Harmony in High Speed Combustion

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- Romick, Aslam, Powers, 2012, The effect of diffusion on the dynamics of unsteady detonation, *Journal of Fluid Mechanics*, 699:453-464.
- Romick, Aslam, Powers, 2015, Verified and validated calculation of unsteady dynamics of viscous hydrogen-air detonation, *Journal of Fluid Mechanics*, to appear.

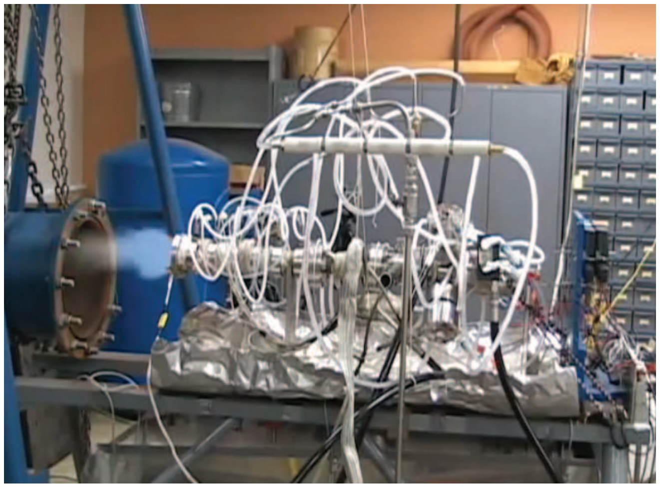
Verification and Validation Overview

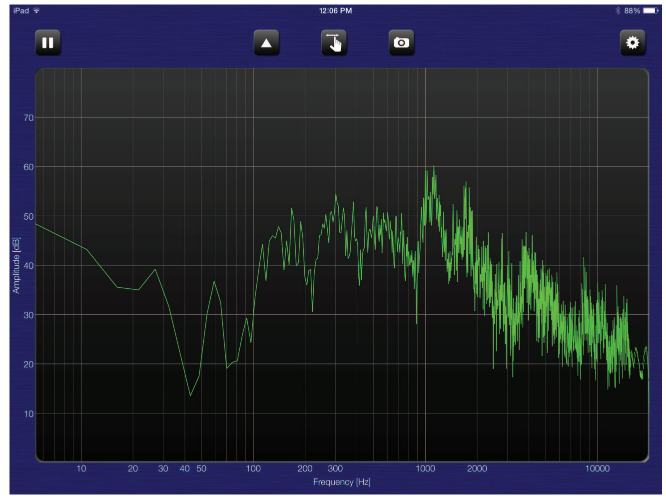
- We will consider here *verification* and *validation* of a multi-scale problem using *Direct Numerical Modeling*, which captures both coarse and fine scales.
- One key algorithm is the *Wavelet Adaptive Multiresolution Method* (WAMR), one of the methods employed in the University of Notre Dame-led *Center for Shock Wave Processing of Advanced Materials* (C-SWARM), a NNSA-supported PSAAP II Center.
- C-SWARM is in Year 1 of a five-year project associated with exascale scientific computing of challenging multi-scale shock physics problems.

Verification and Validation Overview, cont.

- C-SWARM is a joint effort with Notre Dame, Indiana U., and Purdue U.
- Its problem is shocking mechanically pre-activated pressed metallic powders to synthesize new metallic structures.
- We will develop verified and validated predictive codes prepared for an exascale environment.
- The WAMR code, in development at Notre Dame for 20 years, will be used today on a different problem in reactive gas dynamics.

Disharmony in High Speed Combustion



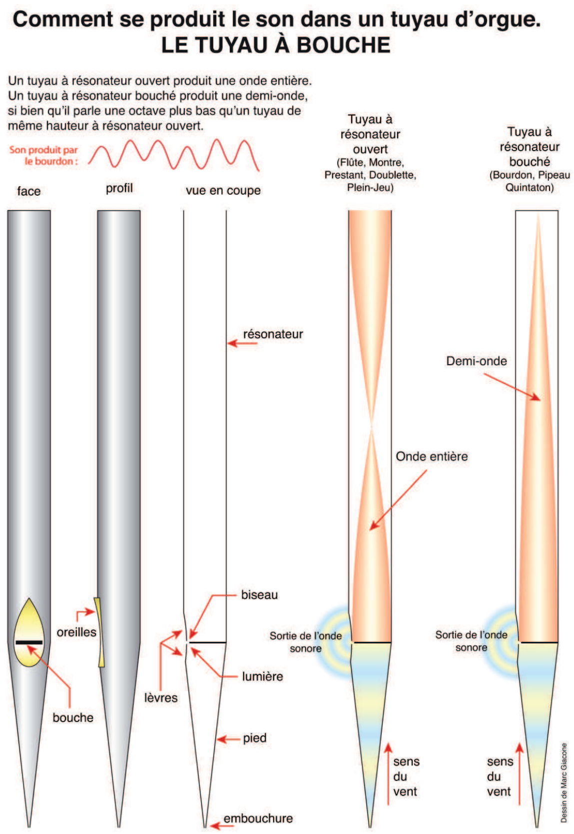


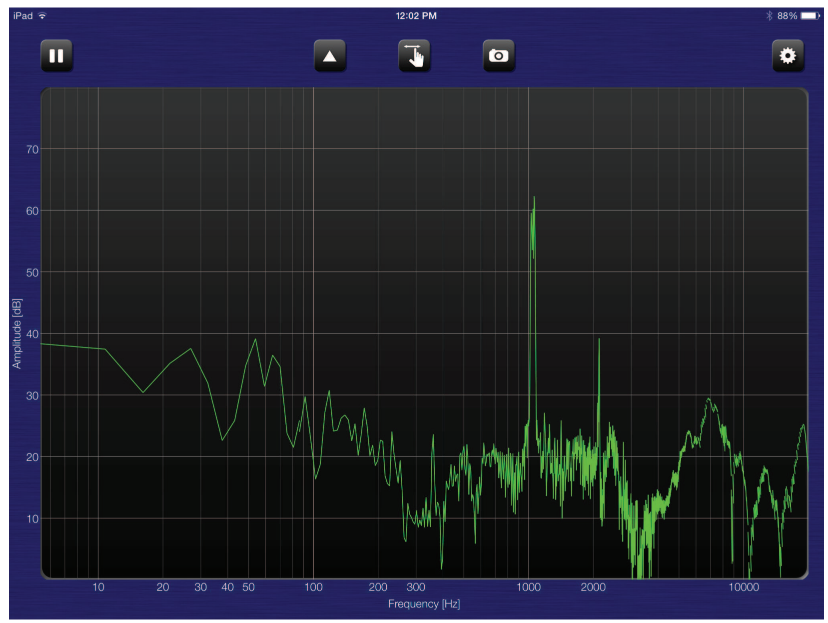
https://www.youtube.com/watch?v=rYxsilgRxi4

Prof. Frank Lu, University of Texas-Arlington.

Described as “25 Hz,” but there is acoustic energy present across the frequency spectrum. Disorder.

Harmony: Organ Pipe Resonance





$a/\ell \sim 1000$ Hz. Higher order harmonic at 2000 Hz. Order.

Motivation

- Combustion dynamics are influenced by various balances of *advection*, *reaction*, and *diffusion*.
- Depending on flow conditions, one may observe simple structures, patterned harmonic structures, or chaotic structures.
- Often, the critical balance is between *advection* and *reaction*, with diffusion serving as only a small perturbation.
- Near stability thresholds, diffusion can play a determining role.
- Full non-linear dynamics can induce complex behavior.
- Extreme care *may or may not be* needed in numerical simulation to carefully capture the multi-scale physics.

Introduction

- Standard result from non-linear dynamics: small scale phenomena can influence large scale phenomena and vice versa.
- What are the risks of using models which ignore diffusion (Euler vs. Navier-Stokes)?
- Might there be risks in using standard filtering strategies: implicit time-advancement, numerical viscosity, LES, and turbulence modeling, all of which introduce *nonphysical diffusion* to filter small scale physical dynamics?

Introduction-Continued

- Powers & Paolucci (*AIAA J.*, 2005) studied the reaction length scales of inviscid H_2-O_2 detonations and found the finest length scales on the order of microns and the largest on the order of centimeters for atmospheric ambient pressure.
- This range of scales must be resolved to capture the dynamics.
- In a one-step kinetic model only a single reaction length scale is induced compared to the multiple length scales of detailed kinetics.
- We examine i) a simple one-step model and ii) a detailed model appropriate for hydrogen.

