Dynamics of Unsteady Inviscid and Viscous Detonations in Hydrogen-Air

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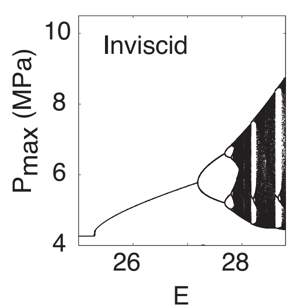
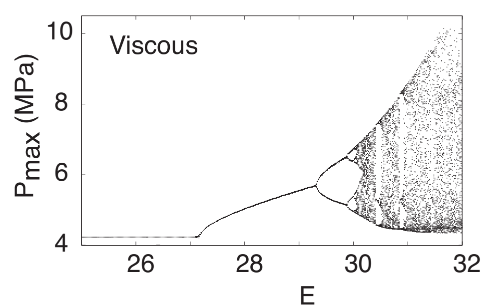
Motivation

- Standard result from non-linear dynamics: small scale phenomena can influence large scale phenomena and vice versa.
- What are the risks of using reactive Euler instead of reactive Navier-Stokes?
- Might there be risks in using numerical viscosity, LES, and turbulence modeling, all of which filter small scale physical dynamics?
  - For one-step kinetics, yes: there are clear and quantifiable risks.
  - For detailed kinetics, definitive calculations await, but probably yes.

Motivation

- It is often argued that viscous forces and diffusive effects are small, do not affect detonation dynamics, and thus can be neglected.
- Tsuboi *et al.*, (*Comb. & Flame*, 2005) report, 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 (*49th AIAA ASM*, 2011) 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) studied the reaction length scales of a steady, inviscid hydrogen detonation and found the finest length scales on the order of sub-microns to microns and the largest on the order of centimeters with ambient conditions of $1\ atm$ and $298\ K$.
- These small scales are continuum manifestations of molecular collisions.
- This range of scales must be resolved to capture the dynamics.

Review of hydrogen detonation

- Sussman (Ph.D. Thesis, 1995) performed one-dimensional simulations using only 20 points in the induction zone.
- Using a massively parallel computing environment, Oran *et al.* (*Comb. & Flame*, 1998) studied the development of detonation cells in a low-pressure hydrogen mixture in two dimensions.
- Eckett (Ph.D. Thesis, 2001) found that 150 points in the induction zone were necessary capture the dynamics of an overdriven, inviscid detonation at an ambient pressure of $1\ atm$.
- Singh *et al.* (*Comb. Theory & Mod.*, 2001) simulated a one-dimensional, unsteady, viscous, detonation in a hydrogen-oxygen-argon mixture using an adaptive mesh.

Review of hydrogen detonation

- Yungster and Radhakrishan (*Comb. Theory & Mod.*, 2004) found that a minimum resolution of near one 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 a parallel computing environment, 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 Equations

- unsteady,
- 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

Unsteady, Compressible, Reactive Navier-Stokes Equations

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

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

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

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

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

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

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

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

Computational Methods

- Inviscid Dynamics
  - High-order shock-fitting algorithm adapted from Henrick *et al.* (*J. Comp. Phys.*, 2006).
  - Equations transformed to a shock-attached frame, jump conditions enforced at shock boundary, and fifth order Runge-Kutta used for time integration.
- Viscous Dynamics
  - Wavelet Adaptive Multiresolution Representation (WAMR) method first developed by Vasilyev and Paolucci (*J. Comp. Phys.*, 1996,1997) employed.
  - An adaptive mesh refinement technique using wavelet functions which have compact support in both space and time enables the use of many less points to accurately represent a flow field.

Case Examined

- Overdriven detonations with ambient conditions of $0.421\ atm$ and $293.15\ K$
- Initial stoichiometric mixture of $2H_2 + O_2 + 3.76N_2$
- $D_{CJ} \sim 1961\, m/s$
- 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):

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

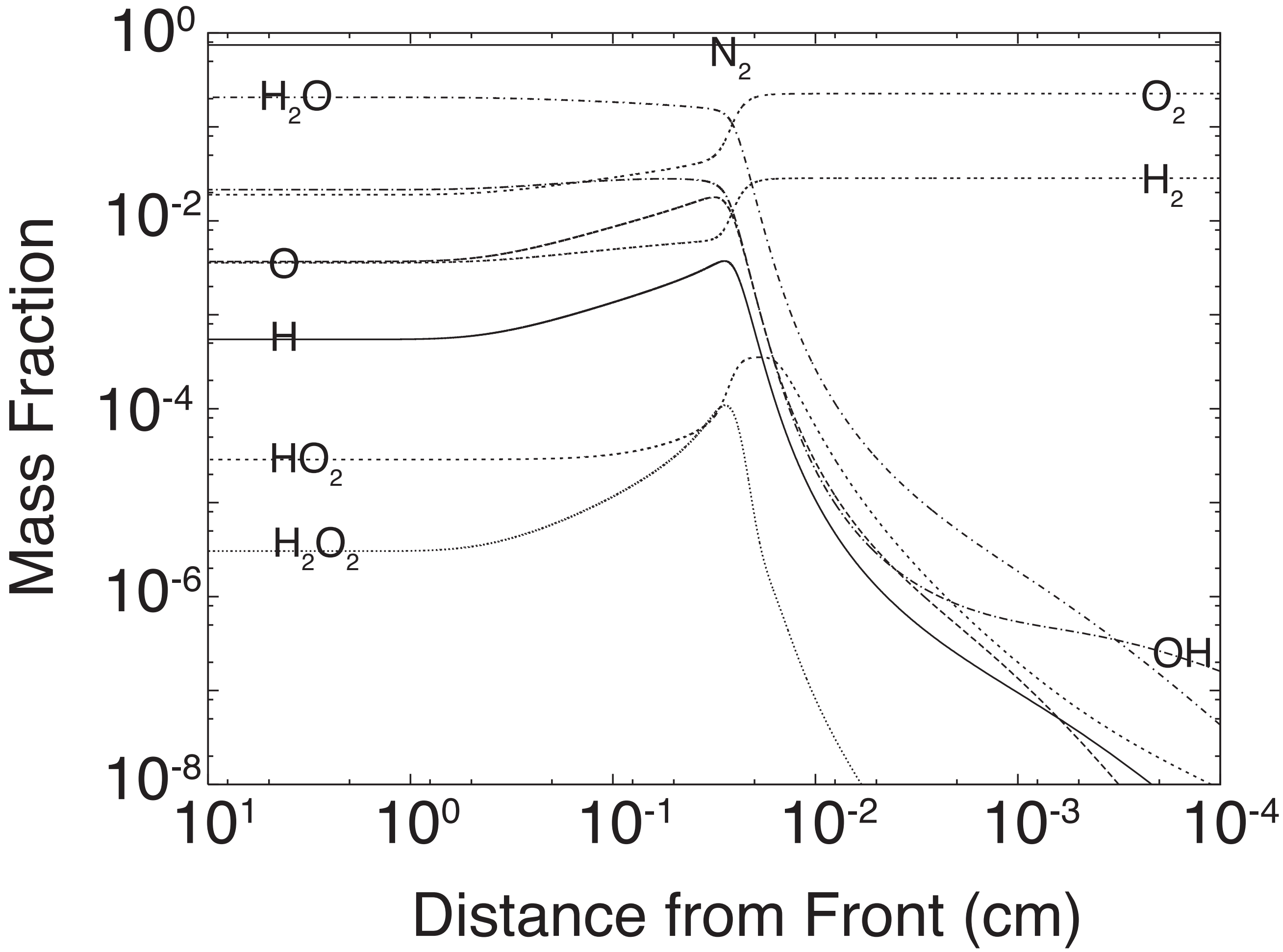
- The finest reaction length scale is $L_r \sim \mathcal{O}\left(10^{-4}\ cm\right)$.
- A simple estimate of a viscous length scale is:

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

- $\lambda < L_\mu < L_r$

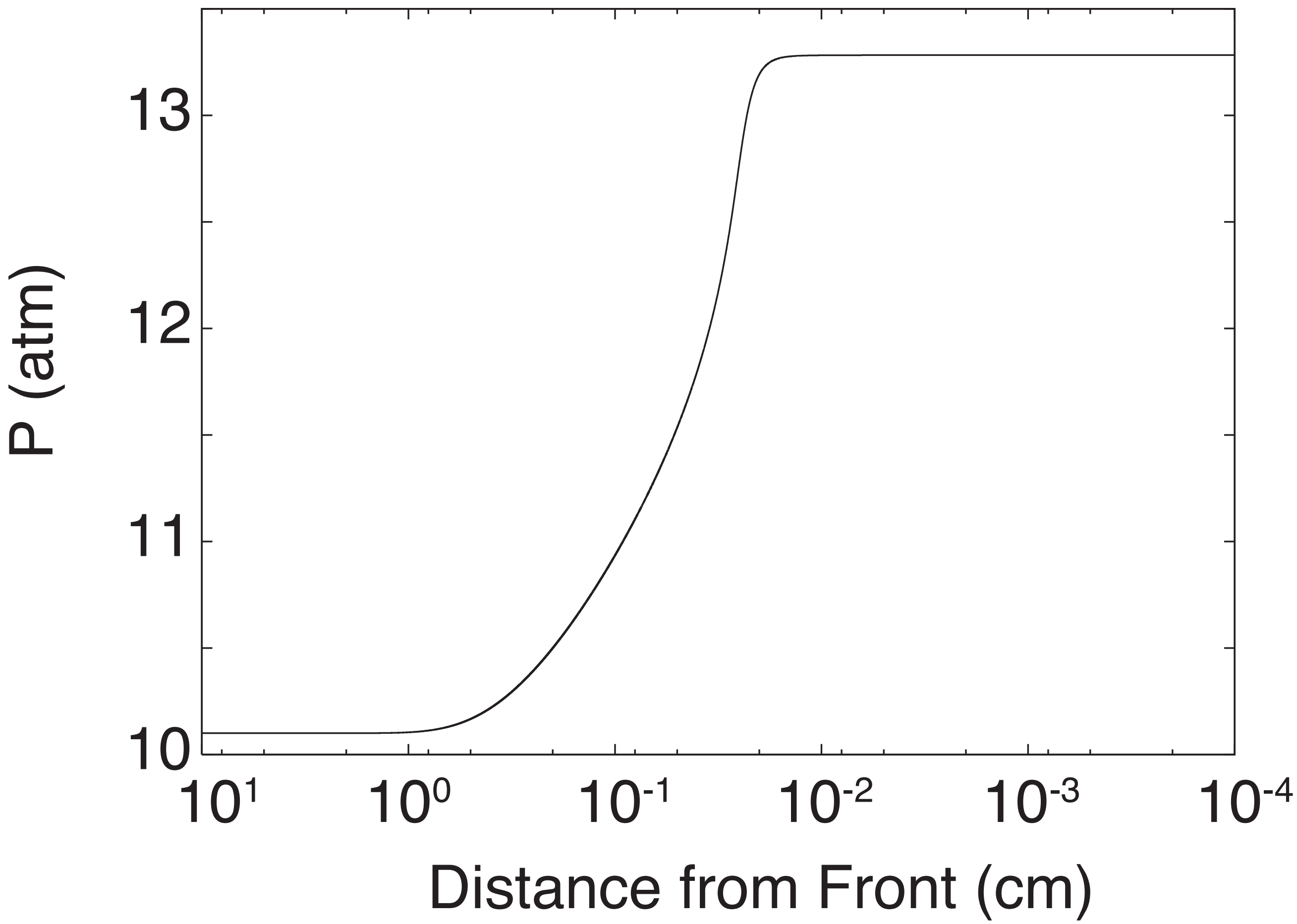
Inviscid Steady-State: Mass Fractions

$f = 1.15$



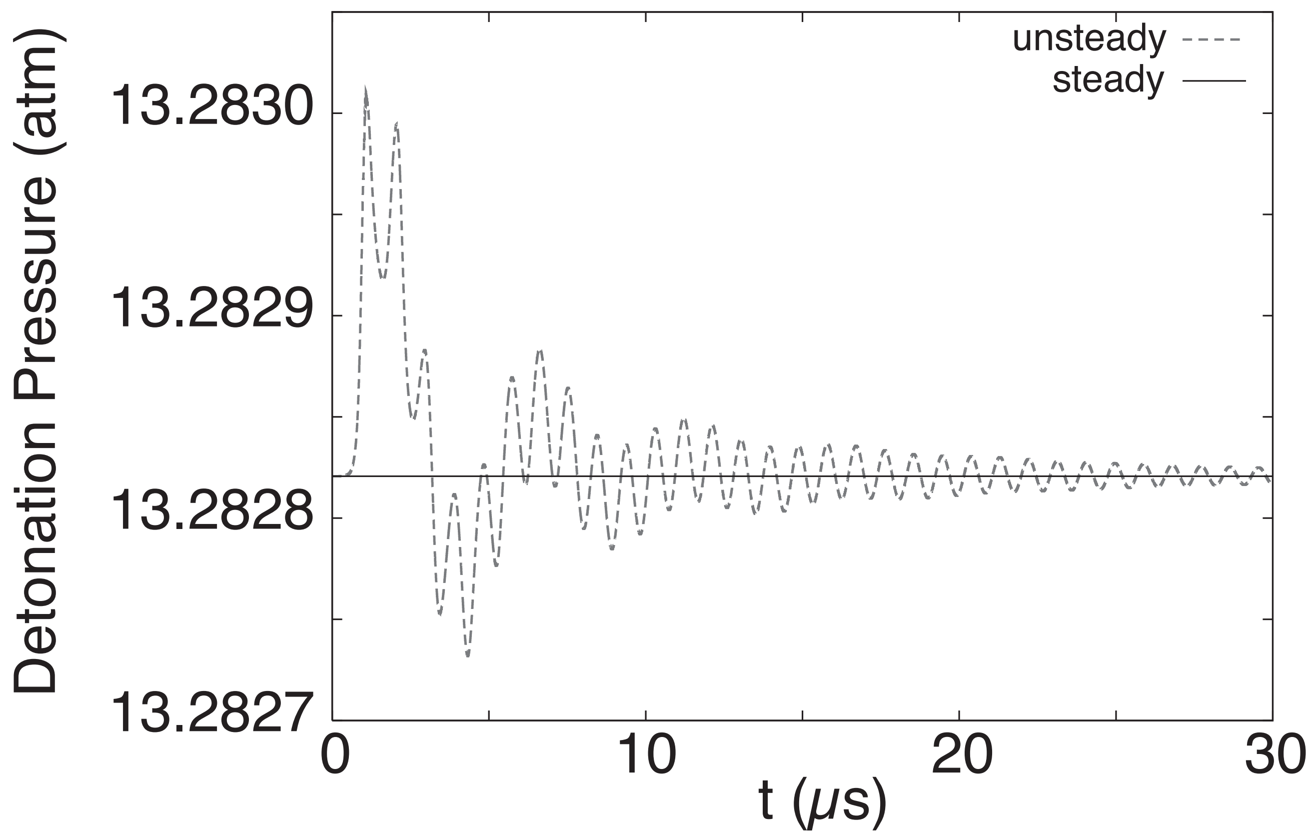
Inviscid Steady-State: Pressure

$f = 1.15$

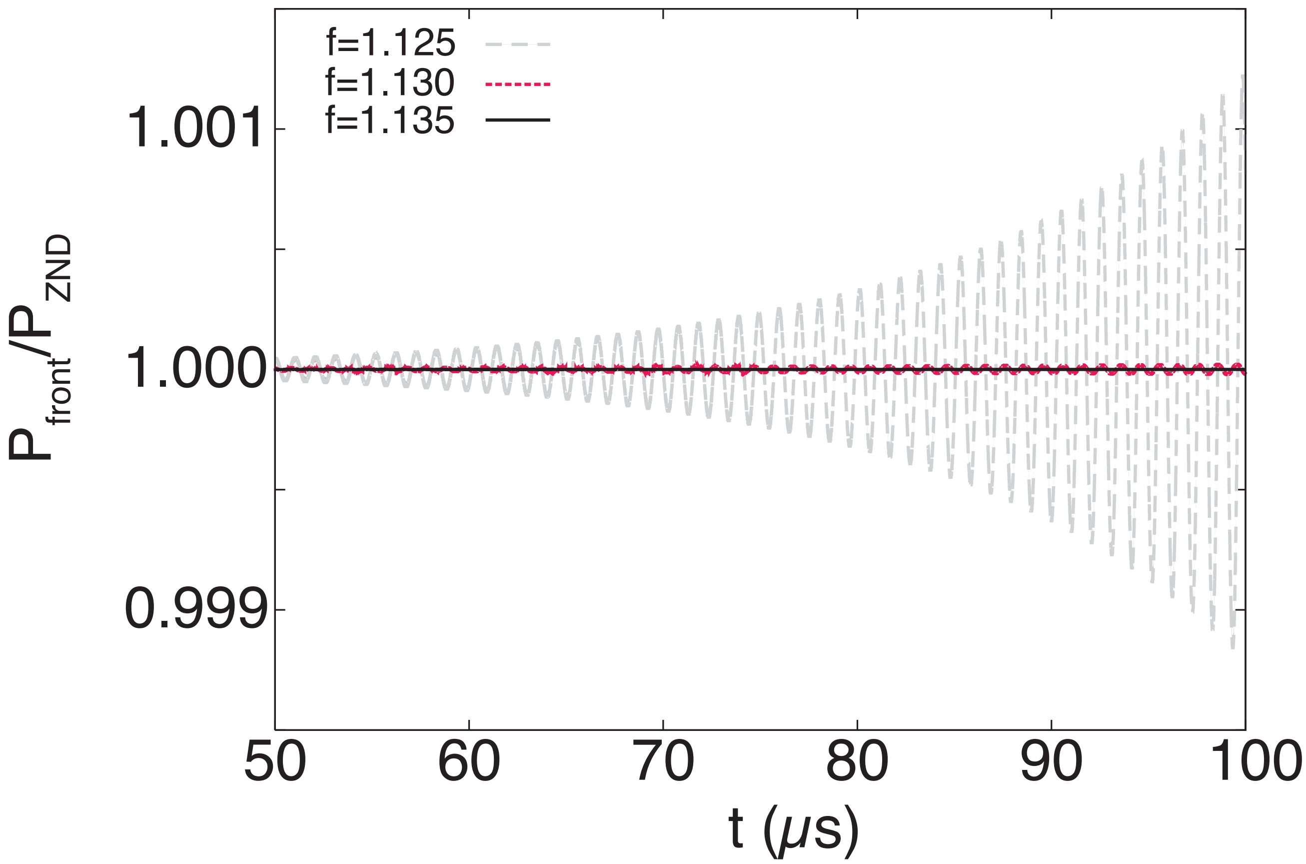


