Verified and Validated Calculation of Unsteady Overdriven Hydrogen-Air Detonation

Christopher M. Romick,
University of Notre Dame, Notre Dame, IN

Tariq D. Aslam,
Los Alamos National Laboratory, Los Alamos, NM

and

Joseph M. Powers

University of Notre Dame, Notre Dame, IN

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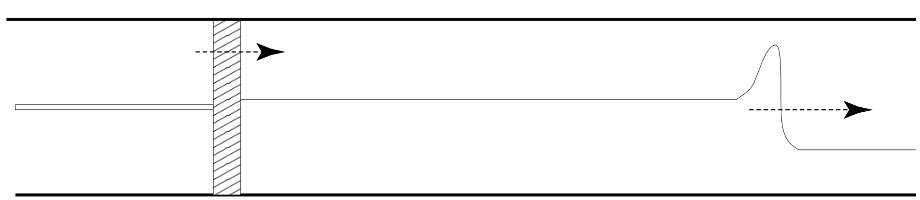
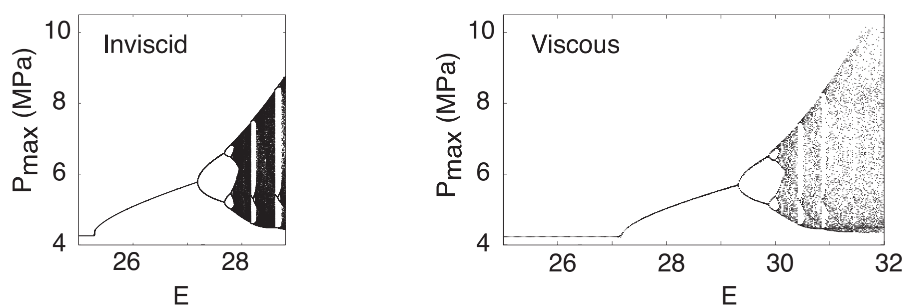
Motivation

- *Verification*: solving the equations correctly. *Validation*: solving the correct equations.
- For a predictive computation both verification and validation are necessary.
- A detonation is a shock-induced combustion wave in which the exothermic energy release contributes to driving the shock.
- It is often argued that viscous forces and diffusive effects are small, do not affect detonation dynamics, and thus can be neglected.
- Standard result from non-linear dynamics: small scale phenomena can influence large scale phenomena and vice versa.
- Might there be risks in using numerical viscosity, LES, and turbulence modeling, all of which filter small scale physical dynamics?



Motivation

- Tsuboi *et al.*, (*Comb. & Flame*, 2005) reported, even when using micron grid sizes, that some structures cannot be resolved.
- Powers, (*JPP*, 2006) showed that two-dimensional detonation patterns are grid-dependent for the reactive Euler equations, but relax to a grid-independent structure for comparable Navier-Stokes calculations.
- Using a one-step kinetics model, we (*JFM*, 2012) showed that when the viscous length scale is similar to that of the finest reaction scale, viscous effects play a critical role in determining the long time behavior of the detonation.
- This suggests grid-dependent numerical viscosity may be problematic and one may want to consider the introduction of physical diffusion.



Review of Hydrogen Detonation

- Powers & Paolucci (*AIAA J.*, 2005) found the finest reaction length scales on the order of sub-microns and the largest on the order of centimeters for steady, inviscid hydrogen-air detonations with ambient conditions of $1\ atm$ and $298\ K$.
- Yungster and Radhakrishan (*Comb. Theory & Mod.*, 2004) found a minimum resolution of near a micron was necessary to capture the dynamics in the inviscid limit at ambient pressure of $0.197\ atm$.
- Daimon and Matsuo (*Phys. Fluids*, 2007) found that as the overdrive is lowered, the long time behavior of the detonation became more complex.
- Using an adaptive mesh in parallel, Ziegler *et al.* (*J. Comp. Phys.*, 2011) examined a viscous double-Mach reflection detonation and found that even with a resolution near a micron only qualitative convergence was achieved.