One-Step Reaction Kinetics Model

One-Dimensional Unsteady Compressible Reactive Navier-Stokes Equations

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

$$\frac{\partial}{\partial t}\left(\rho u\right) + \frac{\partial}{\partial x}\left(\rho u^2 + P - \tau\right) = 0,$$

$$\frac{\partial}{\partial t}\left(\rho\left(e + \frac{u^2}{2}\right)\right) + \frac{\partial}{\partial x}\left(\rho u\left(e + \frac{u^2}{2}\right) + j^q + \left(P - \tau\right) u\right) = 0,$$

$$\frac{\partial}{\partial t}\left(\rho Y_B\right) + \frac{\partial}{\partial x}\left(\rho u Y_B + j_B^m\right) = \rho r.$$

Equations are transformed to a steady moving reference frame.

Constitutive Relations

$$P = \rho R T,$$

$$e = \frac{p}{\rho(\gamma - 1)} - qY_B,$$

$$r = H(P - P_s)a(1 - Y_B)\, e^{-\frac{\tilde{E}}{p/\rho}},$$

$$j_B^m = -\rho \mathcal{D} \frac{\partial Y_B}{\partial x},$$

$$\tau = \frac{4}{3}\mu \frac{\partial u}{\partial x},$$

$$j^q = -k\frac{\partial T}{\partial x} + \rho \mathcal{D} q \frac{\partial Y_B}{\partial x}.$$

with $D = 10^{-4}\,\frac{\mathrm{m}^2}{\mathrm{s}}$, $k = 10^{-1}\,\frac{\mathrm{W}}{\mathrm{mK}}$, and $\mu = 10^{-4}\,\frac{\mathrm{Ns}}{\mathrm{m}^2}$, so for $\rho_o = 1\,\frac{\mathrm{kg}}{\mathrm{m}^3}$, $Le = Sc = Pr = 1.$

Case Examined

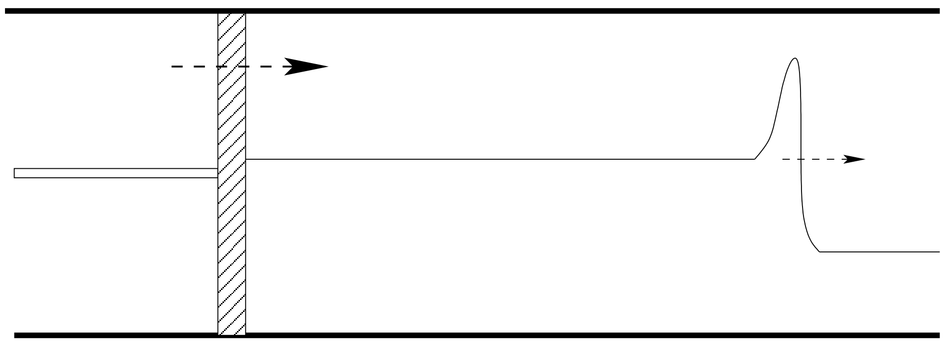
Let us examine this one-step kinetic model with:

- a fixed reaction length, $L_{1/2} = 10^{-6}$ m, which is similar to that of the finest H_2-O_2 scale.
- a fixed diffusion length, $L_\mu = 10^{-7}$ m; mass, momentum, and energy diffusing at the same rate.
- an ambient pressure, $P_o = 101325$ Pa, ambient density, $\rho_o = 1$ kg$/$m^3, heat release $q = 5066250$ m$^2/$s^2, and $\gamma = 6/5$.

Numerical Method

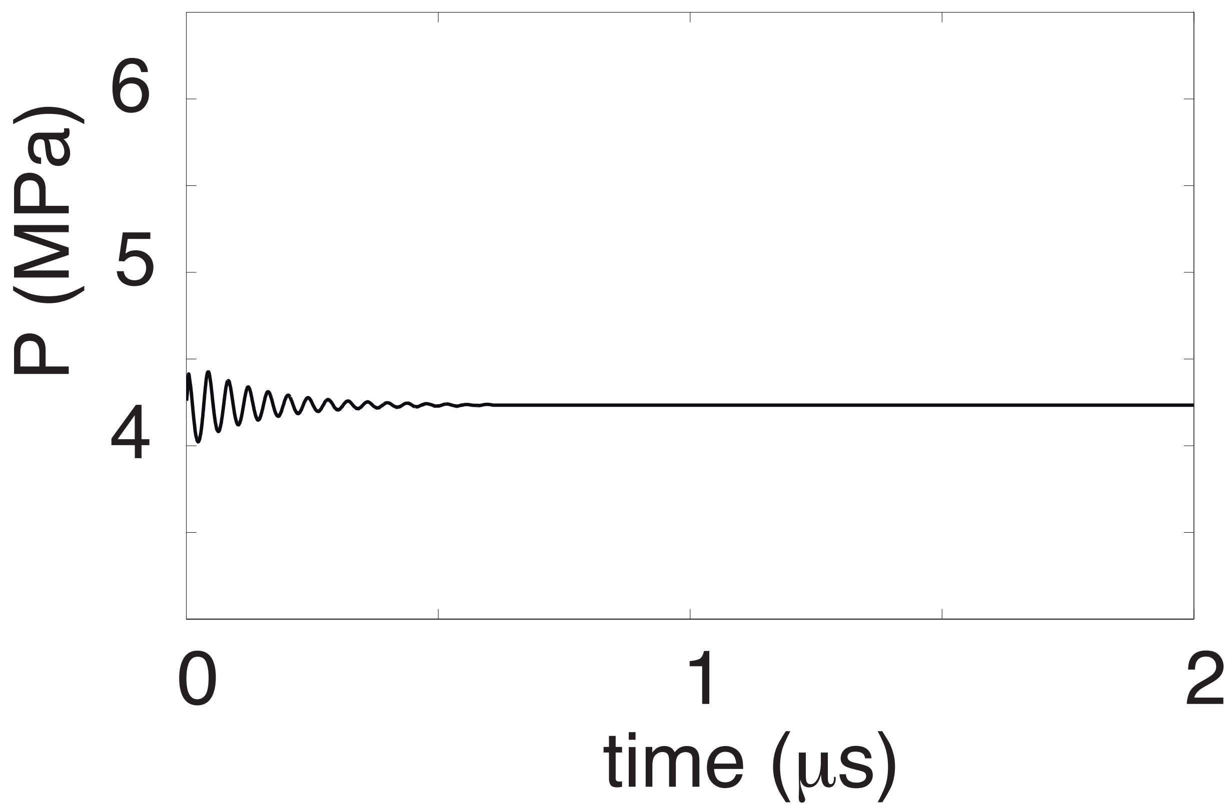
- Finite difference, uniform grid
  $\left(\Delta x = 2.50 \times 10^{-8}\ \text{m}, N = 8001, L = 0.2\ \text{mm}\right)$.
- Computation time = 192 hours for $10\ \mu$s on an AMD 2.4 GHz with 512 kB cache.
- A point-wise method of lines aproach was used.
- Advective terms were calculated using a combination of fifth order WENO and Lax-Friedrichs.
- Sixth order central differences were used for the diffusive terms.
- Temporal integration was accomplished using a third order Runge-Kutta scheme.