Inviscid Transient Behavior: Stable Detonation

$f = 1.15$

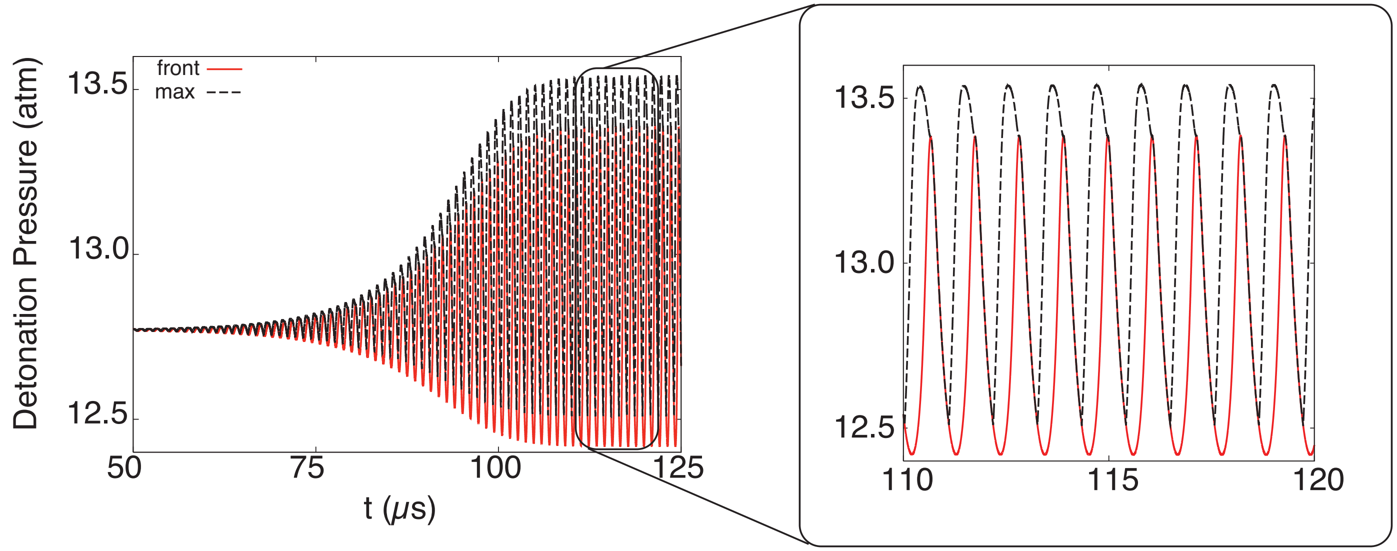


Near Neutral Stability



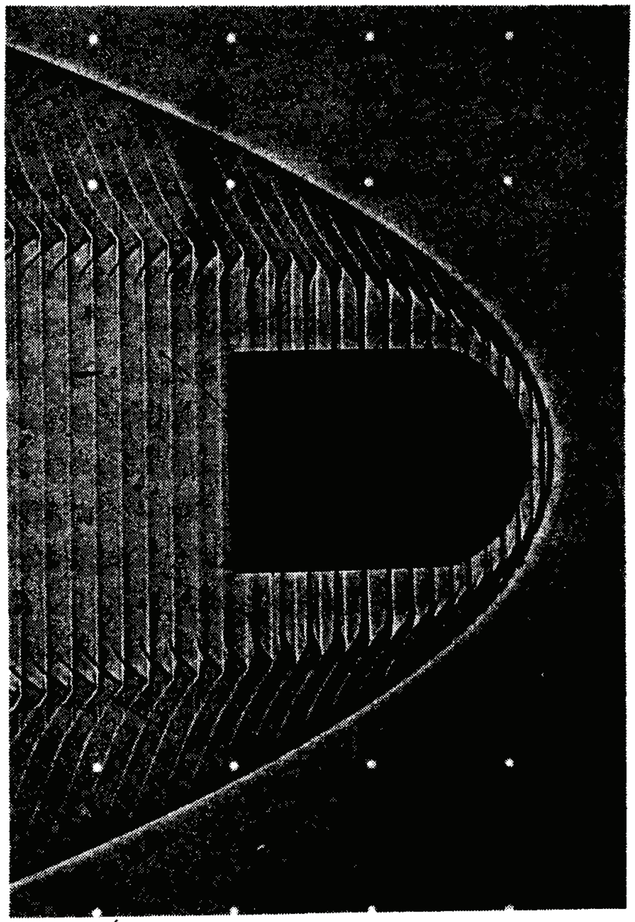
Inviscid Transient Behavior: Unstable Detonation

$f = 1.10$



- 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.

