Verified and Validated Calculation of Multiscale Combustion in Gaseous Mixtures

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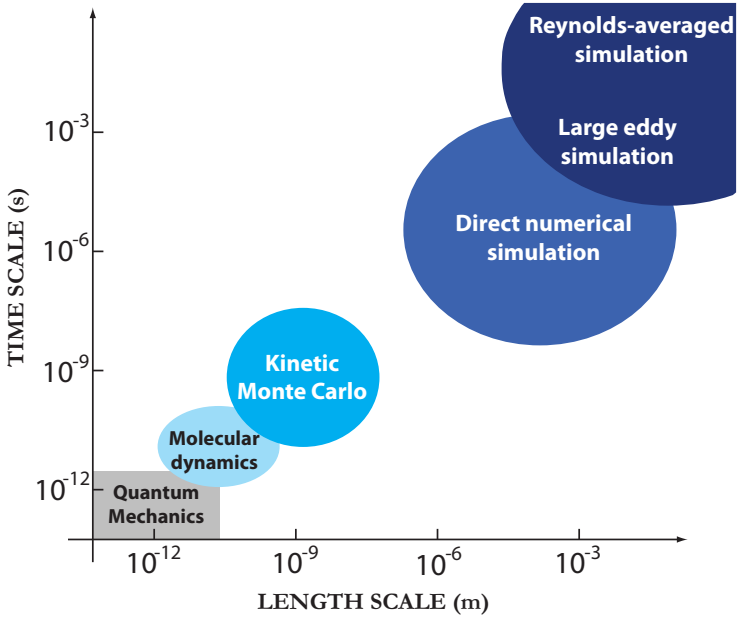
Outline

- Part I: Preliminaries
- Part II: Fundamental linear analysis of length scales of reacting flows with detailed chemistry and multicomponent transport.
- Part III: Direct Numerical Simulation (DNS) of complex flows with a wavelet-based adaptive algorithm implemented in a massively parallel architecture.

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

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

- Segregation of chemical dynamics from transport dynamics is a prevalent notion in reduced kinetics combustion modeling.
- But, can one rigorously mathematically verify an NS 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, *JFM*, 2012.

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 ($a \gg u^2/D$):

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

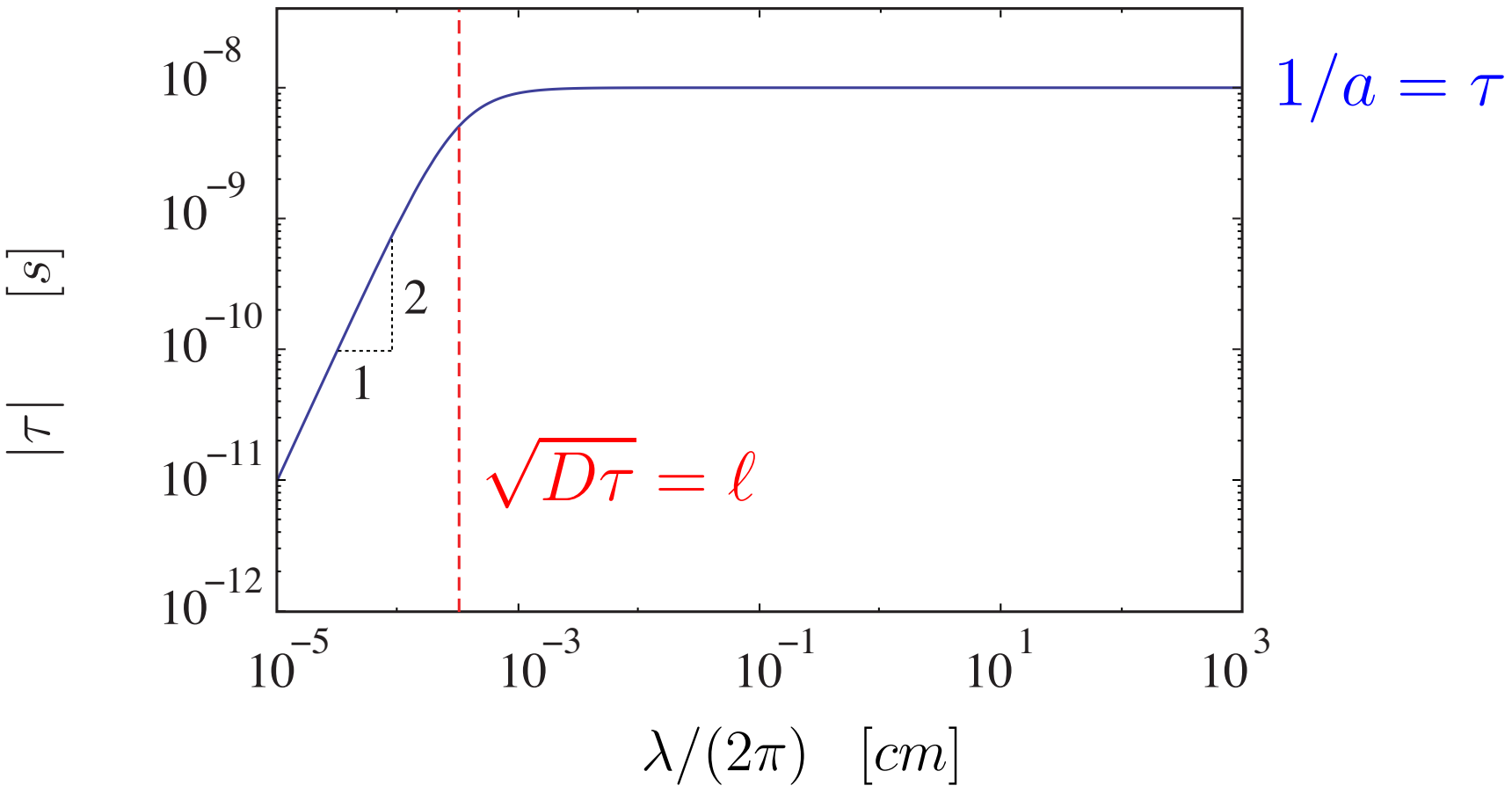
Spatio-Temporal Spectrum

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

- 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:

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

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

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

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

see Al-Khateeb, Powers, Paolucci, *Combustion Theory and Modelling*, 2013.