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

- Overdriven detonations with ambient conditions of $0.421\ atm$ and $293.15\ K$
- Initial stoichiometric mixture of $2H_2 + O_2 + 3.76N_2$
- $D_{CJ} \sim 1972\, m/s$
- Overdrive is defined as $f = D_o^2/D_{CJ}^2$
- Overdrives of $1.001 < f < 1.25$ were examined

Unsteady, Compressible, Reactive NS Equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0,$$

$$\frac{\partial}{\partial t} (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u}\mathbf{u} + p\mathbf{I} - \boldsymbol{\tau}) = \mathbf{0},$$

$$\frac{\partial}{\partial t} \left(\rho \left(e + \frac{\mathbf{u} \cdot \mathbf{u}}{2} \right) \right) + \nabla \cdot \left(\rho \mathbf{u} \left(e + \frac{\mathbf{u} \cdot \mathbf{u}}{2} \right) + (p\mathbf{I} - \boldsymbol{\tau}) \cdot \mathbf{u} + \mathbf{q} \right) = 0,$$

$$\frac{\partial}{\partial t} (\rho Y_i) + \nabla \cdot (\rho \mathbf{u} Y_i + \mathbf{j}_i) = \overline{M_i} \dot{\omega}_i ,$$

$$p = \mathcal{R} T \sum_{i=1}^{N} \frac{Y_i}{\overline{M_i}}, \qquad e = e\left(T, Y_i\right), \qquad \dot{\omega}_i = \dot{\omega}_i \left(T, Y_i\right),$$

$$\mathbf{j}_i = \rho \sum_{\substack{k=1 \\ k \neq i}}^{N} \frac{\overline{M_i} D_{ik} Y_k}{\overline{M}} \left(\frac{\nabla y_k}{y_k} + \left(1 - \frac{\overline{M_k}}{\overline{M}} \right) \frac{\nabla p}{p} \right) - \frac{D_i^T \nabla T}{T},$$

$$\boldsymbol{\tau} = \mu \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T - \frac{2}{3} (\nabla \cdot \mathbf{u}) \mathbf{I} \right),$$

$$\mathbf{q} = -k \nabla T + \sum_{i=1}^{N} \mathbf{j}_i h_i - \mathcal{R} T \sum_{i=1}^{N} \frac{D_i^T}{\overline{M_i}} \left(\frac{\nabla \overline{y}_i}{\overline{y}_i} + \left(1 - \frac{\overline{M_i}}{\overline{M}} \right) \frac{\nabla p}{p} \right).$$

Intrinsic 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):

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

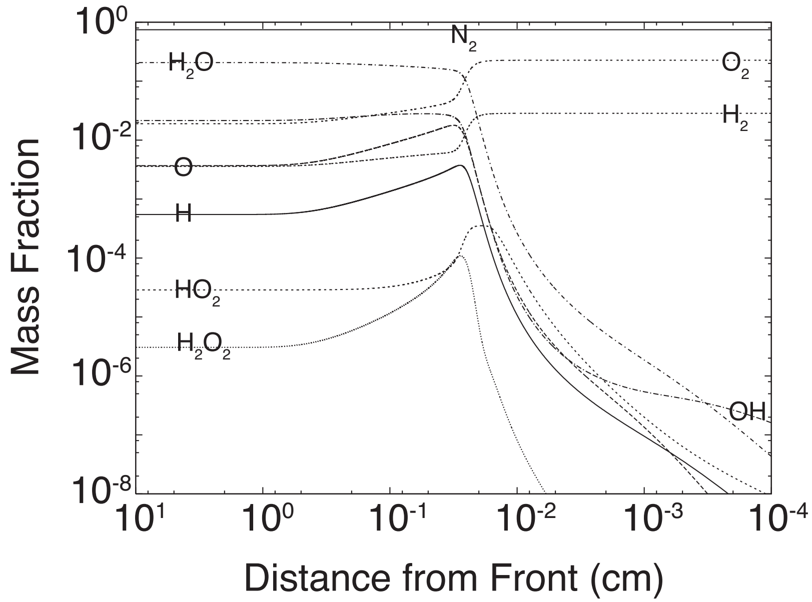
- The finest reaction length scale is $L_r \sim \mathcal{O}\left(10^{-4}\ cm\right)$
- A simple estimate of a viscous length scale is:

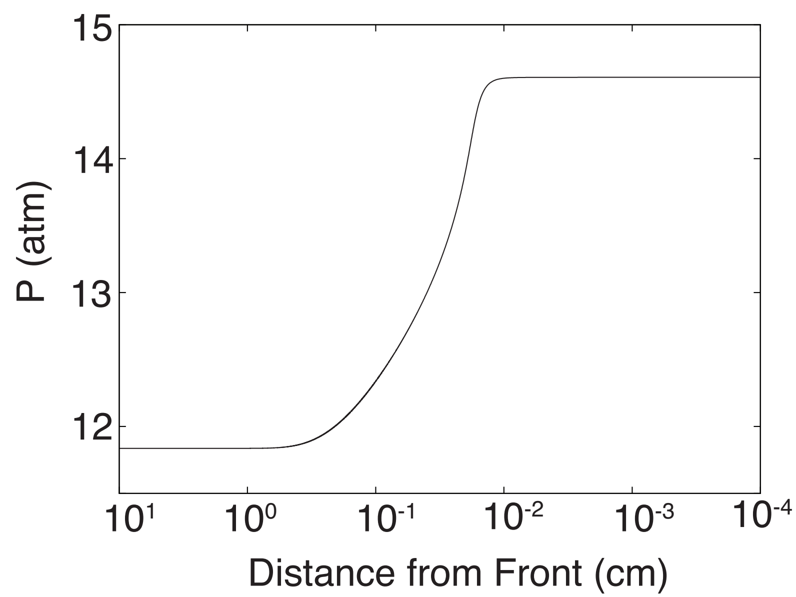
$$L_\mu = \frac{\nu}{c} = \frac{6 \times 10^{-1}\ cm^2/s}{9 \times 10^4\ cm/s} \sim \mathcal{O}\left(10^{-5}\ cm\right)$$

- $\lambda < L_r$ & $\lambda < L_\mu$

Inviscid Steady-State: ZND Profile

$f = 1.25$



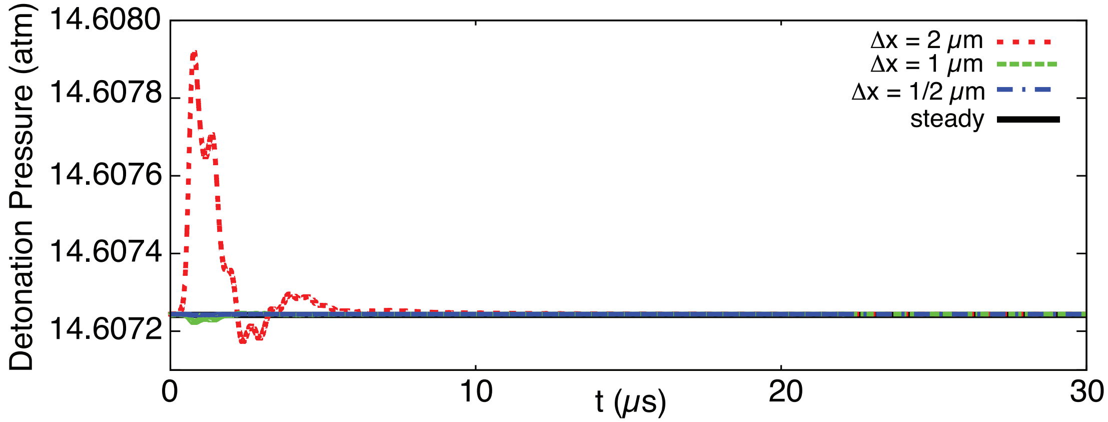


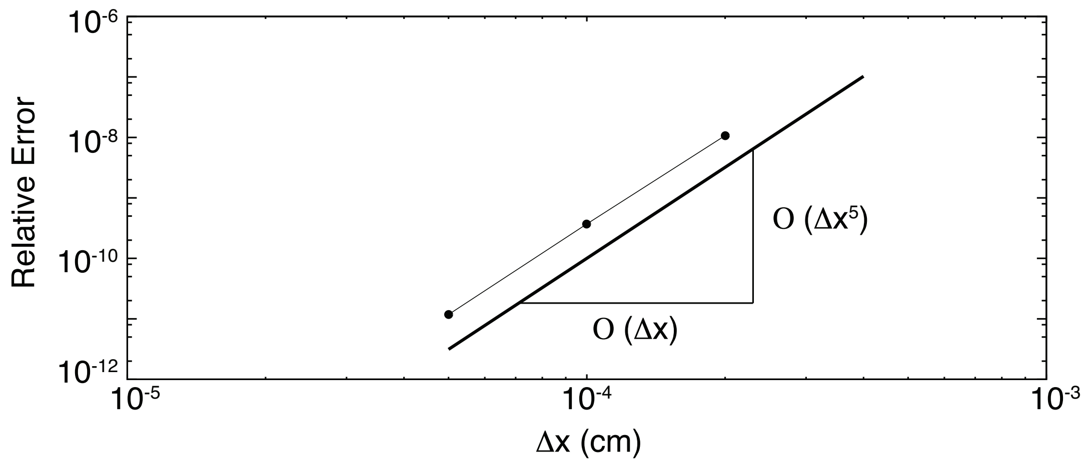
Inviscid Computational Method

- Viscosity, mass diffusion, and thermal conductivity are all set to zero
- Equations transformed to a shock-attached frame
- Jump conditions enforced at shock boundary
- Nominally fifth order shock-fitting algorithm adapted from Henrick *et al.* (*J. Comp. Phys.*, 2006)
- Shock-fitting technique used assures numerical viscosity is minimal
- Fifth order Runge-Kutta used for time integration