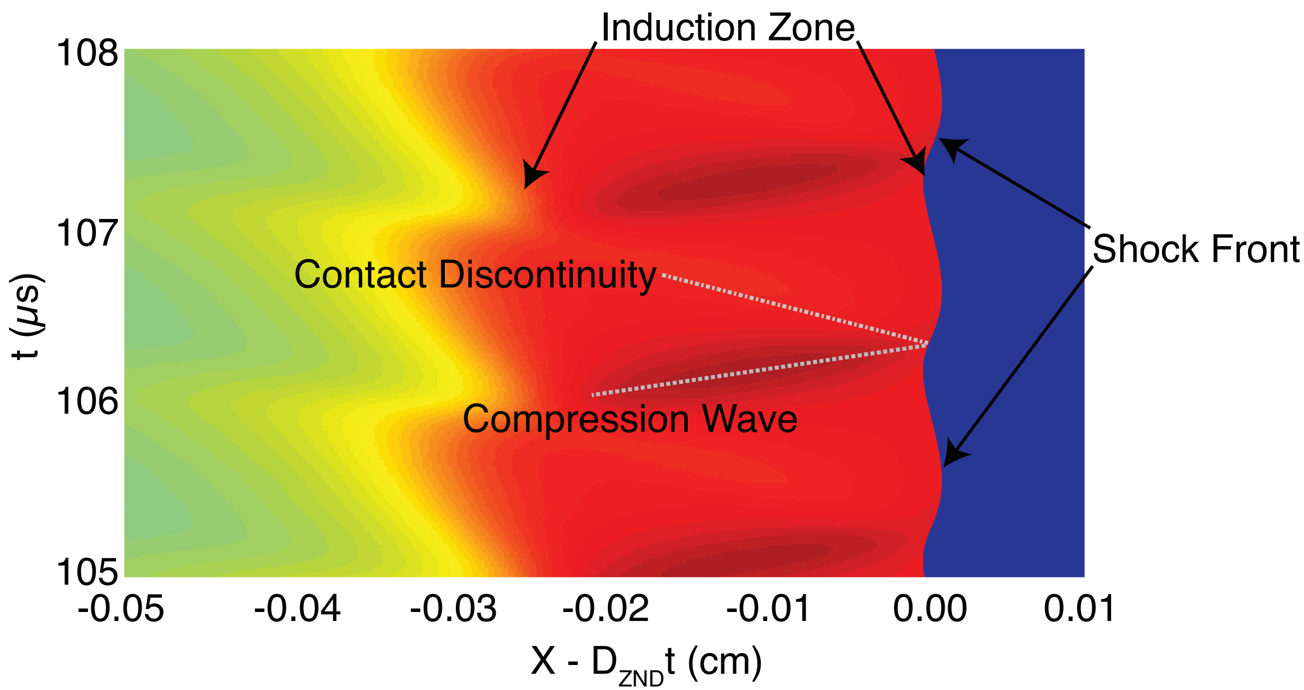
Lehr's High Frequency Instability



- 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 $1.04\ MHz$

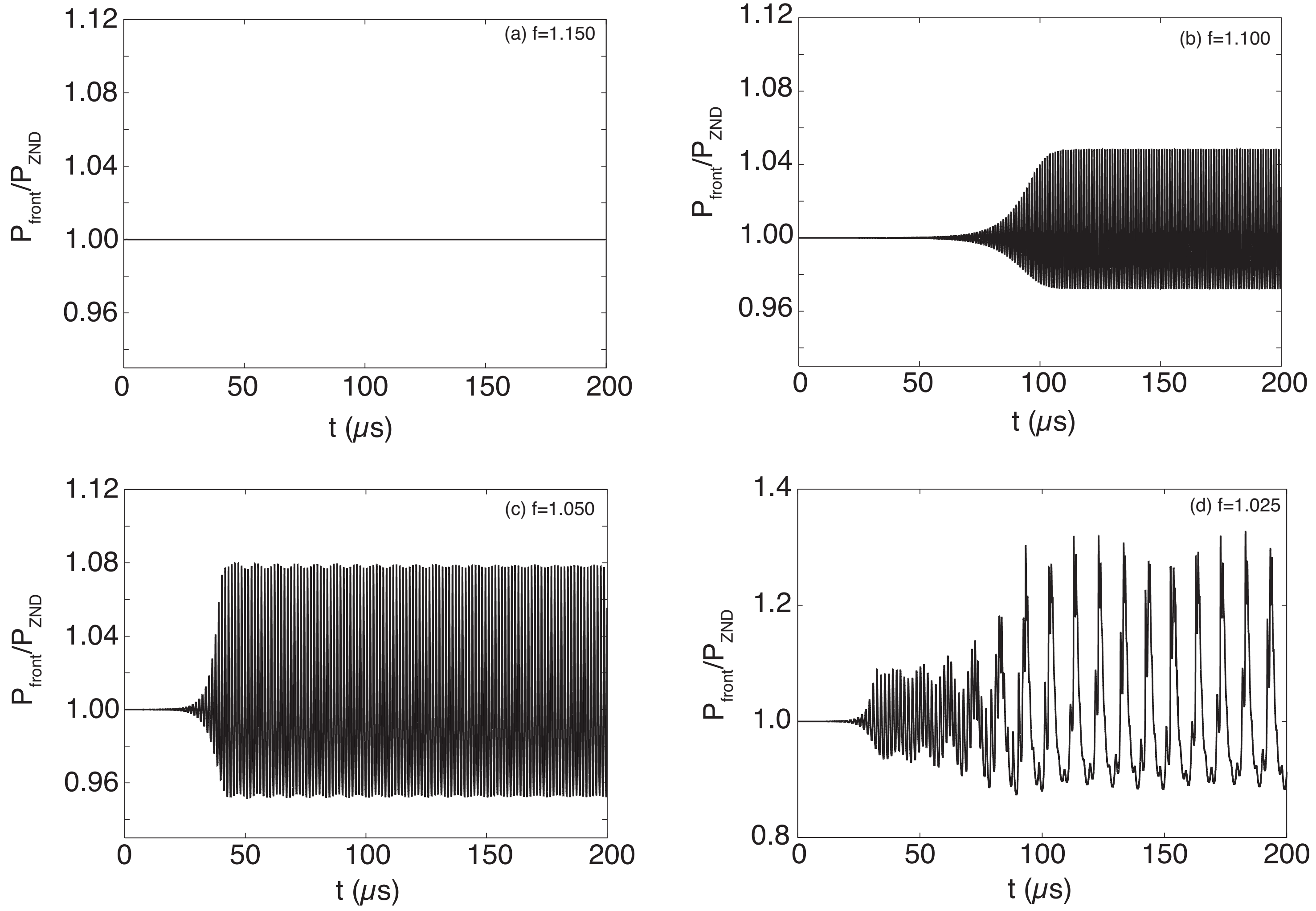
Unstable, Inviscid Detonation: x-t Diagram