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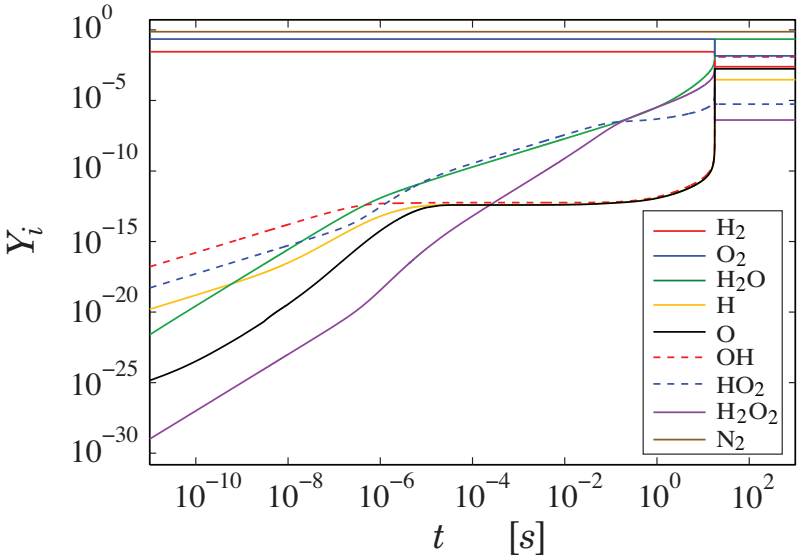
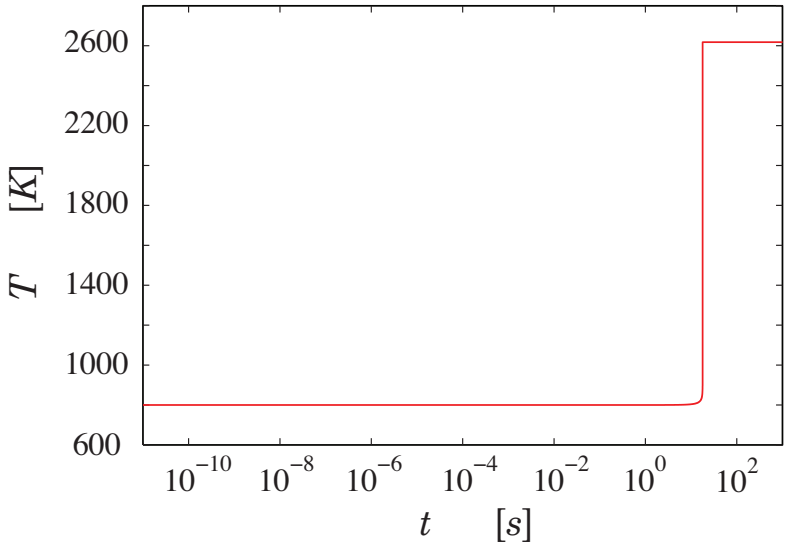
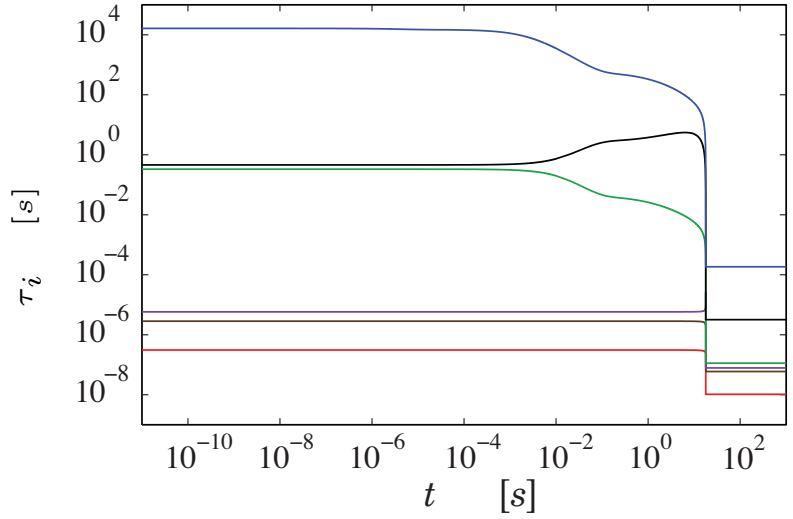
[a] J. A. Miller, R. E. Mitchell, M. D. Smooke, and R. J. Kee, *Proc. Combust. Ins.* **19**, p. 181, 1982.

- Unsteady spatially homogeneous reactive system:





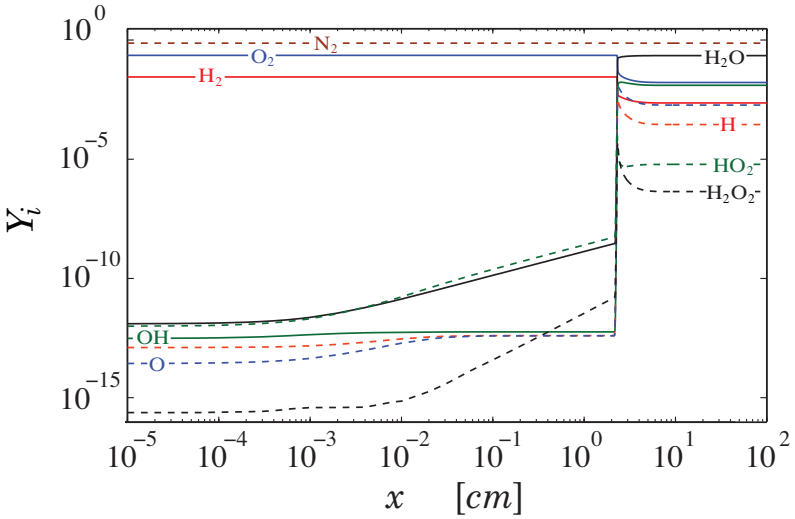


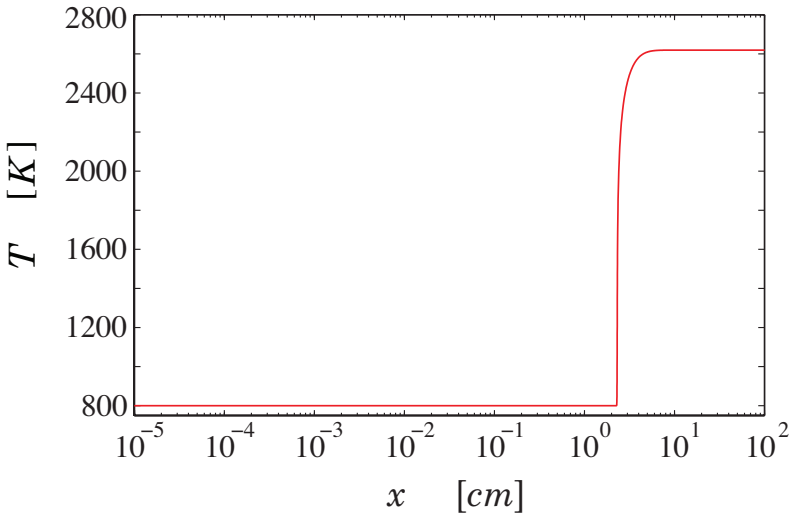
$\tau_{slowest} = 1.8\times10^{-2}\ s$

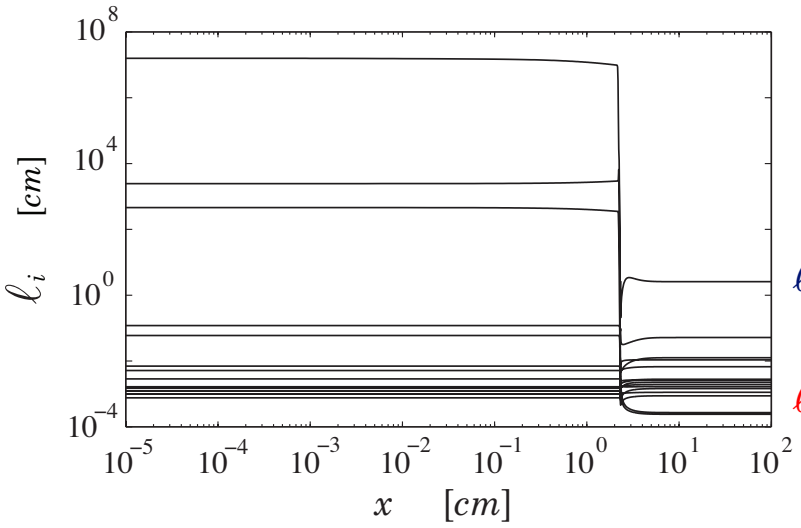
$\tau_{fastest} = 1.0\times10^{-8}\ s$

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

- Steady spatially inhomogeneous reactive system:[a]