Physical Piston Problem



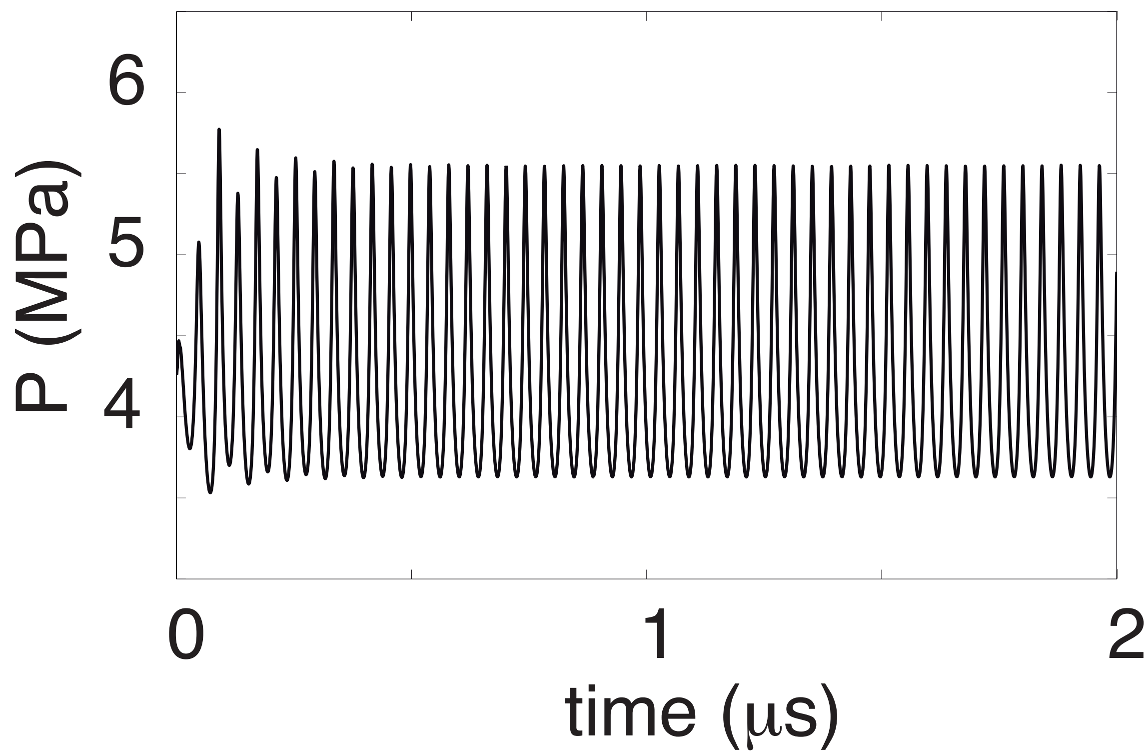
- Initialized with inviscid ZND solution.
- Moving frame travels at the CJ velocity.
- Integrated in time for long time behavior.

Below a Critical Activation Energy, the Detonation is Stable

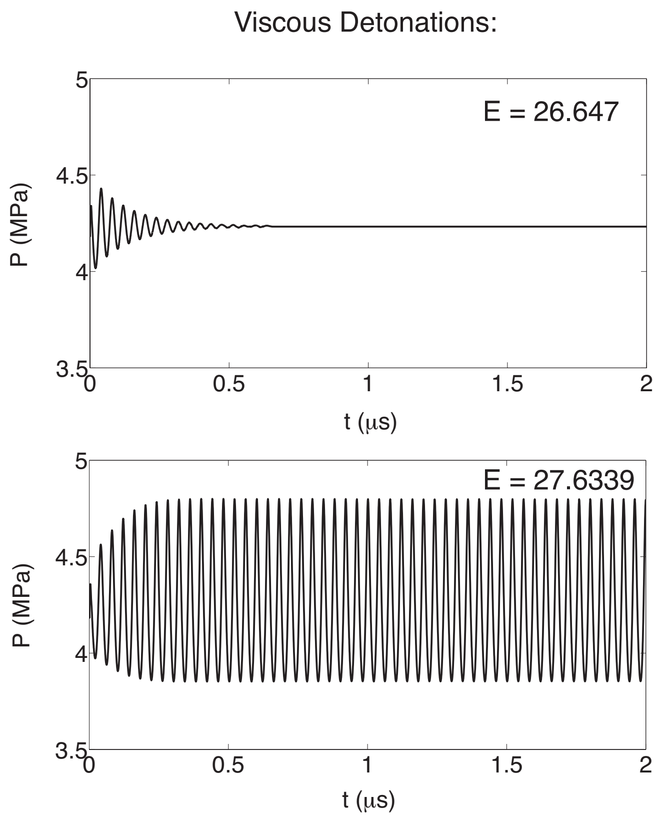


At Higher Activation Energy, Fundamental Harmonic Due to Balance Between Reaction and Advection Between Lead Shock and End of Reaction Zone:

An Organ Pipe Resonance

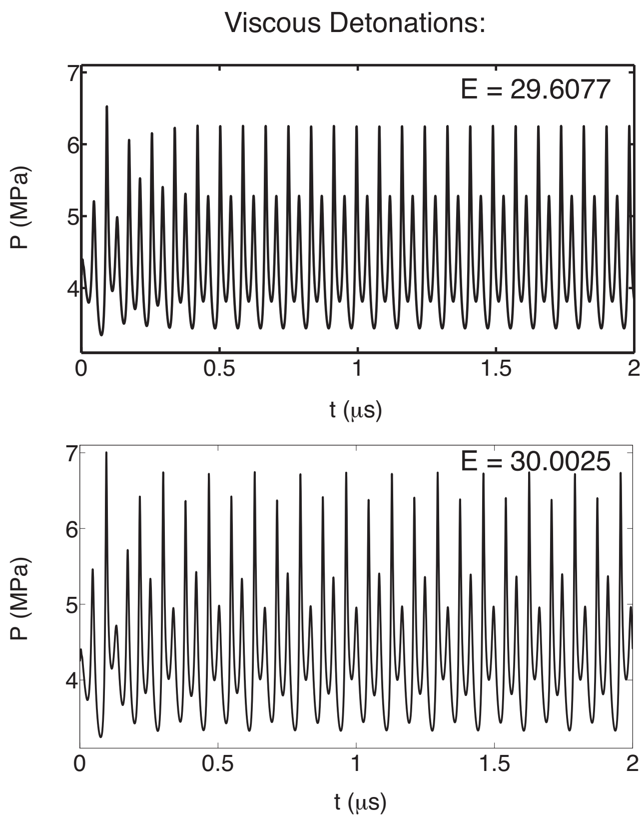


Diffusion Delays Transition to Instability



- Lee and Stewart revealed for $E < 25.26$ the steady ZND wave is linearly stable.
- For the inviscid case Henrick *et al.* found the stability limit at $E_0 = 25.265 \pm 0.005$.
- In the viscous case $E = 26.647$ is still stable; however, above $E_0 \approx 27.1404$ a period-1 limit cycle can be realized.