$f = 1.10$

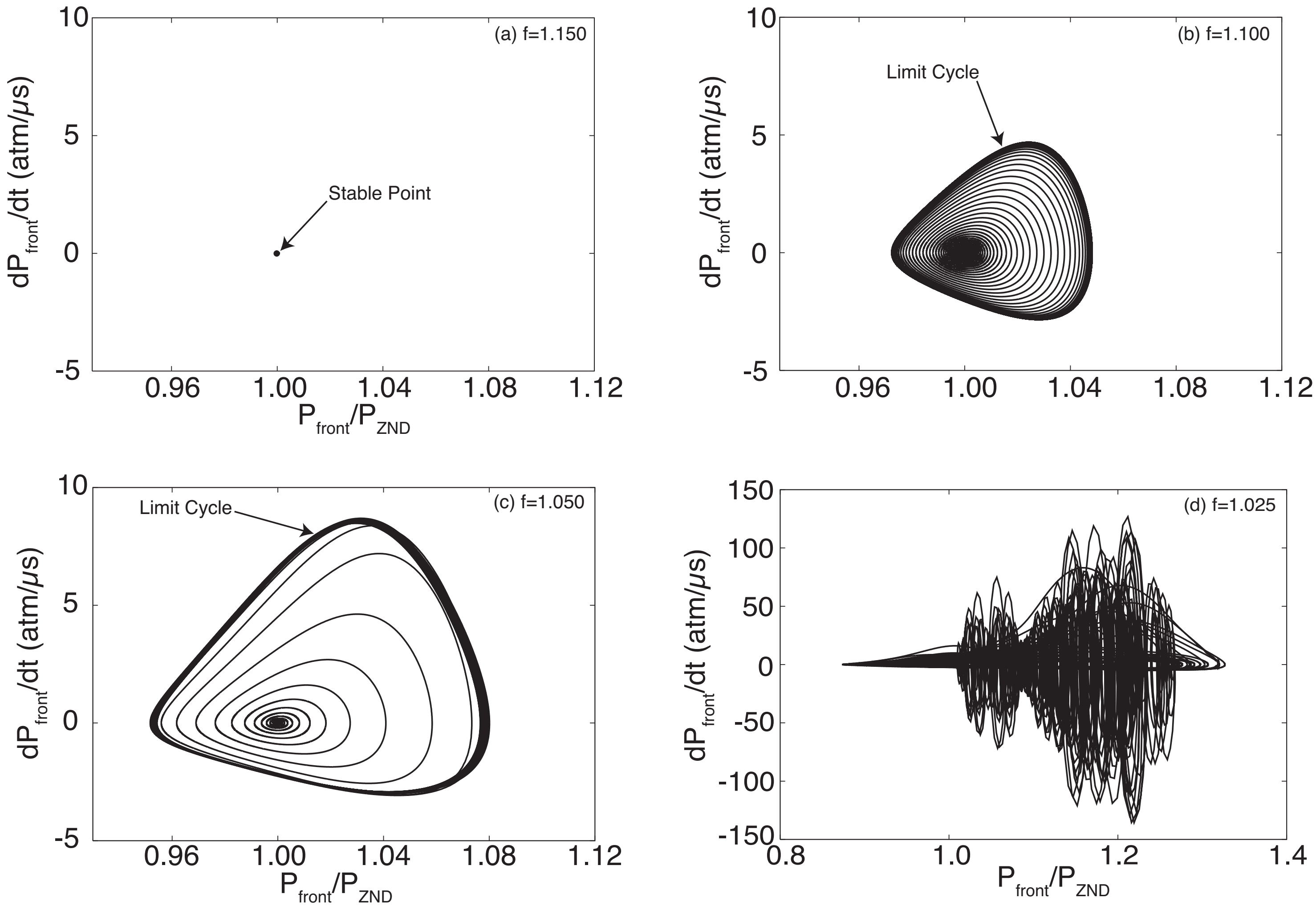


A x-t diagram of density in a Galilean reference frame traveling at $2057\ m/s$.