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

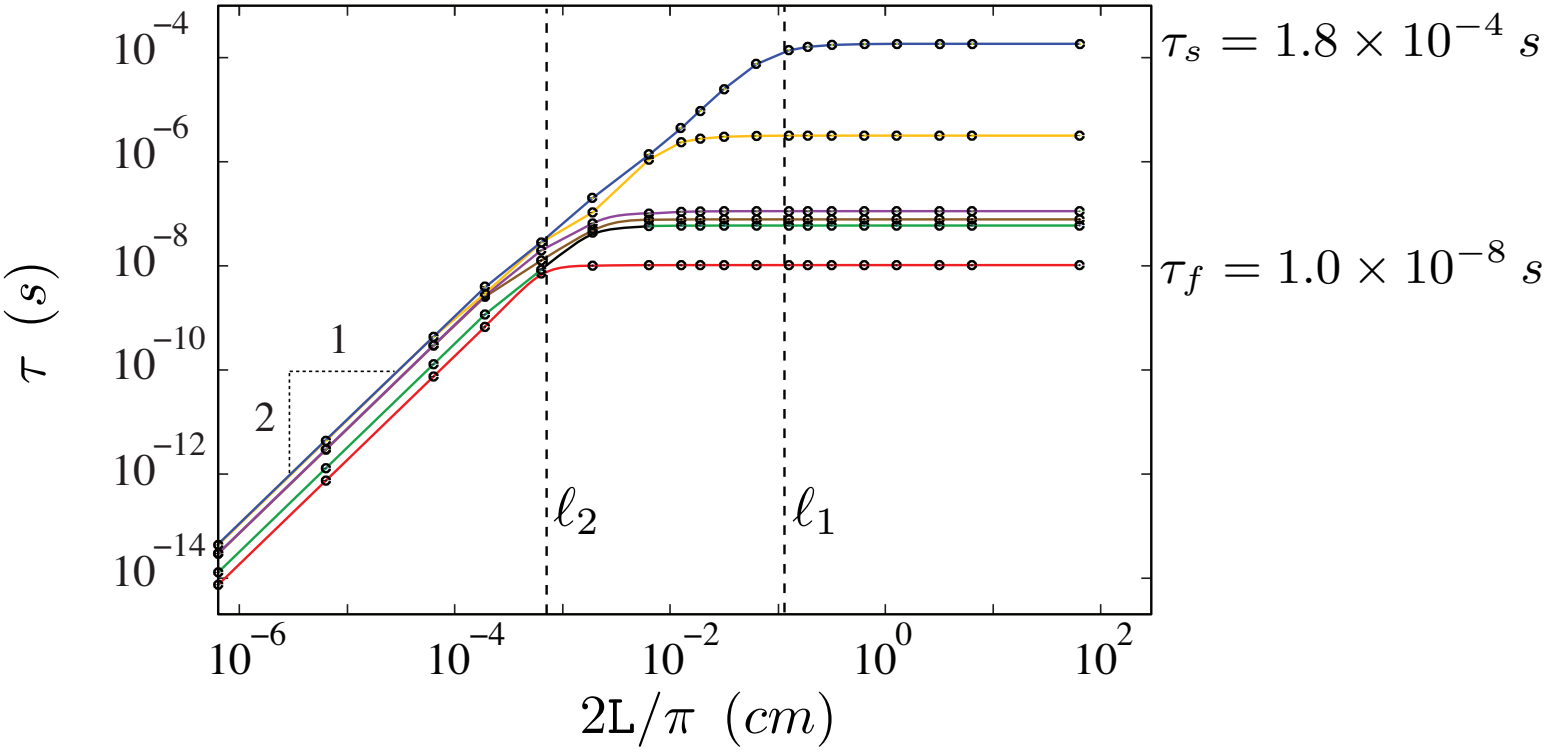
$\ell_{finest} = 2.4\times10^{-4}\ cm$

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

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

Spatio-Temporal Spectrum

- $\ell_1 = \sqrt{D_{mix}\tau_s} = 1.1 \times 10^{-1}\ cm,$
- $\ell_2 = \sqrt{D_{mix}\tau_f} = 8.0 \times 10^{-4}\ cm \approx \ell_{finest} = 2.4 \times 10^{-4}\ cm.$



Conclusions: Part I

- 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 Inert and Reacting Flows

Dynamically Adaptive Algorithm for Solving Time-Dependent PDEs

Given the set of PDEs

$$\frac{\partial u}{\partial t} = F(t, u, u_x, u_{xx}, \ldots),$$

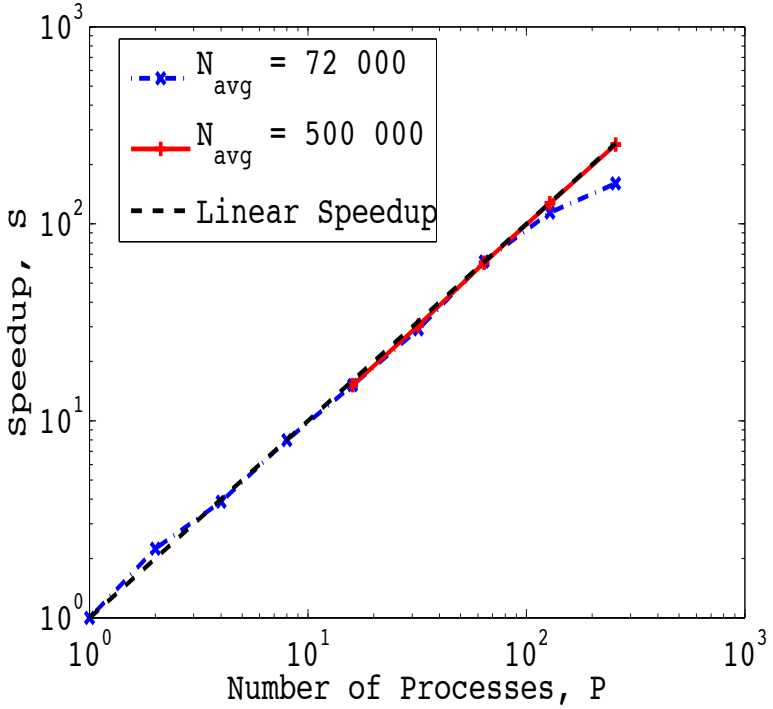
with initial conditions

$$u(x, 0) = u^0.$$

1. Obtain sparse grid, $\boldsymbol{\nu}^m$, based on thresholding of magnitudes of wavelet amplitudes of the approximate solution u^m.
2. Integrate in time using an explicit time integrator with error control to obtain the new solution u^{m+1}.
3. Assign $u^{m+1} \rightarrow u^m$ and return to step 1.