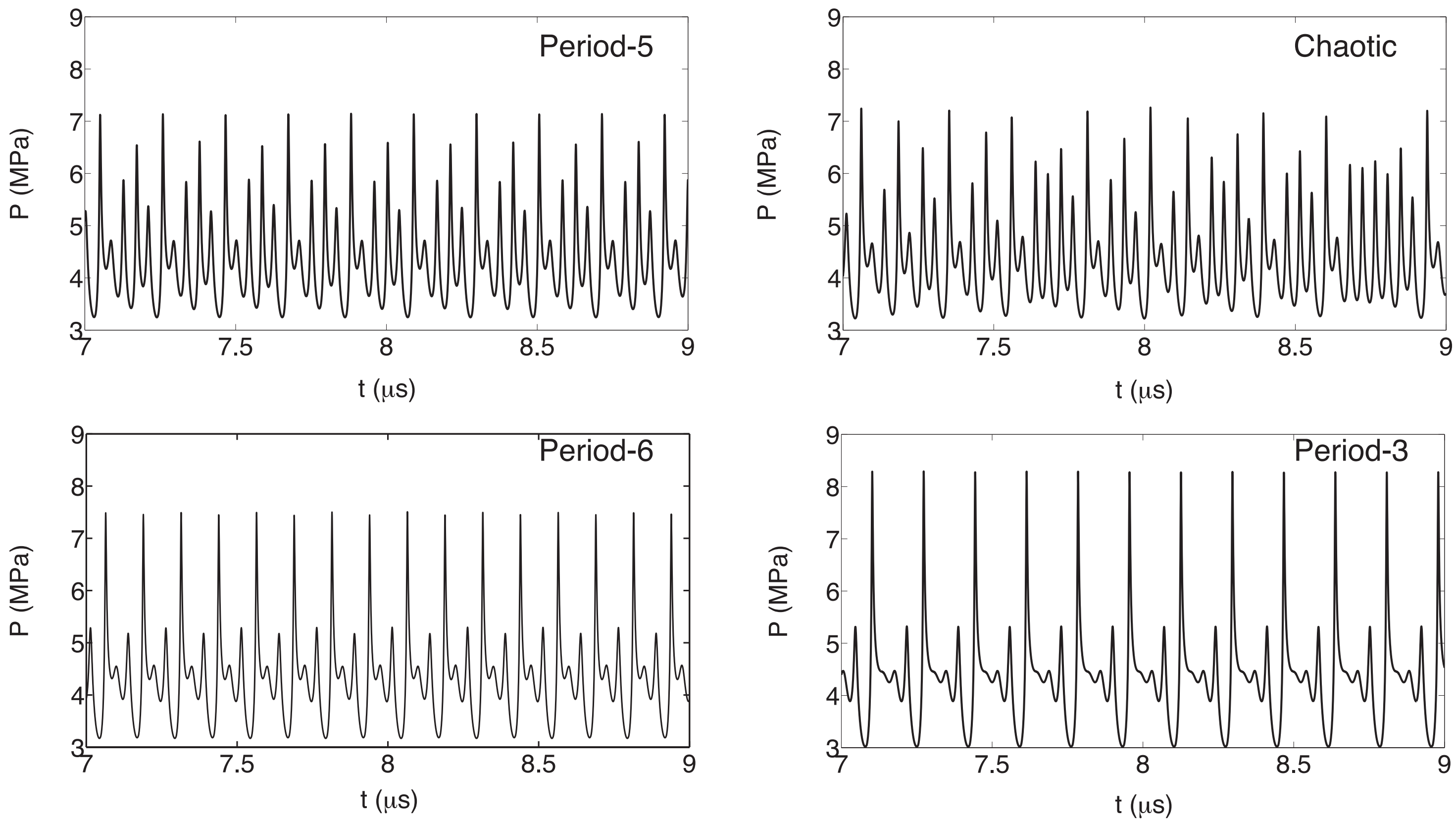
Period-Doubling Phenomena Predicted



- As in the inviscid limit, the viscous case goes through a period-doubling phase.
- For the inviscid case, the period-doubling began at $E_1 \approx 27.2$.
- In the viscous case, the beginning of this period doubling is delayed to $E_1 \approx 29.3116$.

Chaos and Order

Viscous Detonations:



Diffusion Delays Transition to Chaos

- In the inviscid limit, the point where bifurcation points accumulate is found to be $E_\infty \approx 27.8324$.
- For the viscous case, $L_\mu / L_{1/2} = 1/10$, the accumulation point is delayed until $E_\infty \approx 30.0411$.
- For $E > 30.0411$, a region exists with many relative maxima in the detonation pressure; it is likely the system is in the chaotic regime.

Approximations to Feigenbaum's Constant

$$\delta_\infty = \lim_{n\to\infty} \delta_n = \lim_{n\to\infty} \frac{E_n - E_{n-1}}{E_{n+1} - E_n}$$

Feigenbaum predicted $\delta_\infty \approx 4.669201.$

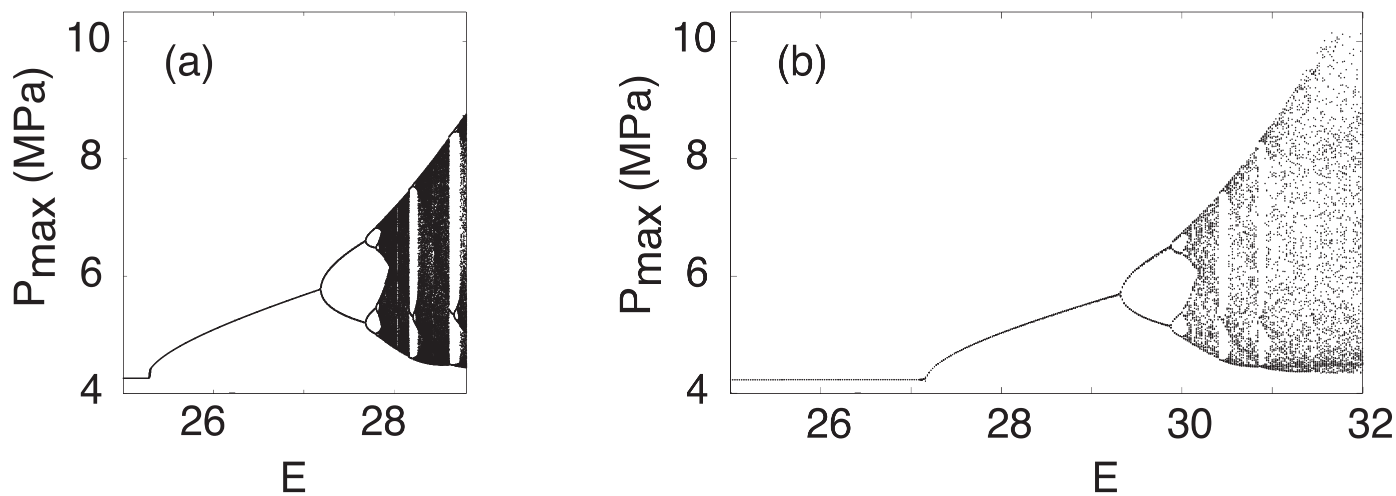
	Inviscid	Inviscid	Viscous	Viscous
n	E_n	δ_n	E_n	δ_n
0	25.2650	-	27.1404	-
1	27.1875	3.86	29.3116	3.793
2	27.6850	4.26	29.8840	4.639
3	27.8017	4.66	30.0074	4.657
4	27.82675	-	30.0339	-

Similar Behavior to Logistics Map:

$$x_{n+1} = rx_n(1 - x_n)$$

- The period-doubling behavior and transition to chaos predicted in both the viscous and inviscid limit have striking similarilities to that of the logistic map.
- Within the chaotic region, there exist pockets of order.
- Periods of 5, 6, and 3 are found within this region.

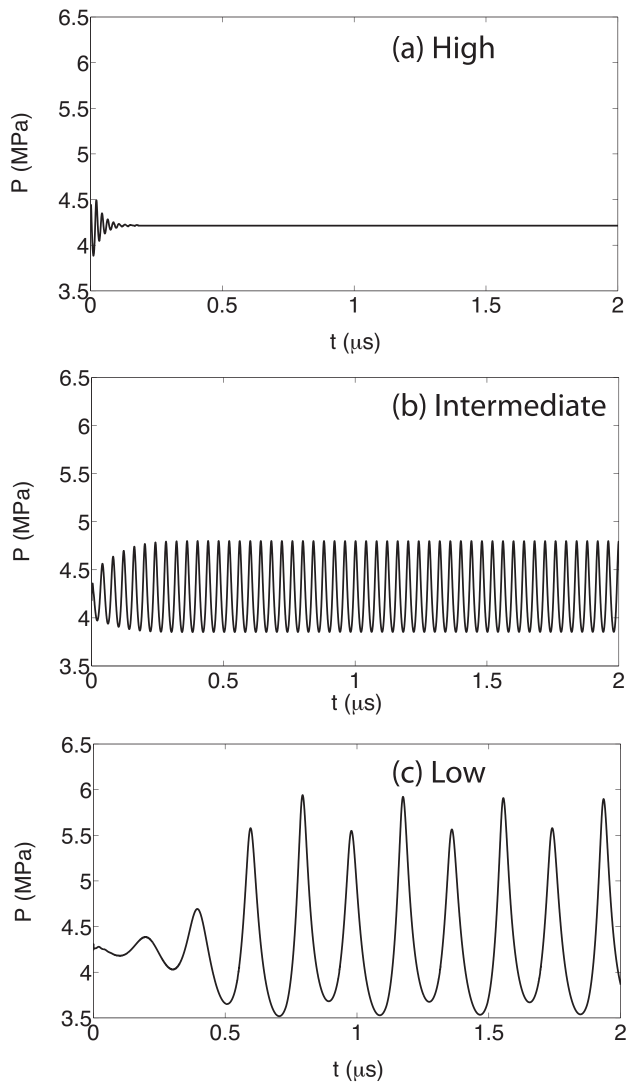
Diffusion Delays Instability: Bifurcation Diagram



a) no diffusion

b) diffusion

Diminishing Diffusion De-Stabiliizes ($E = 27.6339$)



- The system undergoes transition from a stable detonation to a period-1 limit cycle, to a period-2 limit cycle.
- The amplitude of pulsations increases.
- The frequency decreases.