Inviscid Transient Behavior: Various Overdrives

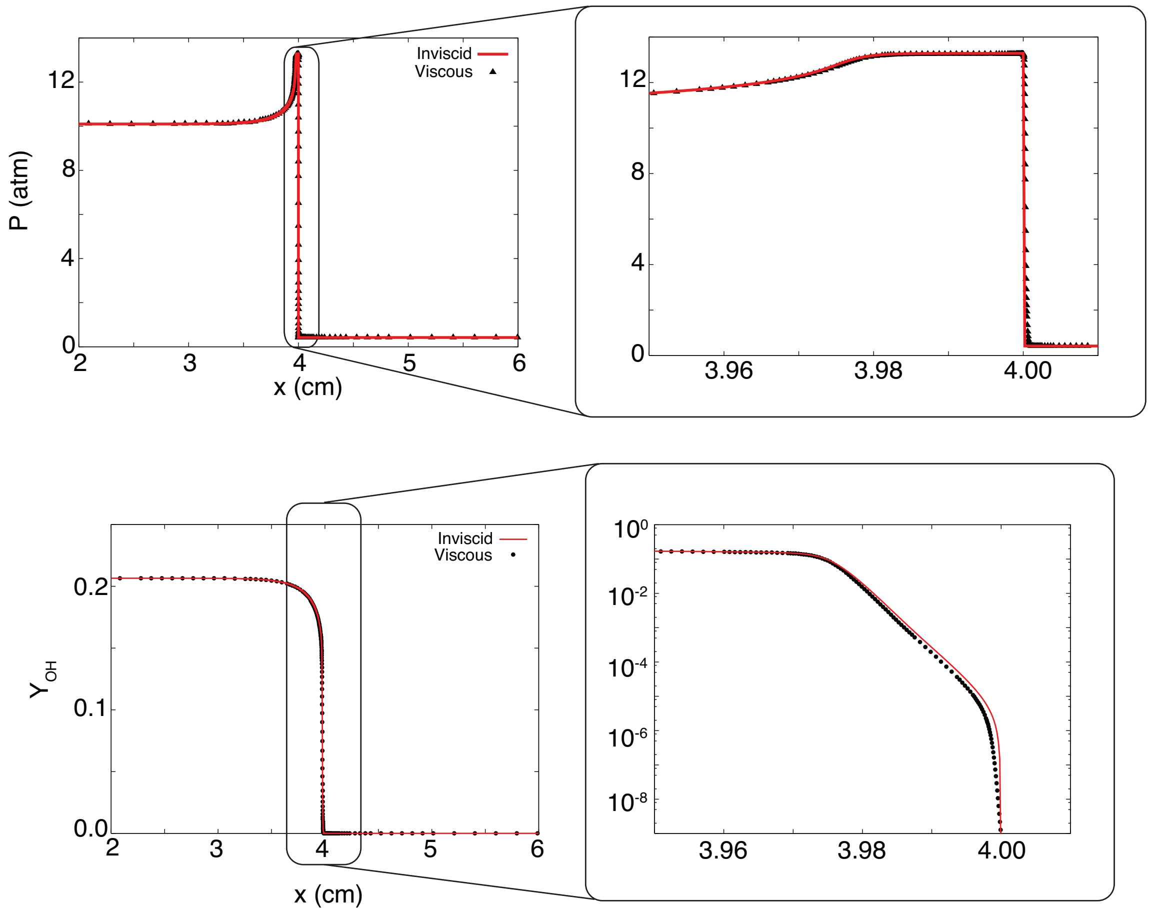


Inviscid Phase Portraits: Various Overdrives



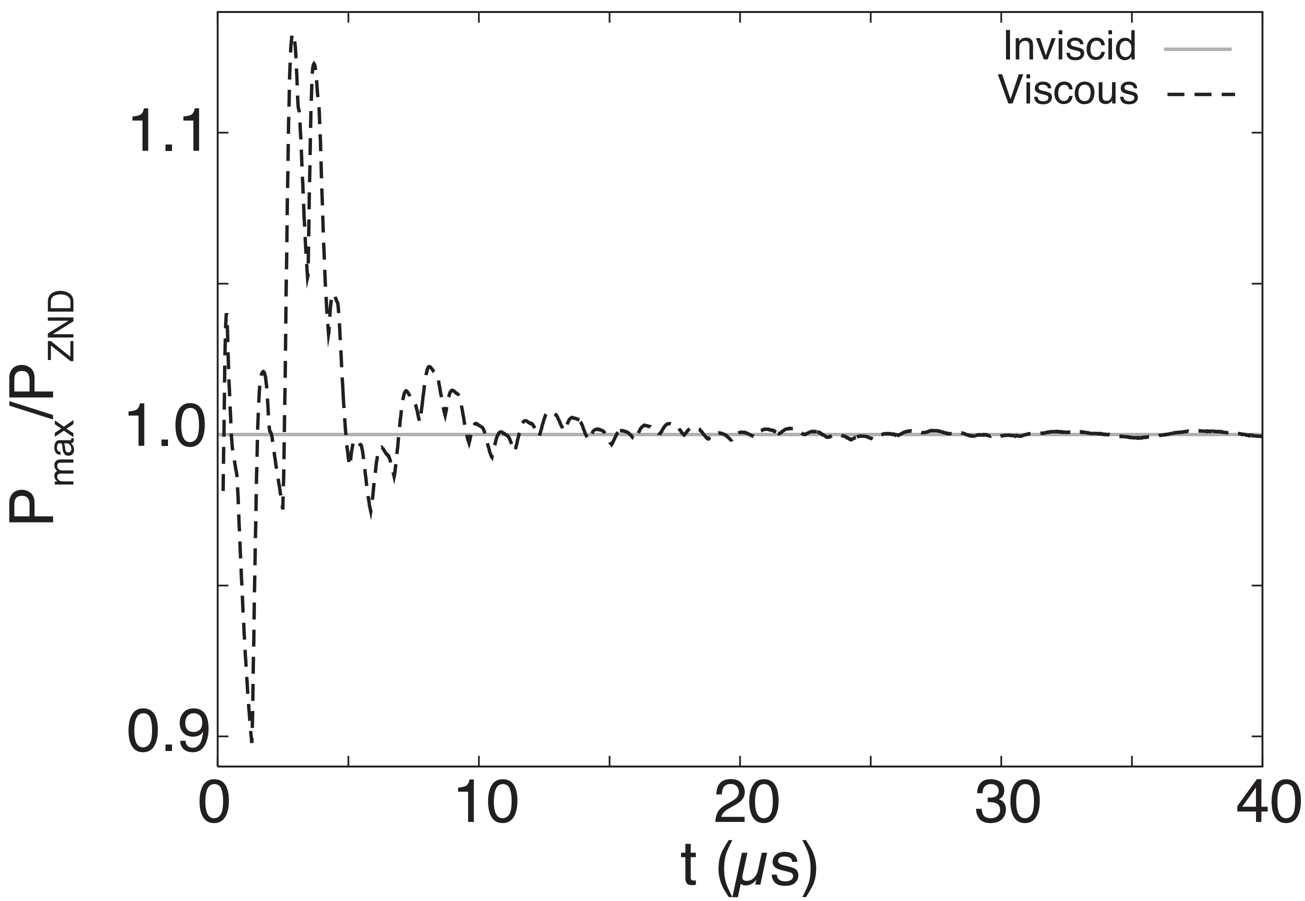