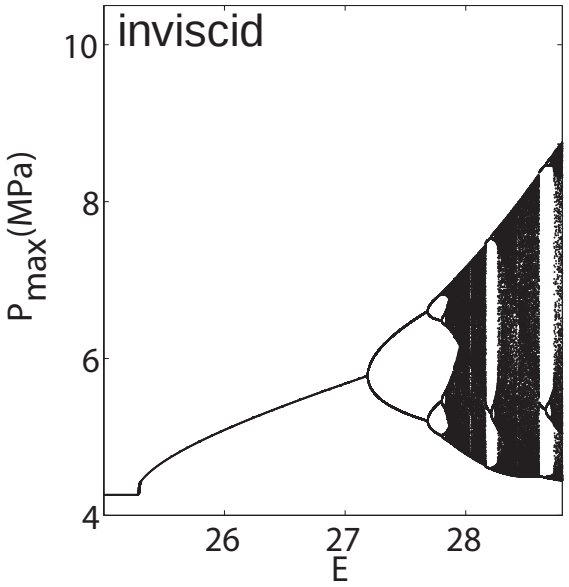
Parallelization

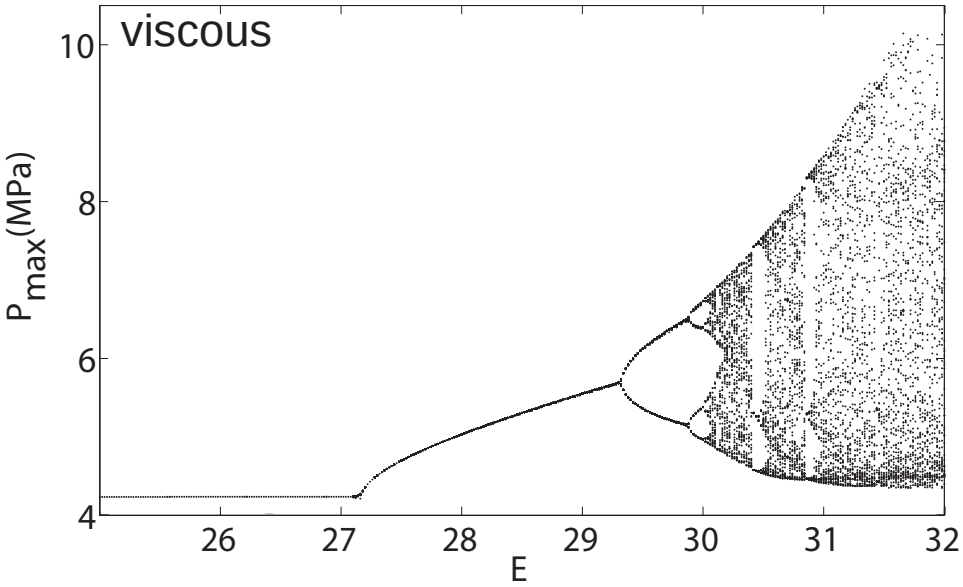
- Parallel algorithm uses an MPI-based domain decomposition.
- Hilbert space-filling curve used for partitioning and load-balancing.
- Strong scaling up to 256 cores with $> 90\%$ parallel efficiency.
- Chemkin-II and Transport Libraries used for evaluation of thermodynamics, transport properties, and reaction source terms.



Dual Quad-Core, 2.7 GHz L5520 Intel Nehalem nodes (8 cores/node), 12 GB RAM, Infiniband interconnect

Effect of Diffusion on Long-Time Detonation Dynamics





- Standard 1D problem with one-step kinetics, see Powers, *et al.*, 2006.
- 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.

Model: Reactive Navier-Stokes (NS) Equations

- Unsteady, compressible, one-dimensional
- Detailed mass action kinetics with Arrhenius temperature-dependency
- Ideal mixture of calorically imperfect ideal gases
- Physical viscosity and thermal conductivity
- Multicomponent mass diffusion with Soret and DuFour effects

Case Examined

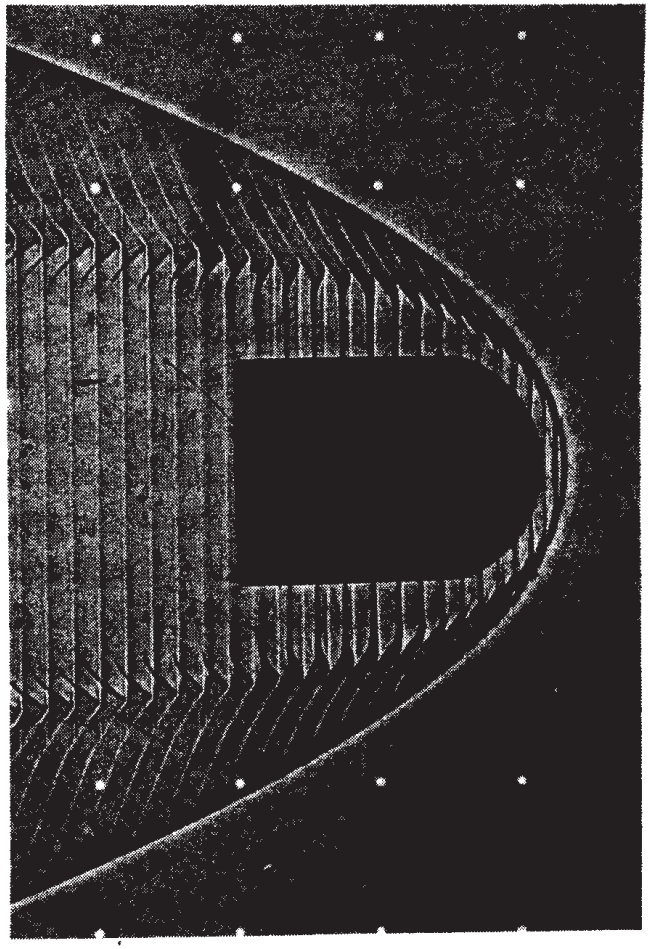
- Initially quiescent stoichiometric mixture of $2H_2 + O_2 + 3.76N_2$ at $1\ atm$ and $293.15\ K$ accelerated using a piston
- Form of piston velocity was chosen to force a detonation to form $\sim 1\ \mu s$

$$u_p = u_{p_i}\left(1 + \tanh\left[a\left(t - t_a\right)\right]\right) - \left(u_{p_i} - u_{p_f}\right)\left(1 + \tanh\left[b\left(t - t_b\right)\right]\right),$$

$$u_{p_i} = 1650\, m/s,\ a = 10^8\ 1/s,\ b = 10^7\ 1/s, t_a = 10^{-7}\ s,\ t_b = 10^{-6}\ s.$$