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

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

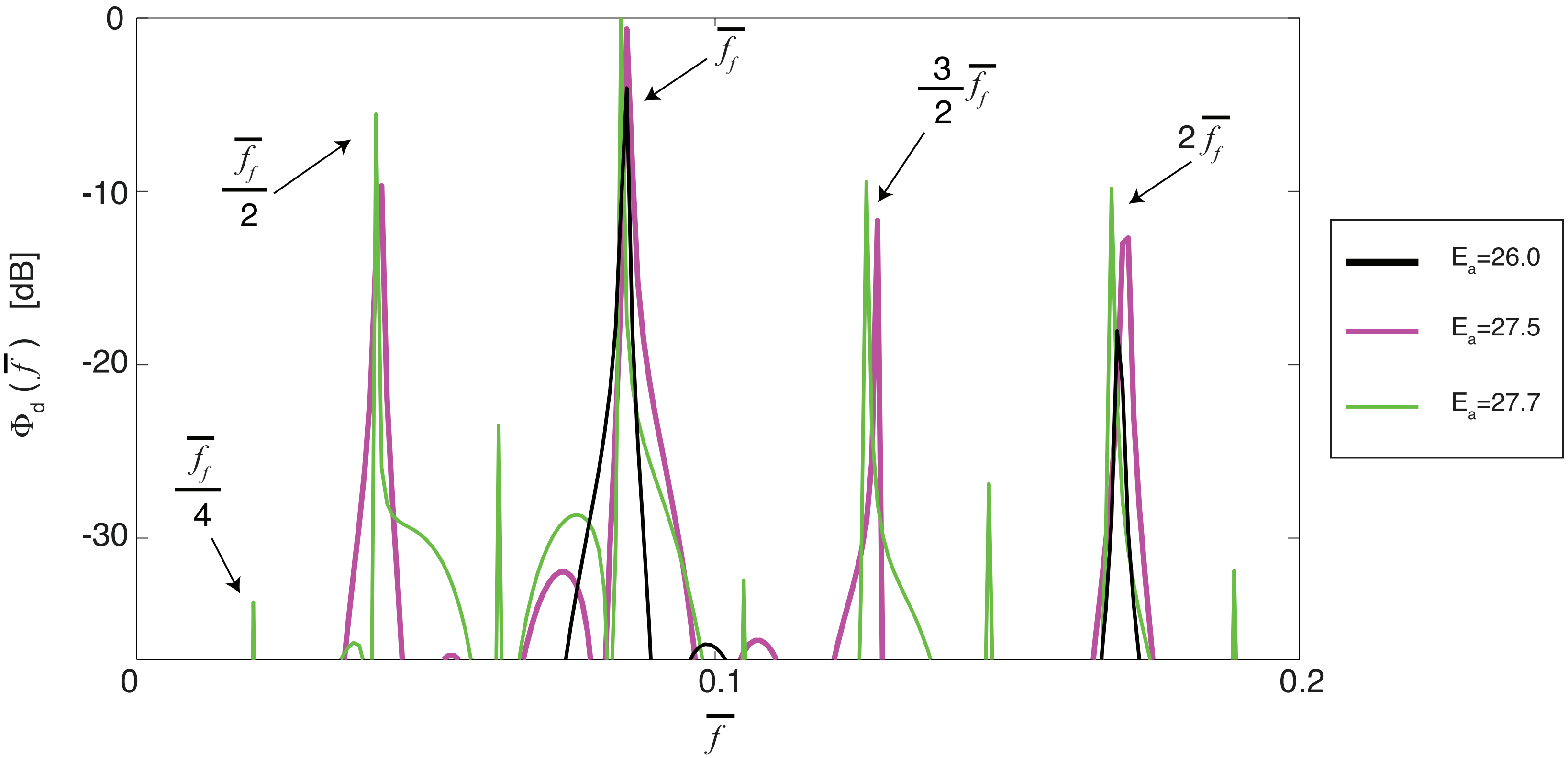
$$\Phi_d(\bar{f}_k) = \frac{2}{N^2}|P_k|^2, \qquad k = 1, 2, \ldots, (N/2 - 1),$$

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

where P_k is the standard discrete Fourier Transform of p,

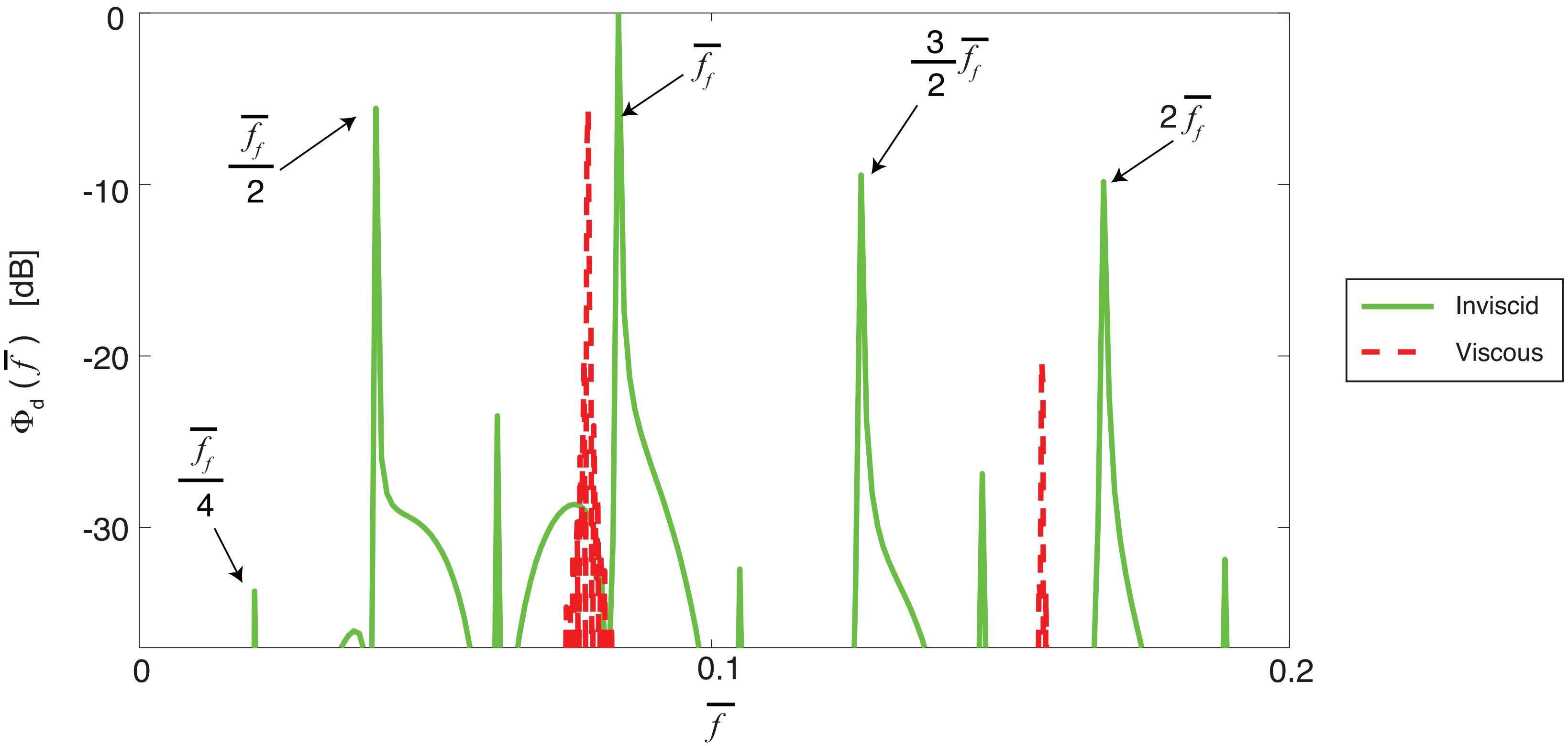
$$P_k = \sum_{n=0}^{N-1} p_n \exp\left(-\frac{2\pi \imath n k}{N}\right), \qquad k = 0, 1, 2, \ldots, N/2.$$