Stable, Viscous Detonation: Long Time Structure

$f = 1.15$



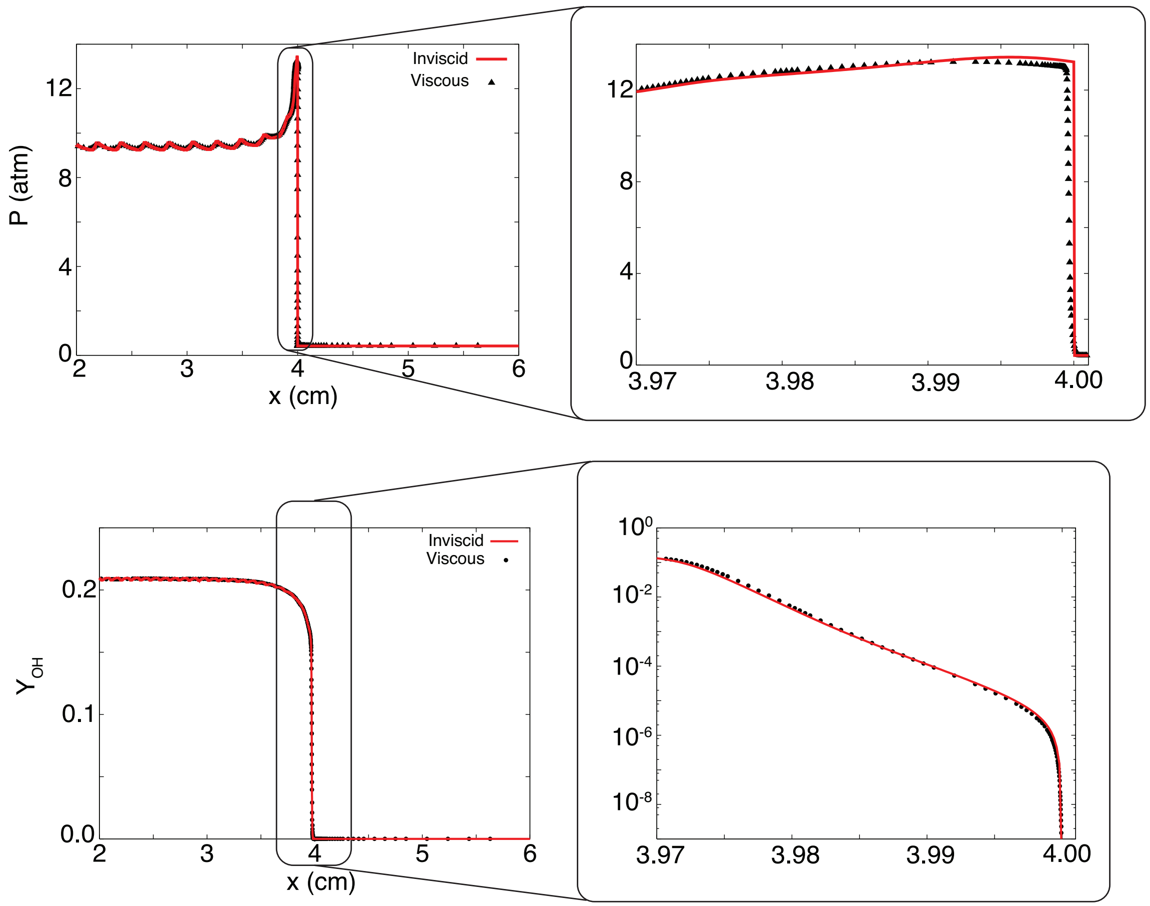
Stable, Viscous Detonation: Transient Behavior