- Final piston velocities $1200\ m/s < u_{p_f} < 1500\ m/s$ were examined

Validation: Lehr's High Frequency Instability

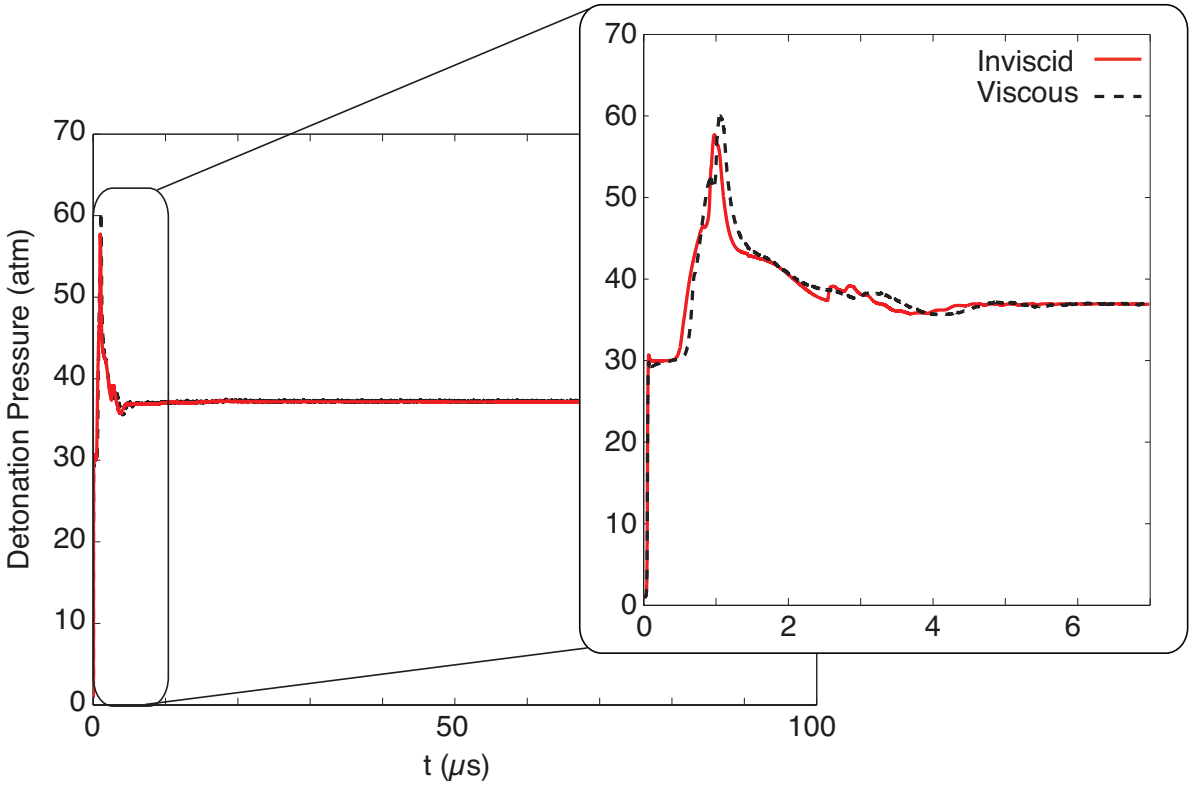


(*Astro. Acta*, 1972)

- Shock-induced combustion experiment (*Astro. Acta*, 1972)
- Stoichiometric mixture of $2H_2 + O_2 + 3.76N_2$ at $0.421\ atm$
- Observed $1.04\ MHz$ frequency for projectile velocity corresponding to $f \approx 1.1$
- For $f = 1.1$, the predicted frequency of $0.97\ MHz$ agrees with observed frequency and the prediction by Yungster and Radhakrishan of $1.06\ MHz$

Stable Detonation

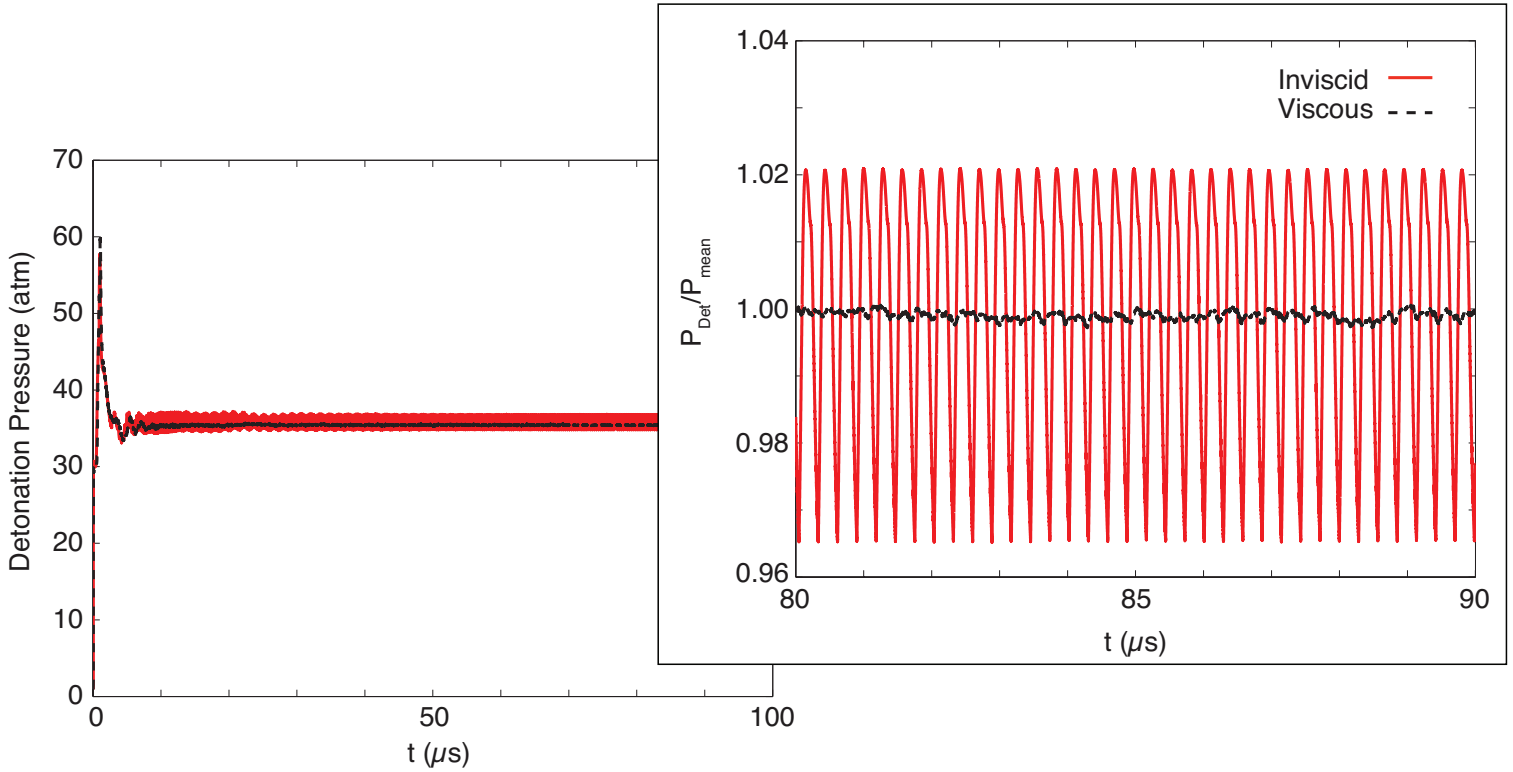
$u_{p_f} = 1500\, m/s$



The viscous case smooths the initialization; due to this slightly weaker shock, it takes longer to ignite the detonation. This delay increases the von Neumann spike. Additionally, the viscosity causes the detonation to take longer to relax to steady state.