Higher Order Harmonics Predicted as Activation Energy Increases

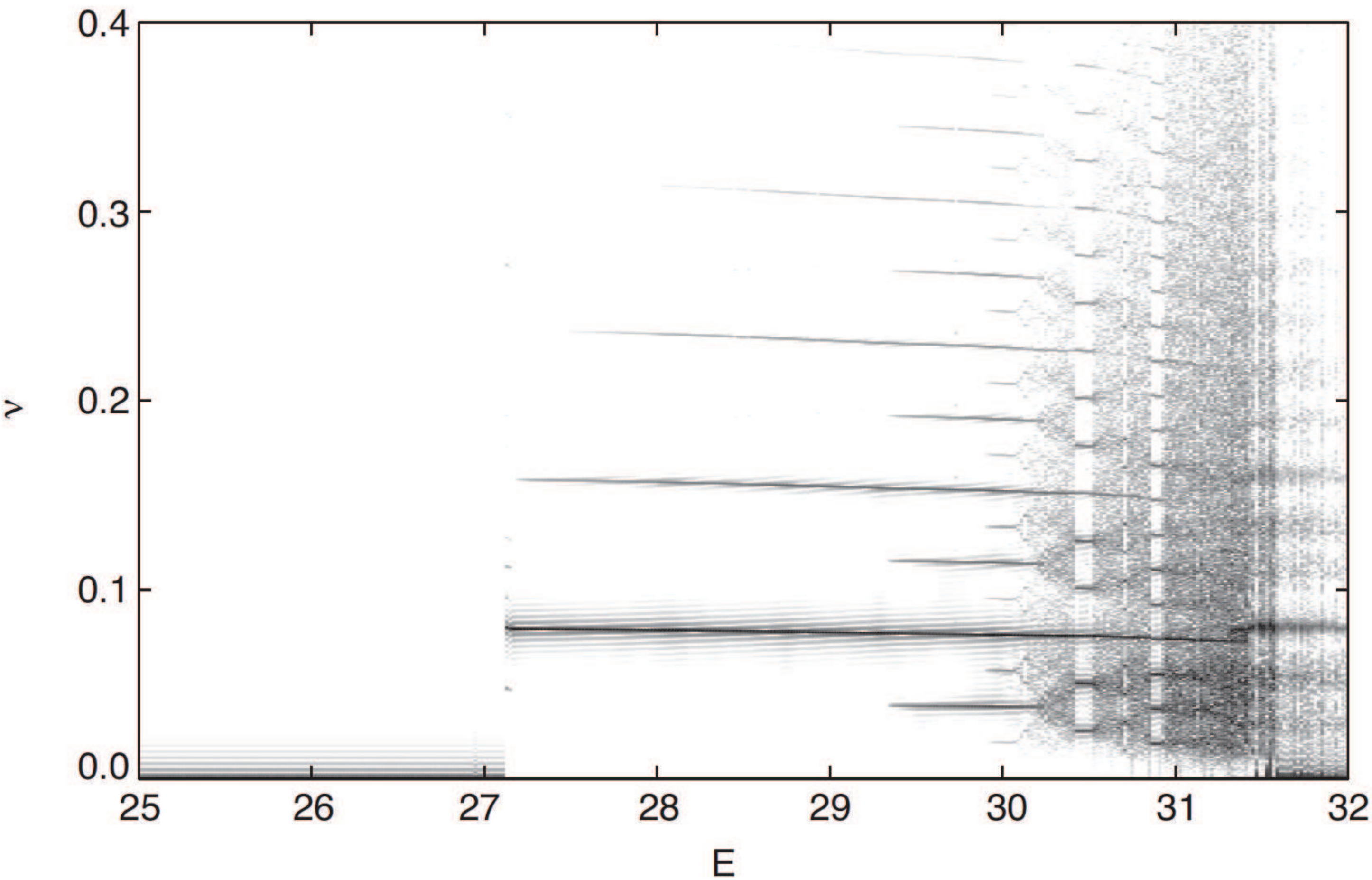


Diffusion Modulates the Amplitude and Shifts the Frequency

$E_a = 27.7$



Bifurcation of Oscillatory Modes: Baroque Harmonies!



Simple One-Step Model: Conclusions

- Dynamics of one-dimensional detonations are influenced by mass, momentum, energy diffusion, especially so in the region of high frequency instability.
- In general, the effect of diffusion is stabilizing.
- Bifurcation and transition to chaos show similarities to the logistic map.
- The structures are deterministic and often harmonious, but with possible baroque complexity.

Detailed Reaction Kinetics Model

Unsteady, Compressible, Reactive Navier-Stokes Equations

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

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

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

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

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

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

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

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

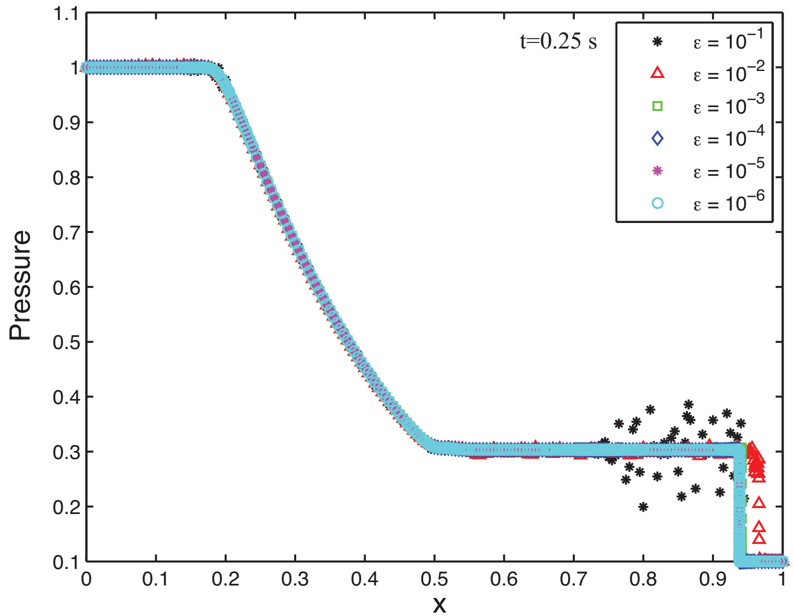
Computational Methods

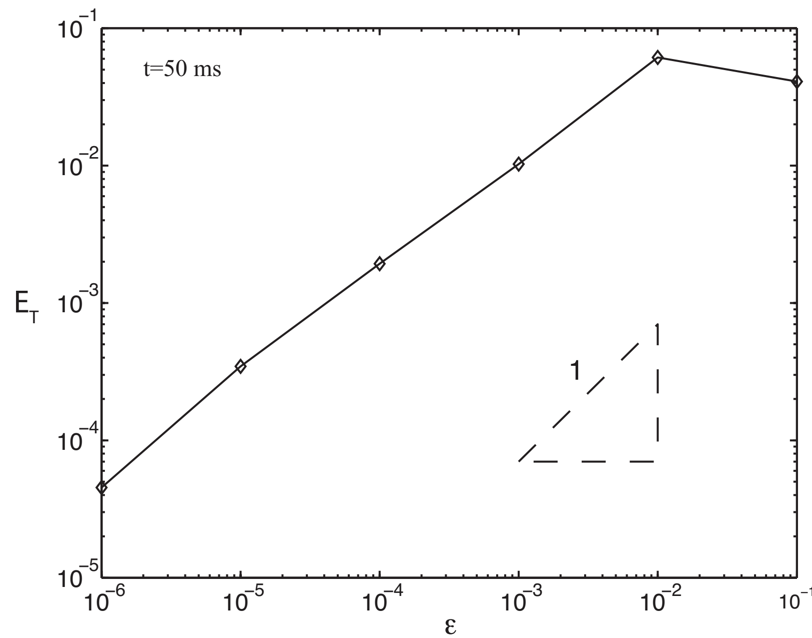
- Inviscid
  - Shock-fitting : Fifth order algorithm adapted from Henrick *et al.*, *JCP.*
  - Shock-capturing : Second order min-mod algorithm
- Viscous
  - Wavelet method (WAMR), developed by Vasilyev and Paolucci, *JCP*
  - User-defined threshold parameter ϵ controls error: *automatic verification!*

$$\begin{aligned} u^J(\mathbf{x}) &= \underbrace{\sum_{\mathbf{k}} u_{0,\mathbf{k}} \Phi_{0,\mathbf{k}}(\mathbf{x}) + \sum_{j=0}^{J-1} \sum_{\{\lambda : |d_{j,\lambda}| \geq \epsilon\}} d_{j,\lambda} \Psi_j(\mathbf{x})}_{u_\epsilon^J} \\ &+ \underbrace{\sum_{j=0}^{J-1} \sum_{\{\lambda : |d_{j,\lambda}| < \epsilon\}} d_{j,\lambda} \Psi_j(\mathbf{x})}_{R_\epsilon^J} \end{aligned}$$

- All methods used a fifth order explicit Runge-Kutta scheme for time integration