Inviscid Transient Behavior: Stable Detonation

$f = 1.25$

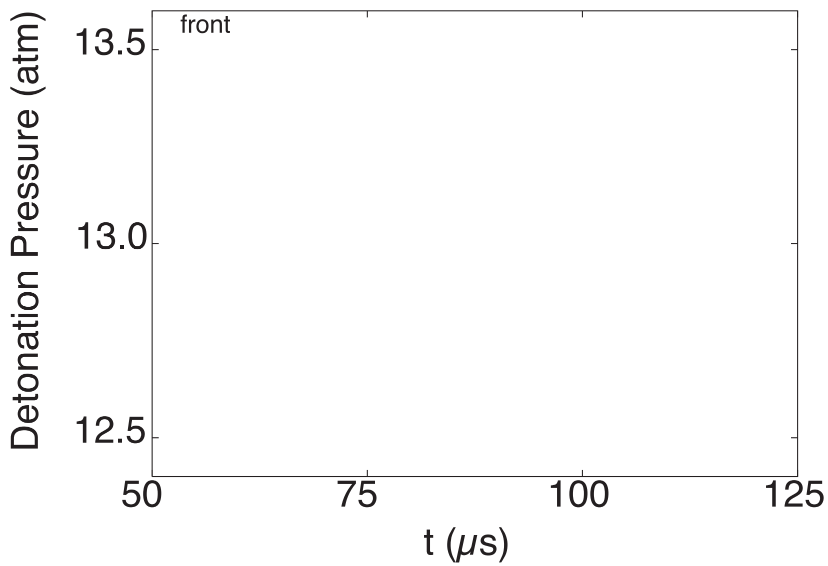




Convergence rate of 4.97

Inviscid Unstable Detonation

$f = 1.10$

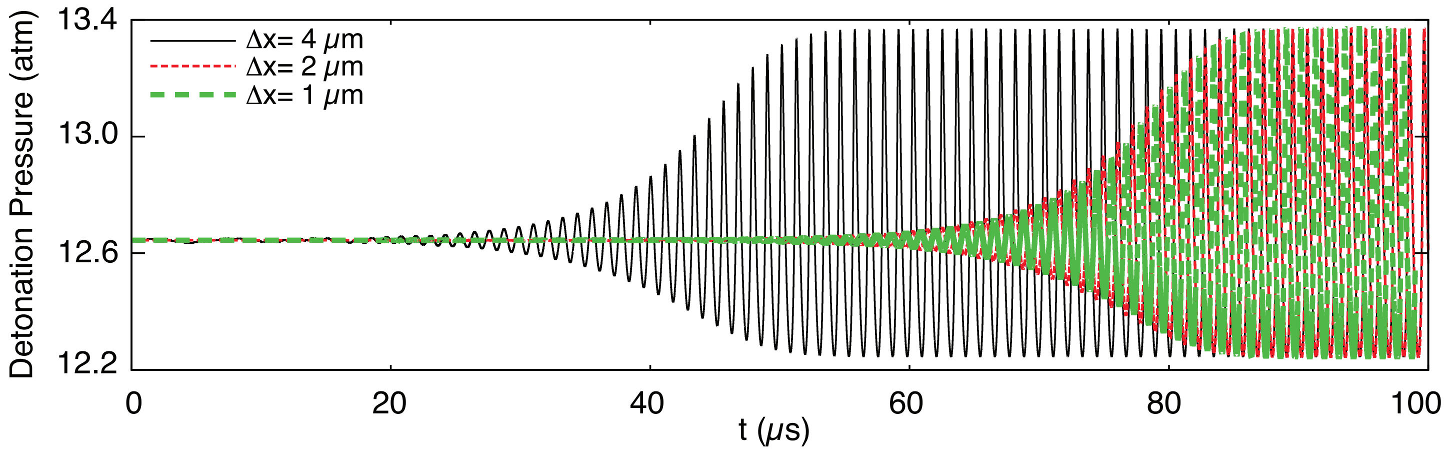


A single frequency oscillation occurs at a frequency of $0.97\ MHz$

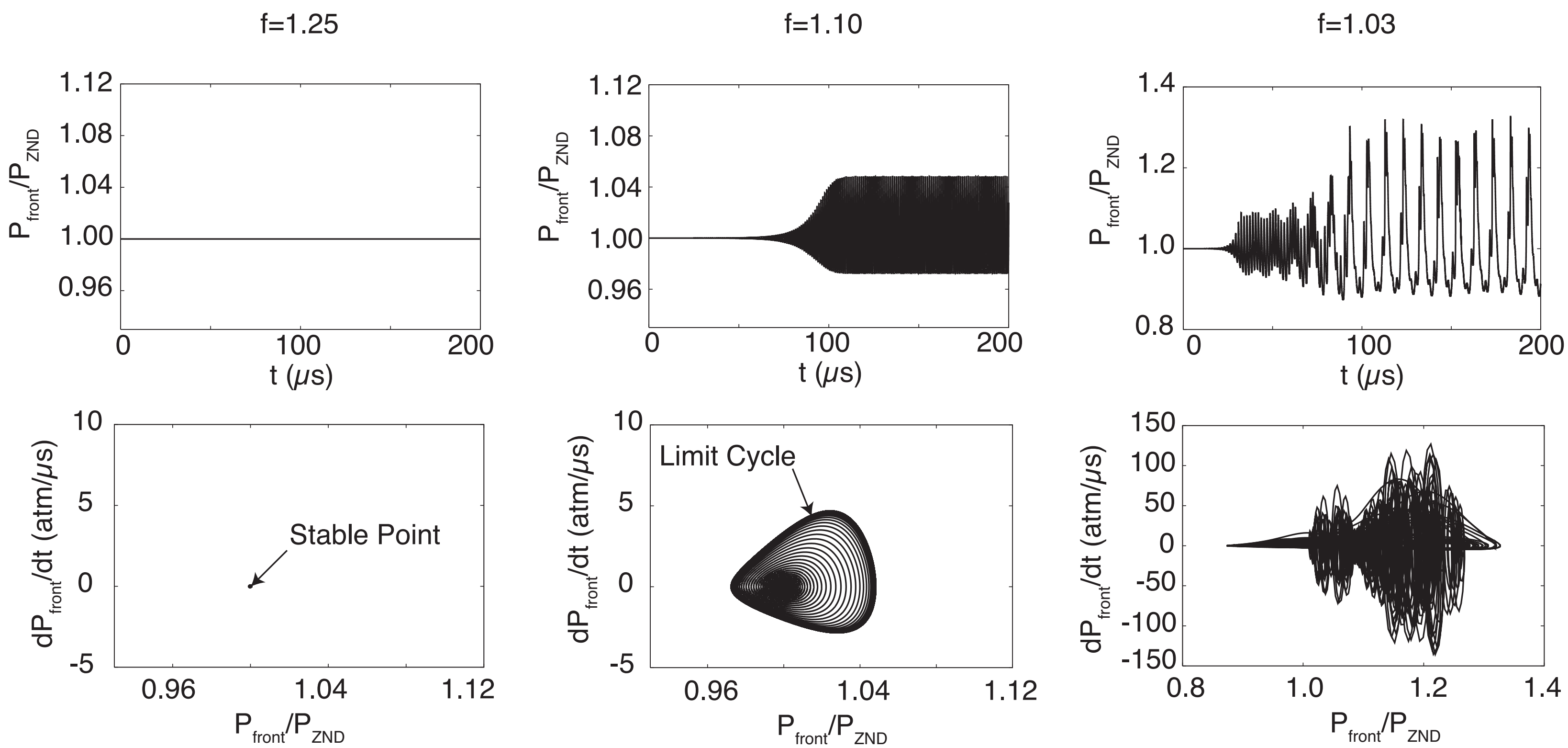
Maximum Pressure and Frequency Convergence

$f = 1.08$

Case	$\Delta\ x$	Max Pressure	Frequency
1	4 μm	13.36749 atm	0.899336 MHz
2	2 μm	13.36927 atm	0.899549 MHz
3	1μm	13.36980 atm	0.899612 MHz



Inviscid Bifurcation Behavior



Viscous Computational Method

- The Wavelet Adaptive Multiresolution Representation (WAMR) method was used.
- First developed by Vasilyev and Paolucci (*J. Comp. Phys.*, 1996 & 1997).
- The basis functions have compact support in both space and scale.
- The nature of the wavelet basis allows multiscale signals to be efficiently represented relative to many other common methods.
- User-defined threshold parameter controls error and guarantees a verified solution.

