

2-D Viscous Detonation

Initial Conditions:

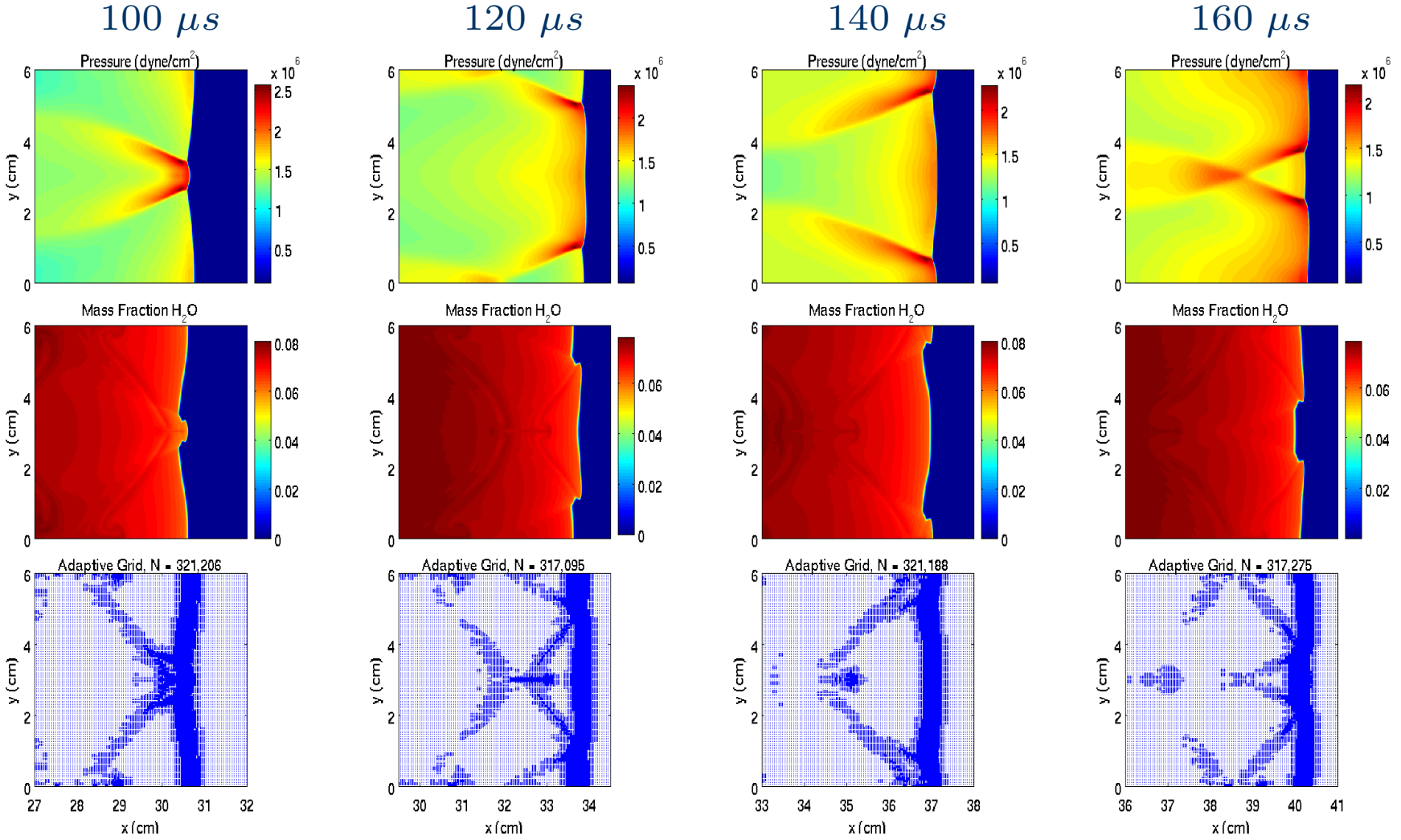


Domain: $[0, 60] \times [0, 6]$ cm
Front: $x = 15.0$ cm
Unreacted pocket:
$[1.05 \times 1.43]$ cm
at $x = 14.7$ cm
$P = 4.7 \times 10^5$ dyne/cm^2
$T = 2100$ K
128 cores
391 hrs runtime