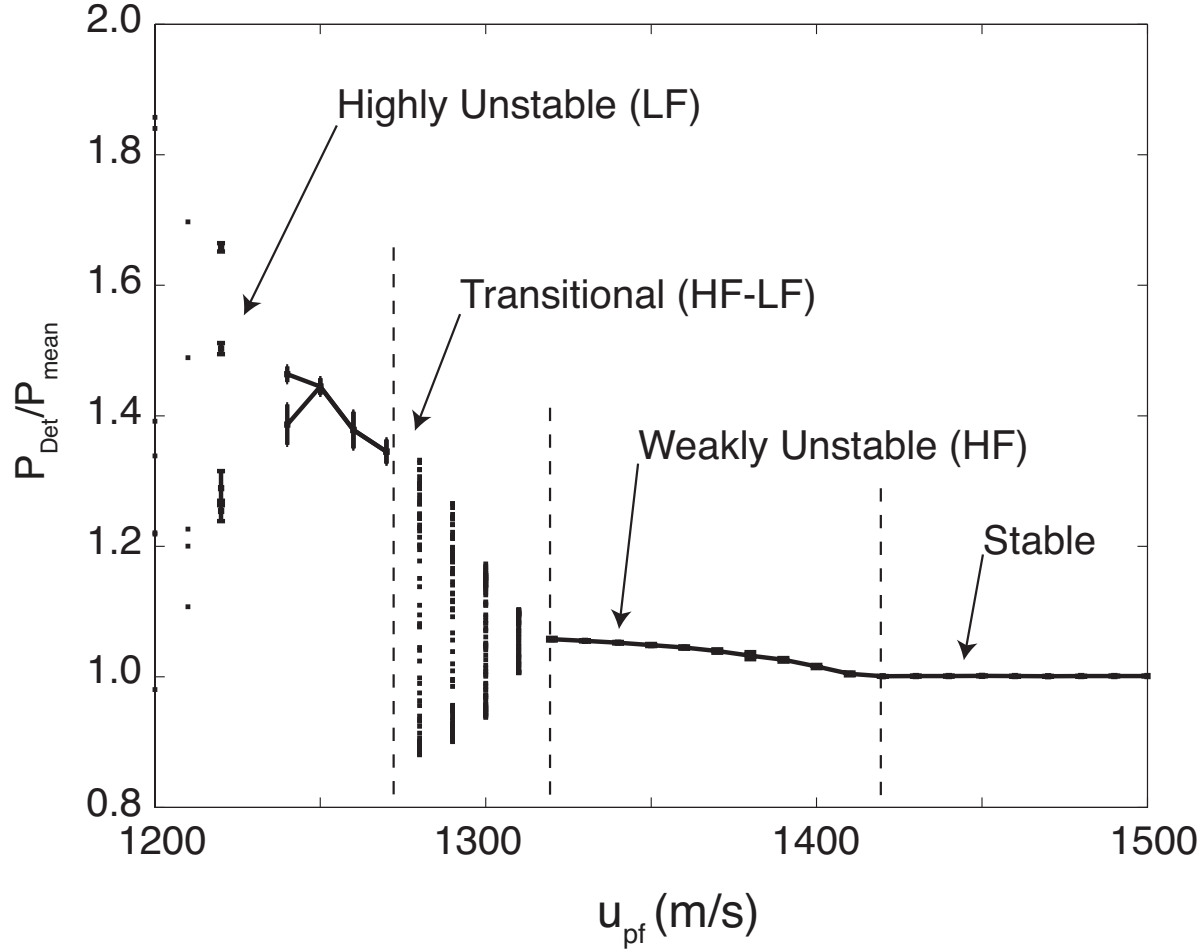
Unstable Detonation

$u_{p_f} = 1420\, m/s$



The addition of physical viscosity delays the onset of the initial appearance of instability. The small variations present in the viscous case are due to the detonation traversing a non-uniform grid and will be reduced as the tolerance of the WAMR is reduced.

Bifurcation Plot - Viscous



Harmonic Analysis - PSD

- Harmonic analysis can be used to extract the multiple frequencies of a signal
- The discrete one-sided mean-squared amplitude Power Spectral Density (PSD) for the pressure was used

$$\Phi_d(0) = \frac{1}{N^2}|P_o|^2,$$

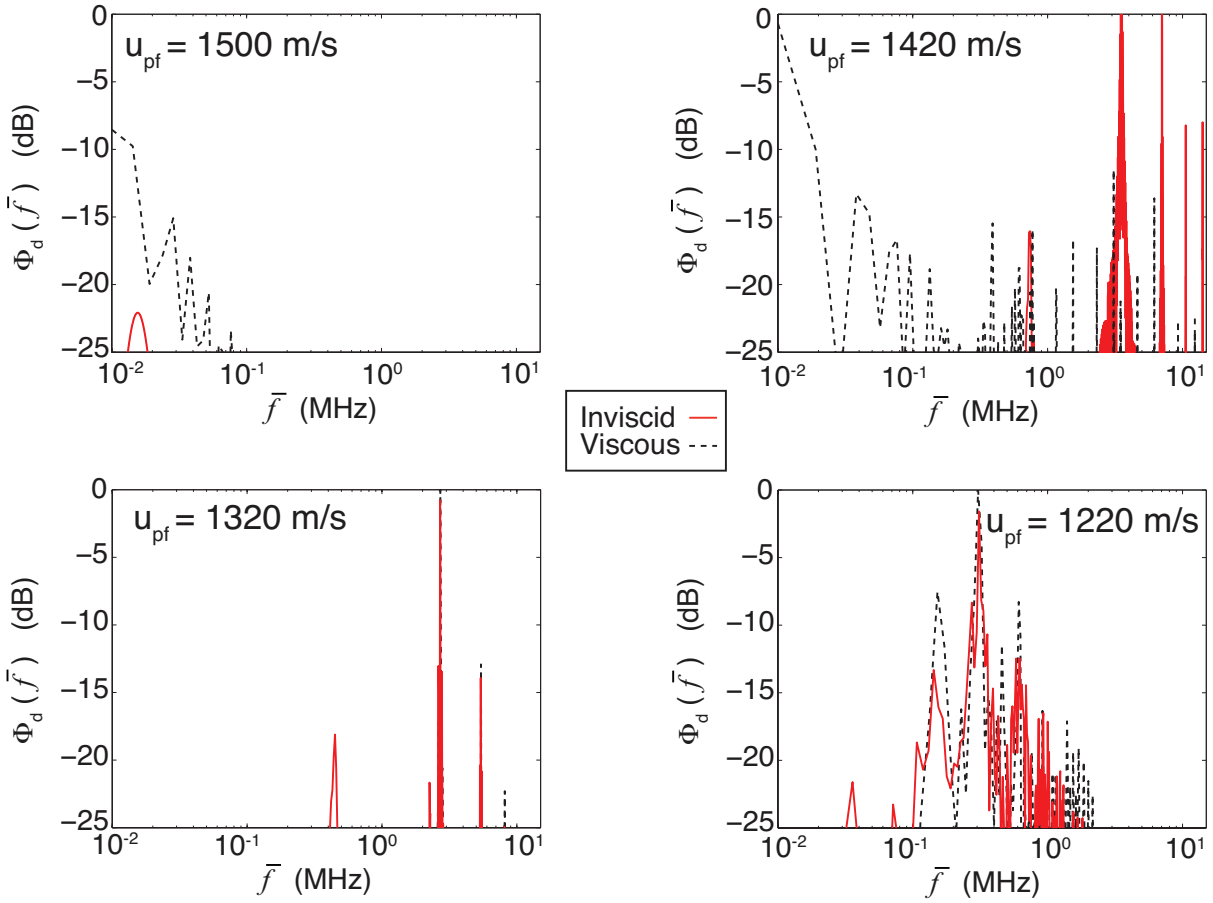
$$\Phi_d(\bar{f}_k) = \frac{2}{N^2}|P_k|^2, \qquad k = 1, 2, \ldots, (N/2 - 1),$$