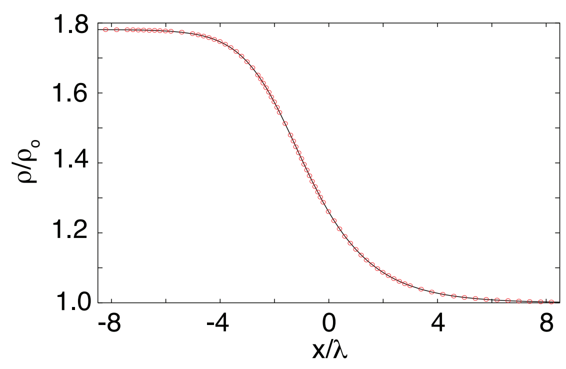
Demonstration of WAMR

- $Ma = 1.55$ shock propagating in argon
- The structure of the viscous (NS) steady shock is governed by two ordinary differential equations:

$$\frac{du}{dx} = \frac{\rho_o \mathcal{R} T}{\overline{M}} \frac{u_o}{u} - \rho_o u_o u - p_o - \rho_o u_o^2$$

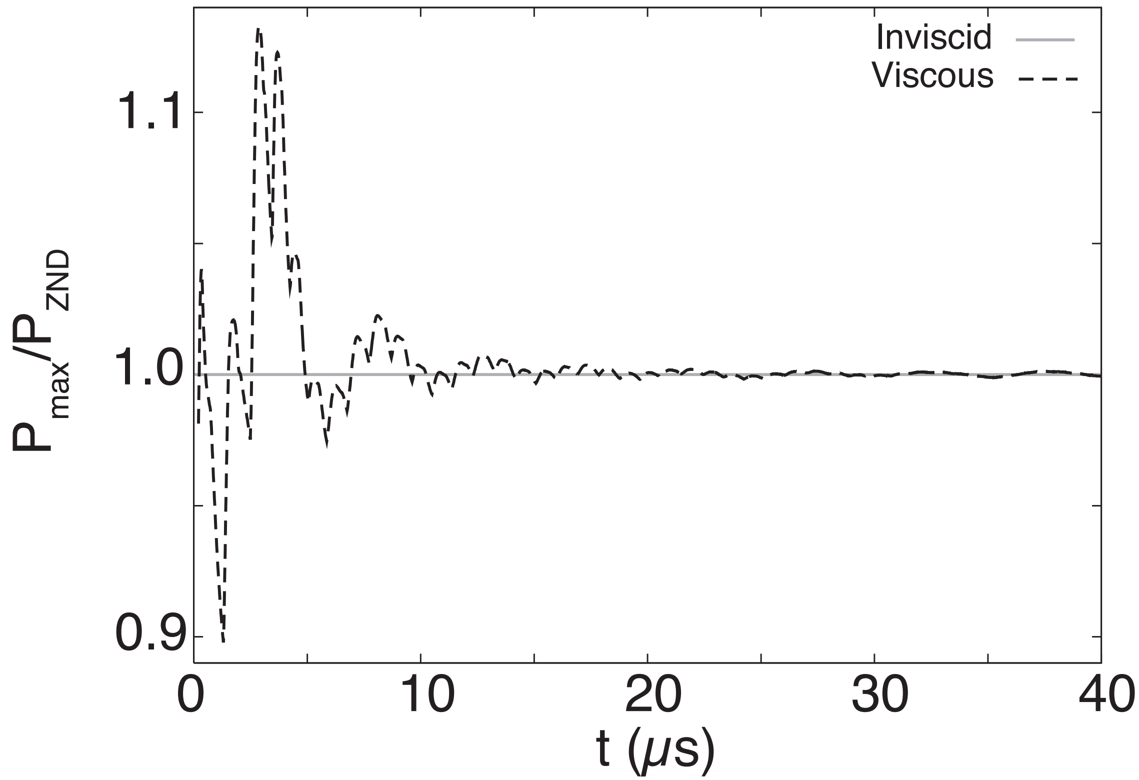
$$\frac{dT}{dx} = \frac{2\rho_o u_o \mathcal{R} T - (\gamma - 1)\overline{M}\left(\rho_o u_o \left(2e_o + (u + u_o)^2\right) + 2p_o(u + u_o)\right)}{2(\gamma - 1)\overline{M}}$$

- Shooting problem from the shocked values (ρ_s, u_s, p_s) to the ambient conditions (ρ_o, u_o, p_o)
- WAMR prediction is indistinguishable from the steady wave solution