Automatic Verification with WAMR

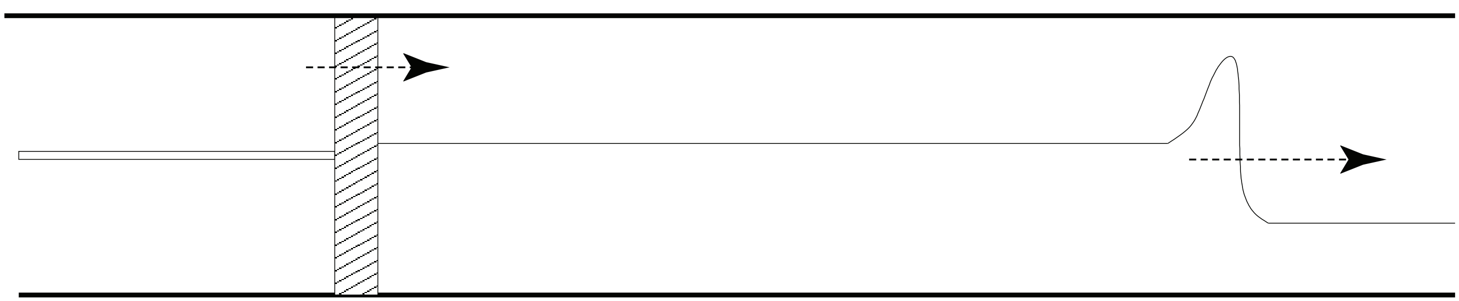




- Sod shock tube result from Brill, Grenga, Powers, and Paolucci, 11th World Congress on Computational Mechanics, 2014.
- The error is controlled by WAMR.

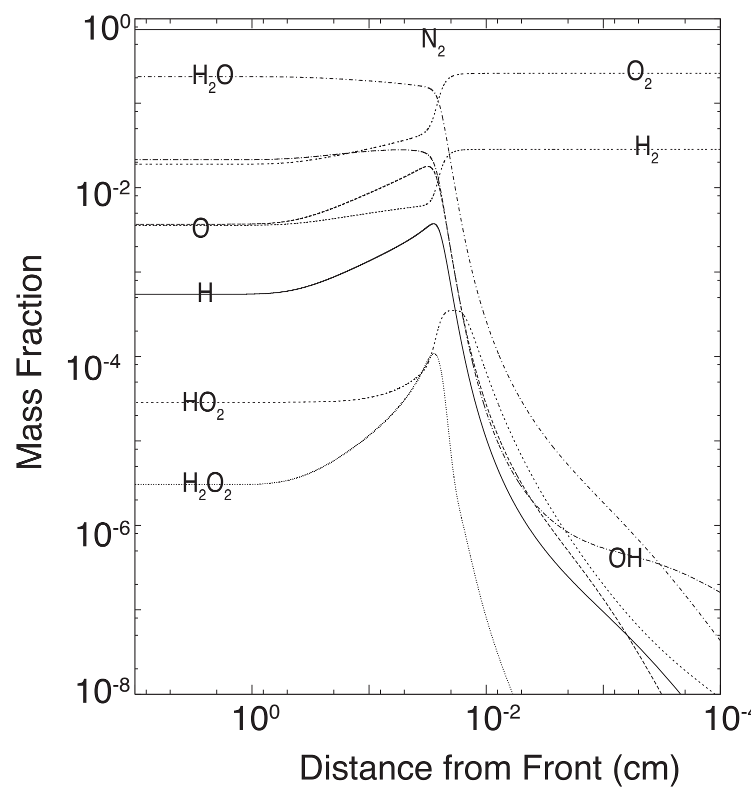
Cases Examined

- 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 $1.018 < f < 1.150$ were examined