$$\Phi_d(N/2) = \frac{1}{N^2}|P_{N/2}|^2,$$

where P_k is the standard discrete Fourier Transform of p,

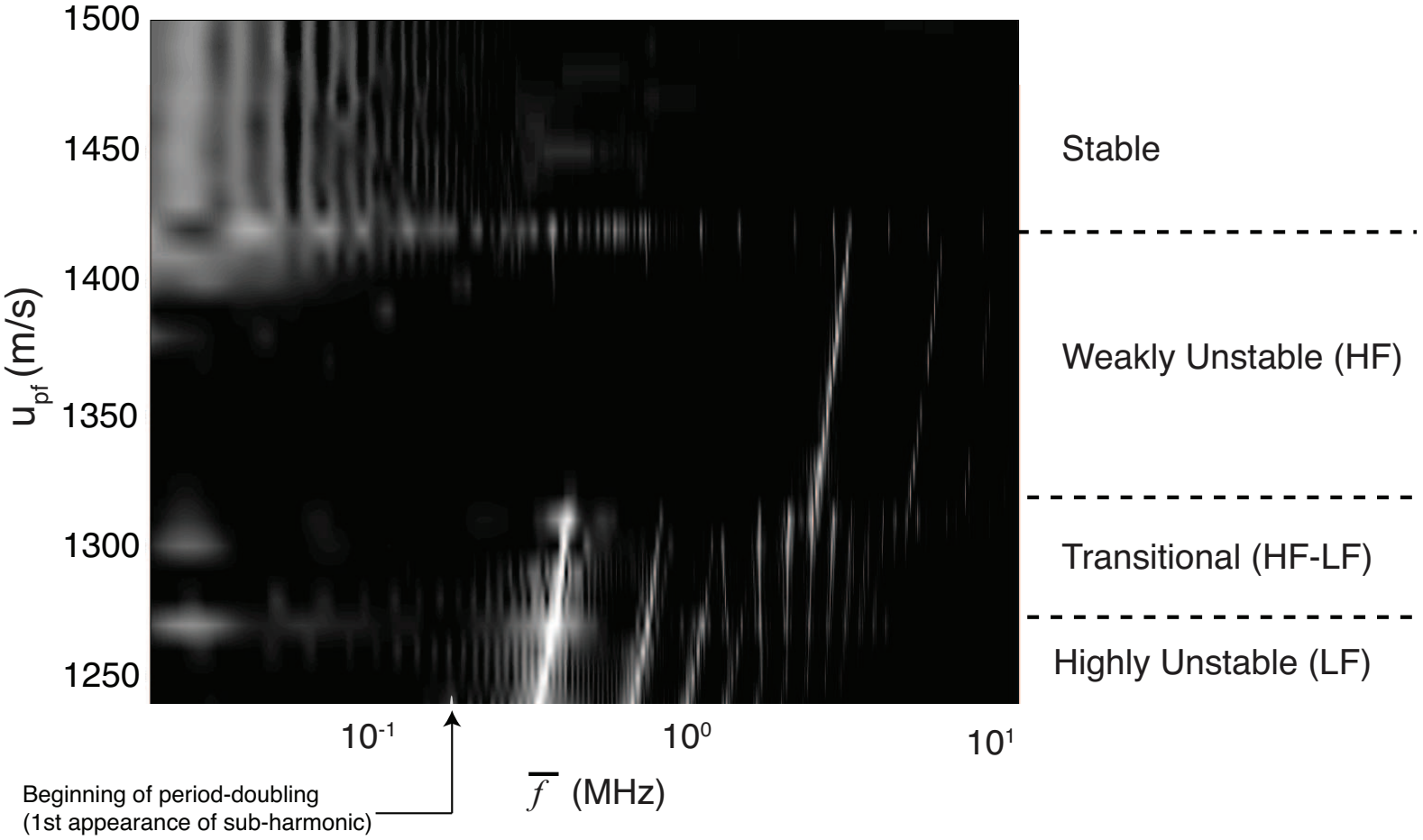
$$P_k = \sum_{n=0}^{N-1} p_n \exp\left(-\frac{2\pi\imath nk}{N}\right), \qquad k = 0, 1, 2, \ldots, N/2.$$

Inviscid vs. Viscous - Frequency Domain



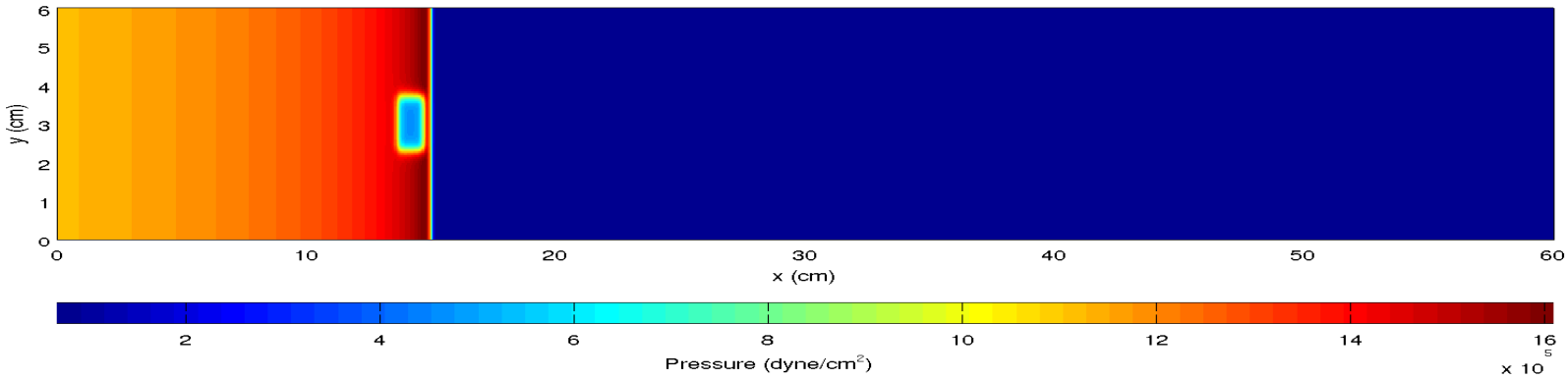
The inviscid case under goes a transition to instability before the viscous case; it also enters the dual mode oscillations before the viscous case. At the lower piston velocities the inviscid case appears to be chaotic sooner.

Overview of the Frequency Domain - Viscous



2-D Viscous Detonation

Initial Conditions:

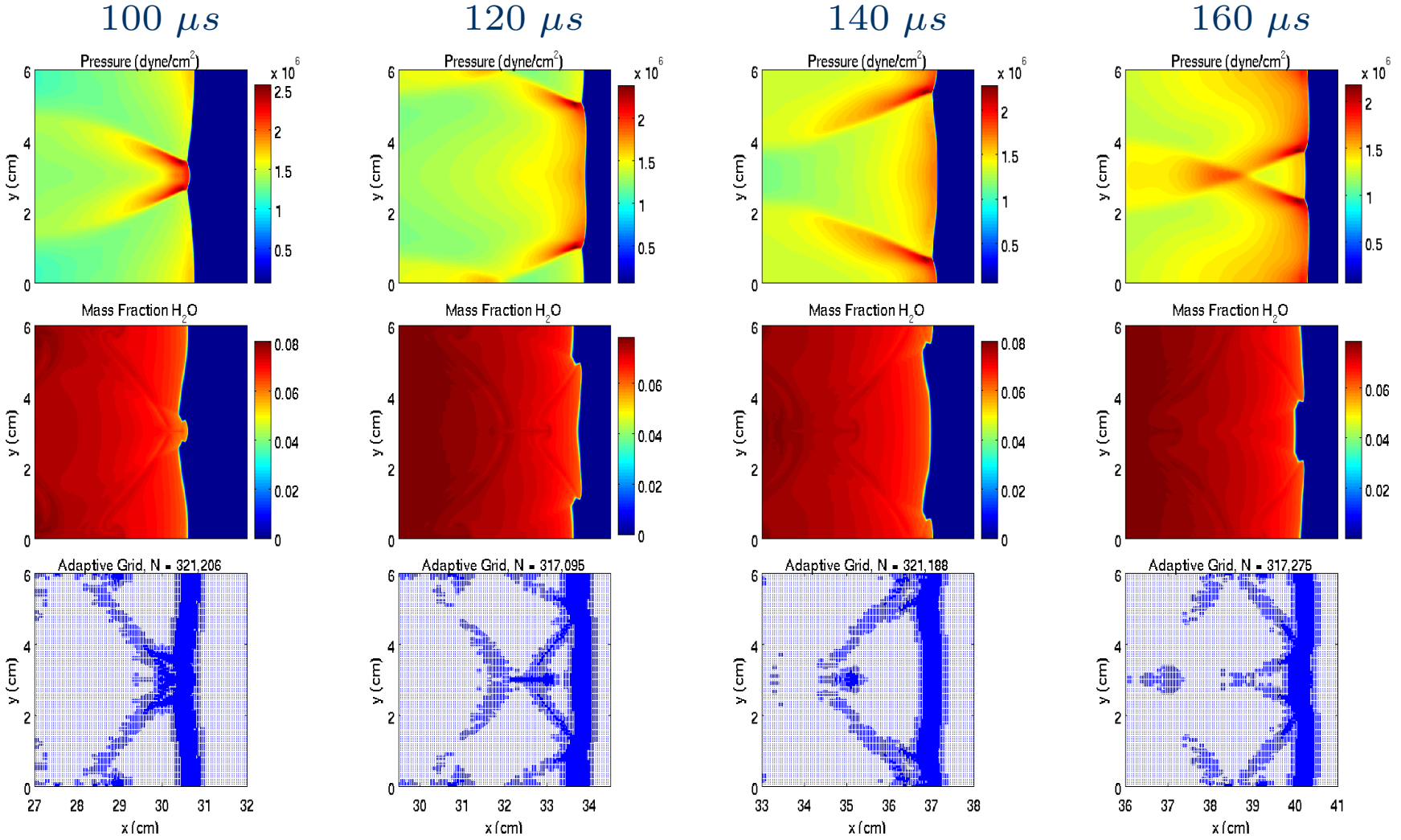


Domain: $[0, 60] \times [0, 6]$ cm
Front: $x = 15.0$ cm
Unreacted pocket:
$[1.05 \times 1.43]$ cm
at $x = 14.7$ cm
$P = 4.7 \times 10^5$ dyne/cm^2
$T = 2100$ K
128 cores
391 hrs runtime

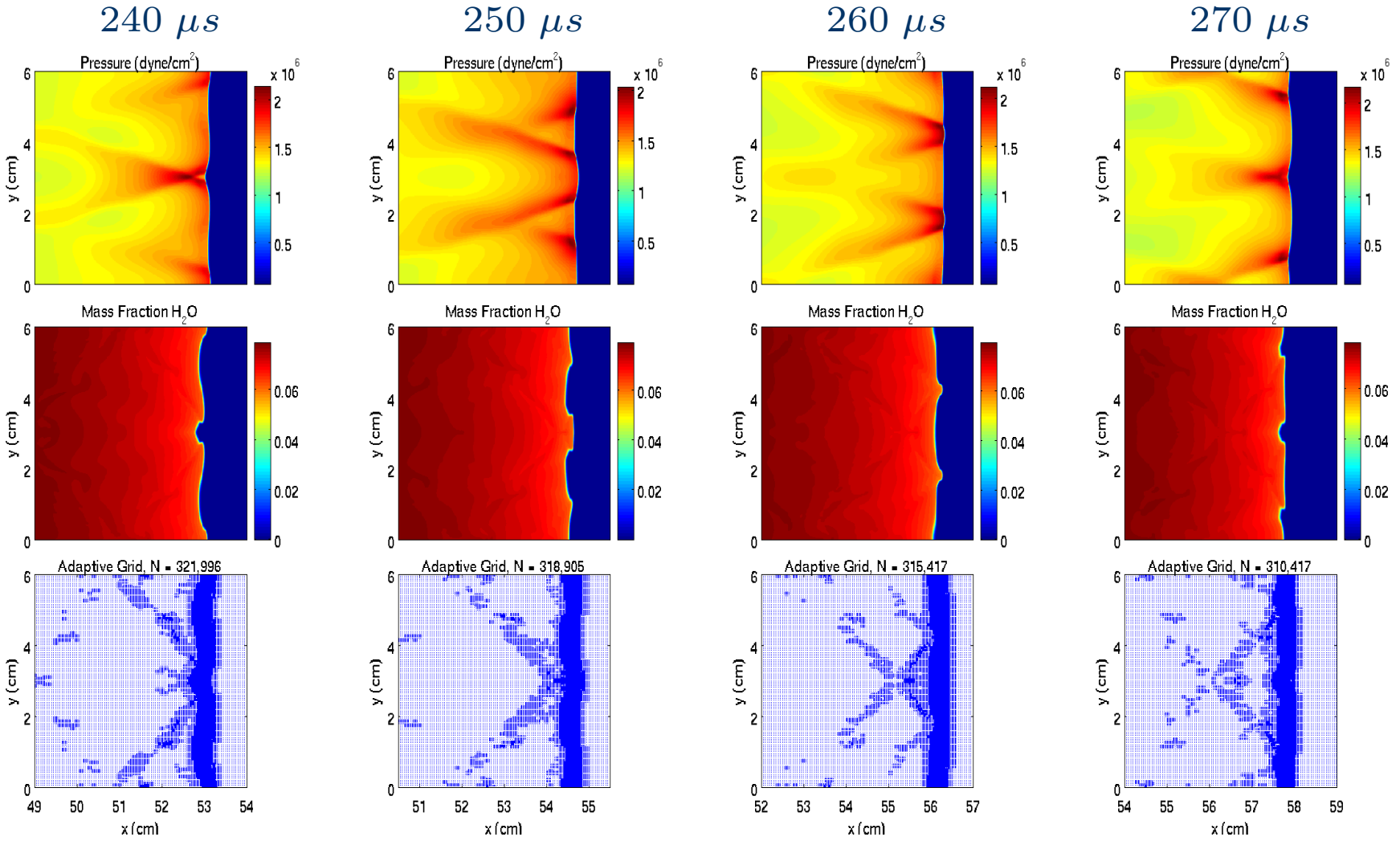
$2H_2 : O_2 : 7Ar$ mixture
9 species, 37 reactions

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

- $100\ \mu m \times 100\ \mu m$ 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 and validated 2D calculations for realistic reacting gas mixtures with detailed kinetics and multicomponent transport are realizable with modern adaptive algorithms working within a massively parallel computing architecture.
- It is possible for 2D calculations to span over five orders of magnitude: from near mean-free path scales ($10^{-4}\ cm$) to small scale device scales ($10\ cm$).
- Micro-scale viscous shock dynamics can dramatically influence oscillatory detonation dynamics on the macro-scale (see Romick, *et al.*, 2012).
- Validation against unsteady calculations awaits 3D extensions.
- 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.