Stable, Viscous Detonation

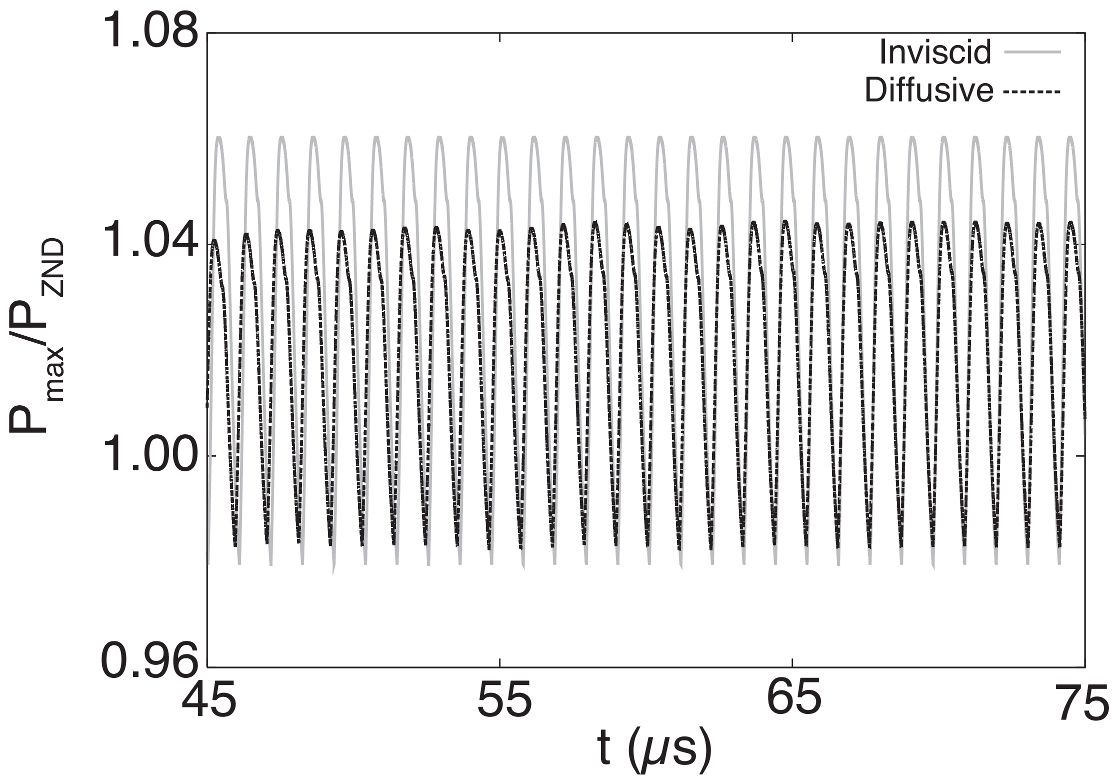
$f = 1.15$



The diffusive detonation relaxes to a steady propagating wave, similar to the inviscid case.

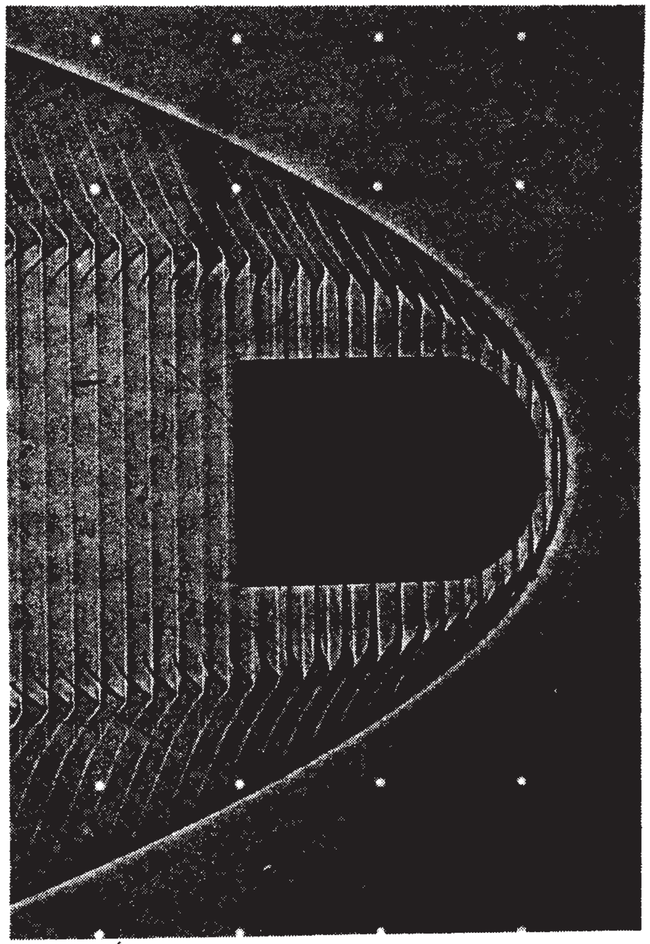
Unstable, Viscous Detonation

$f = 1.10$



The addition of viscous effects have a stabilizing effect, decreasing the amplitude of the oscillations. The pulsation frequency relaxes to $0.97\ MHz$.