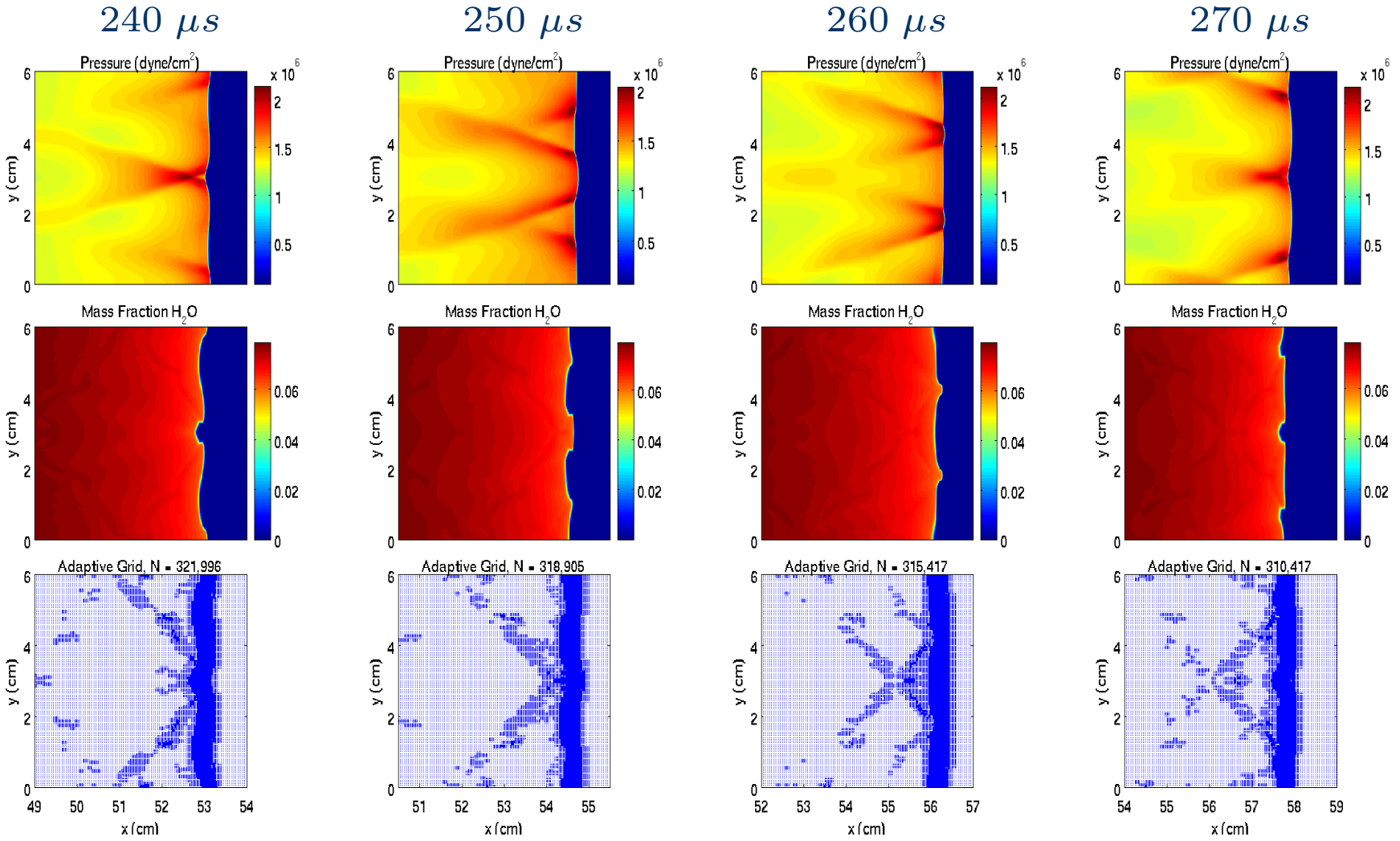
$2H_2 : O_2 : 7Ar$ mixture
9 species, 37 reactions

Wavelet parameters:
$\epsilon = 1 \times 10^{-3}$
$p = 6, \quad n = 5$
$[N_x \times N_y]_{j_0} = [600 \times 60]$
$J - j_0 = 10$

2-D Viscous Detonation (cont.)



2-D Viscous Detonation (cont.)



Inert Viscous Cylindrical Implosion

- WAMR algorithm employed
- $100\ \mu m \times 100\ \mu m$ square domain,
- Pure argon,
- Initial uniform temperature, $T = 300\ K$,
- Initial pressure ratio is $4\ atm : 0.2\ atm$ between argon on either side of an octagonal diaphragm,
- $T_{max}(r = 0, t \sim 40\ ns) \sim 2400\ K$.

Conclusions

- Verified 1D and 2D combustion physics spanning over five orders of magnitude–from near mean-free path scales ($10^{-4}\ cm$) to small scale device scales ($10\ cm$)–can be calculated today with modern adaptive algorithms working within a massively parallel computing architecture.
- Micro-scale viscous shock dynamics can influence oscillatory detonation dynamics on the macro-scale.
- Some 1D detonations can be validated; others await 3D extension.
- Realization of verified and validated DNS would remove the need for common, but problematic, modeling assumptions (shock-capturing, turbulence modeling, implicit chemistry with operator splitting, reduced kinetics/flamelets).
- Such 3D V&V could be viable in an exascale environment; however, routine desktop DNS calculations remain difficult to envision at macro-device scales.