$f = 1.15$



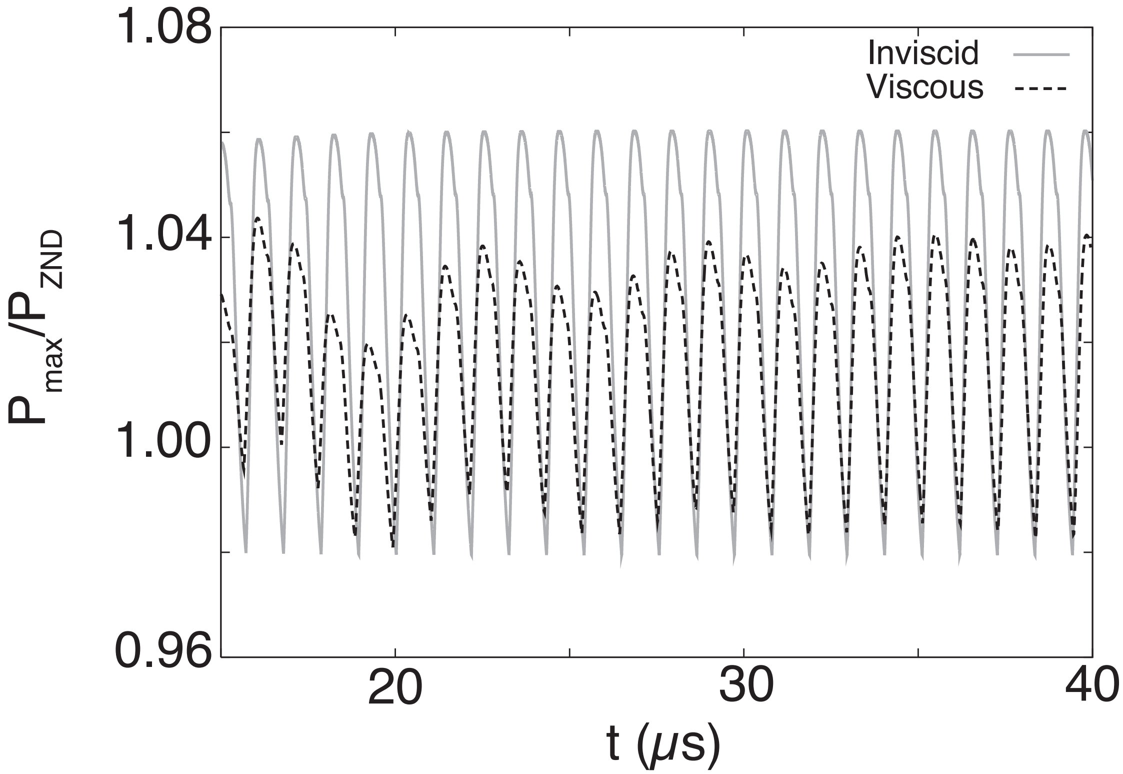
Unstable, Viscous Detonation: Long Time Structure

$f = 1.10$



Unstable, Viscous Detonation: Transient Behavior

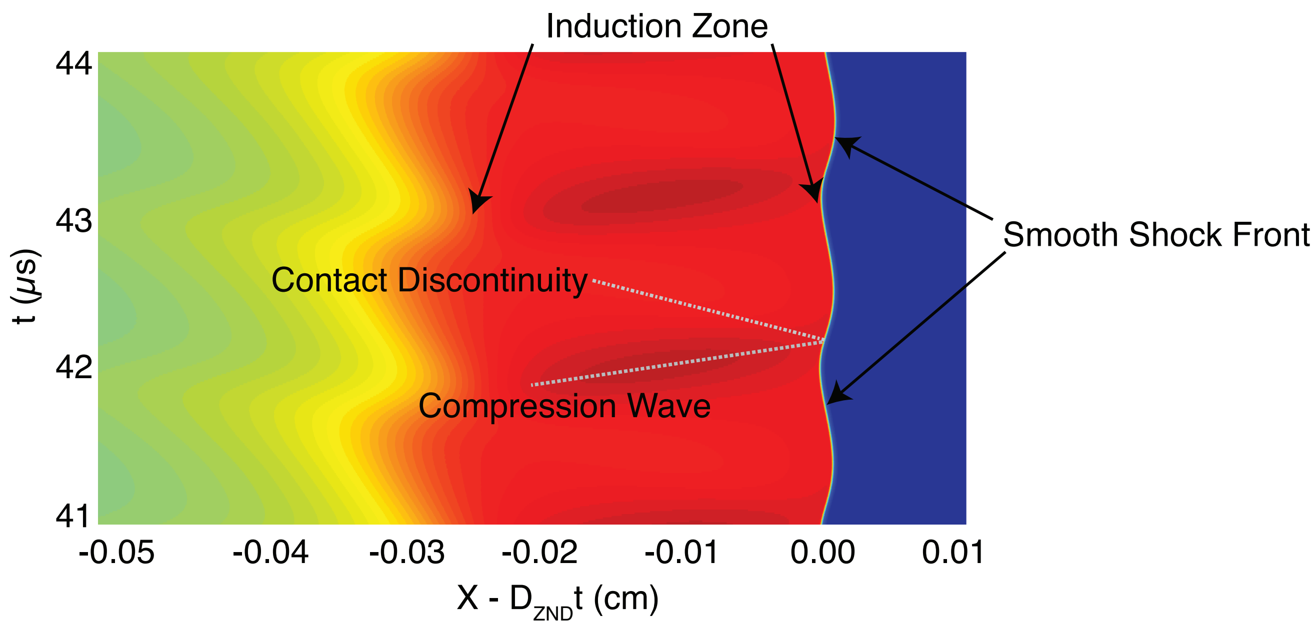
$f = 1.10$



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 $2057\ m/s$.

Conclusions

- Unsteady, inviscid detonation dynamics can be accurately simulated when all reaction length scales admitted by detailed kinetics are fully resolved using a fine grid; the shock-fitting technique used assures numerical viscosity is minimal.
- At high overdrives, the detonations are stable.
- As the overdrive is decreased, the long time behavior becomes progressively more complex.
- In the inviscid limit a critical overdrive, $f = 1.130$, is found below which oscillations at a single frequency appear.
- As the overdrive is lowered, the amplitude of these oscillations increases.

Conclusions

- Lowering the overdrive yet further gives rise to oscillations at multiple frequencies.
- The predicted $0.97\ MHz$ frequency for a $f = 1.10$ overdriven detonation agrees well with the frequency of $1.04\ MHz$ observed by Lehr in his experiments of shock-induced combustion flow around spherical projectiles.
- The structure of the overdriven detonation relative to the inviscid limit is modulated by the addition of mass, momentum, and energy diffusion.
- The addition of viscous effects has a stabilizing effect on the long time behavior of a detonation; the amplitude of the oscillations is significantly reduced.