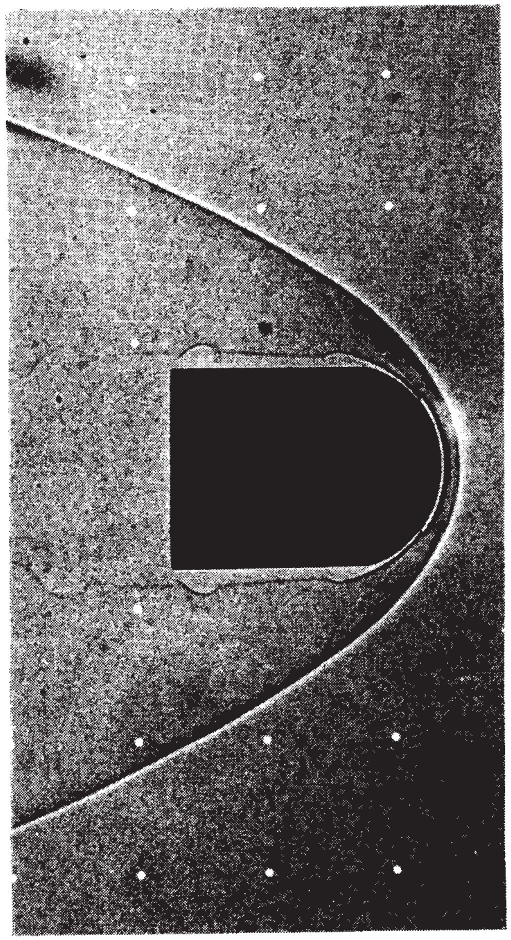
Validation: Lehr's High Frequency Instability



(*Astro. Acta*, 1972)

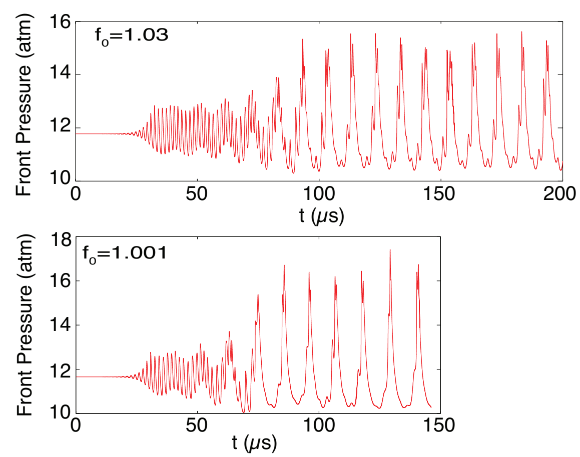
- Shock-induced combustion experiment (*Astro. Acta*, 1972)
- Stoichiometric mixture of $2H_2 + O_2 + 3.76N_2$ at $0.421\ atm$
- Observed $1.04\ MHz$ frequency for projectile velocity corresponding to $f \approx 1.1$
- For $f = 1.1$, the predicted frequency of $0.97\ MHz$ agrees with observed frequency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

Validation: Lehr's Low Frequency Instability



(*Astro. Acta*, 1972)

- Lehr observed a $0.15\ MHz$ frequency at a projectile velocity below the CJ detonation velocity
- For $f_0 \approx 1$, the main frequency is near $0.10\ MHz$, even though there are multiple modes



Conclusions

- Shock fitting coupled with fifth order spatial discretization assures numerical viscosity is minimal, thus giving rise to verified calculations of unsteady, inviscid detonation dynamics when all reaction length scales are fully resolved.
- At high overdrives, the detonations are stable; as the overdrive is decreased, the long time behavior becomes progressively more complex.
- The addition of diffusion has a stabilizing effect on the long time behavior of a detonation; the amplitude of the oscillations can be significantly reduced.
- Comparison with Lehr's experiments gives some, yet limited validation.
  - The predicted frequency of $0.97\ MHz$ for a $f = 1.1$ overdriven detonation agrees with the frequency observed by Lehr of $1.04\ MHz$.
  - The low frequency observed by Lehr $(0.15\ MHz)$ at a velocity below the CJ velocity is similar to the predicted frequency of $0.10\ MHz$ at low overdrives.

Verification of WAMR

- Error proportional to thresholding parameter