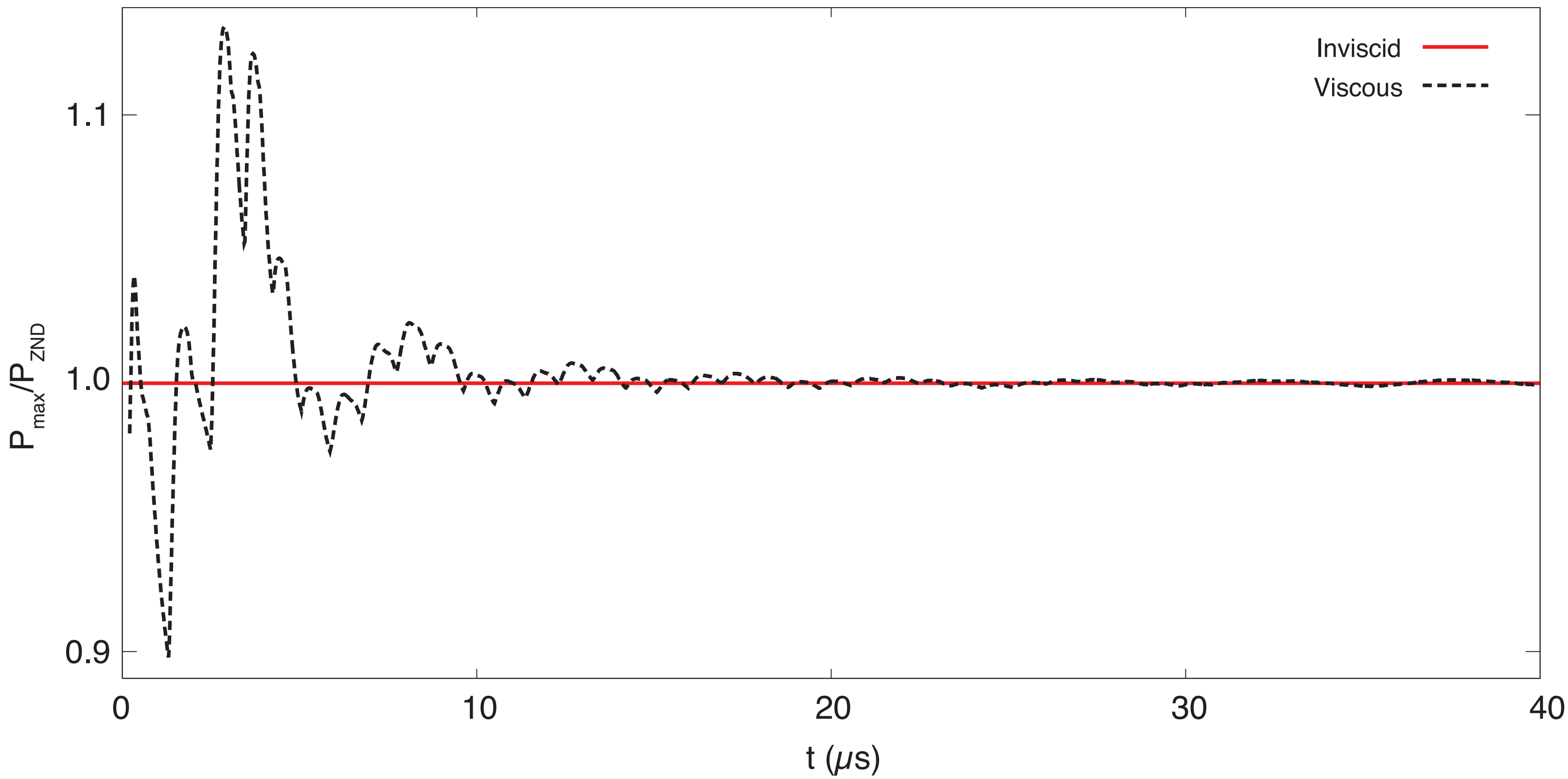
Typical Stable Steady Wave Profile

$f = 1.15$



Stable Detonation at High Overdrive

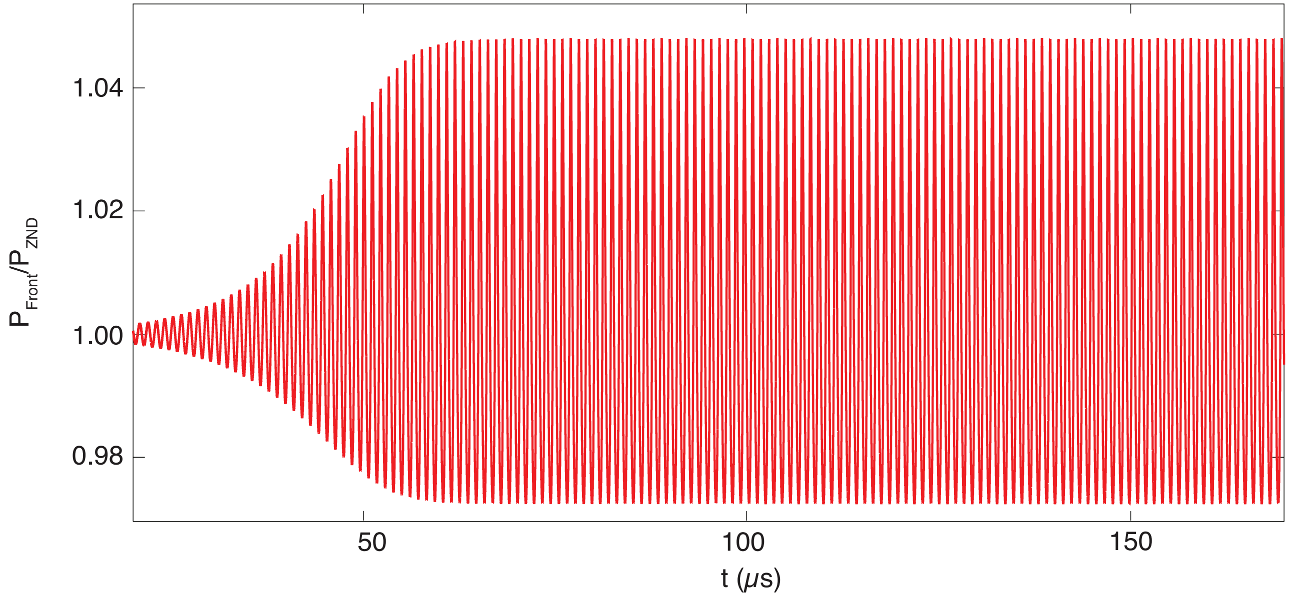
$f = 1.15$



For high enough overdrives, the detonation relaxes to a steady propagating wave in the inviscid case as well as in the diffusive case.

Lower Overdrive: High Frequency Instability, No Diffusion

$f = 1.10$

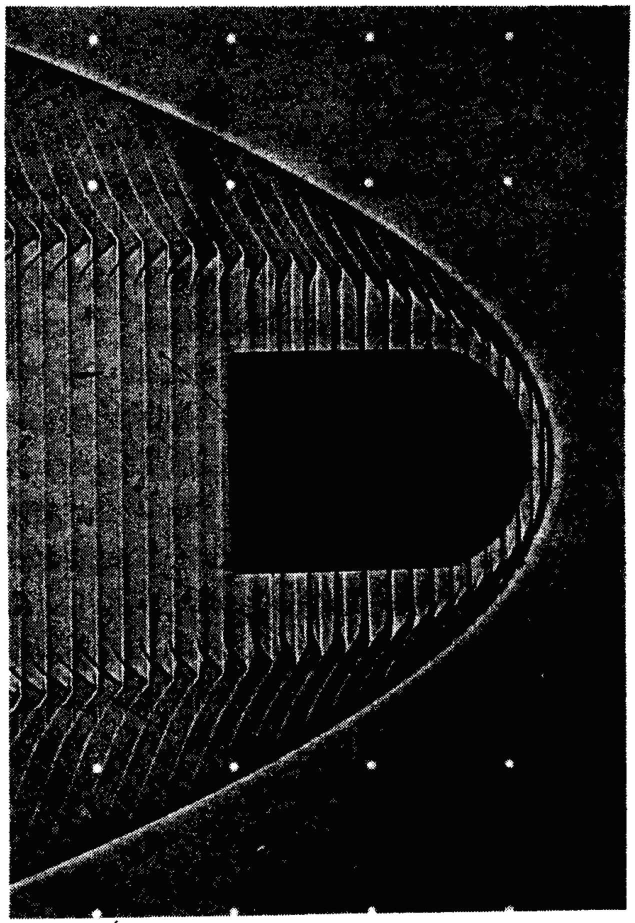


A single fundamental frequency oscillation occurs at a frequency of $0.97\ MHz$.

This frequency agrees with the experimental observations of Lehr (*Astro. Acta*, 1972).

Organ pipe oscillation between shock and end of reaction zone: $\nu \simeq a/\ell$ = (1000 m/s)/(0.0001 m)$\simeq$ 10 MHz.

Validation with Lehr's High Frequency Instability

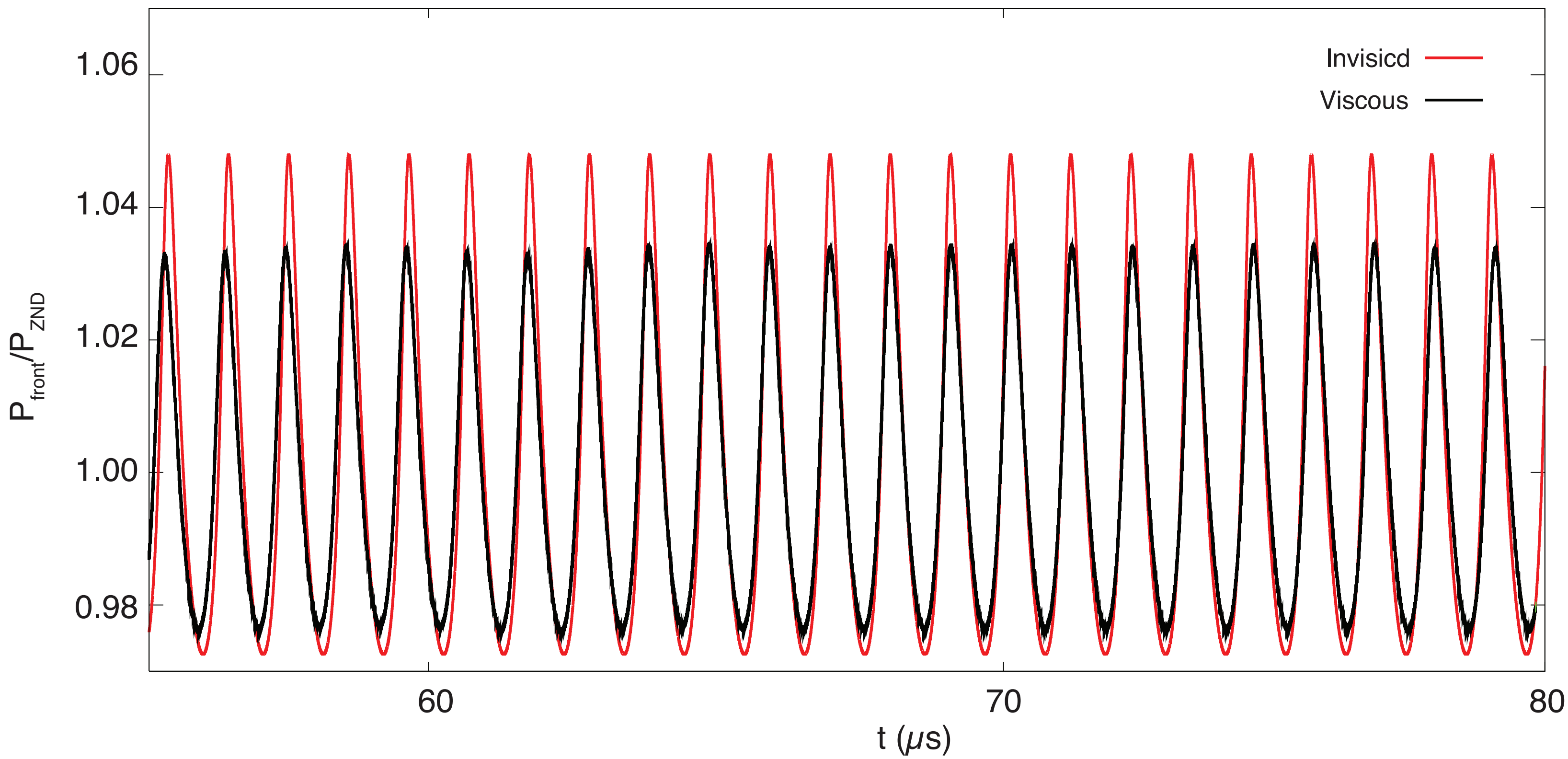


(*Astro. Acta*, 1972)

- Shock-induced combustion experiment (*Astro. Acta*, 1972)
- Stoichiometric mixture of $2\text{H}_2 + \text{O}_2 + 3.76\text{N}_2$ at 0.421 atm
- Observed 1.04 MHz frequency for projectile velocity corresponding to $f \approx 1.10$
- For $f = 1.10$, the predicted frequency of 0.97 MHz agrees with observed frequency and the prediction by Yungster and Radhakrishan of 1.06 MHz

High Frequency Mode - Viscous vs. Inviscid

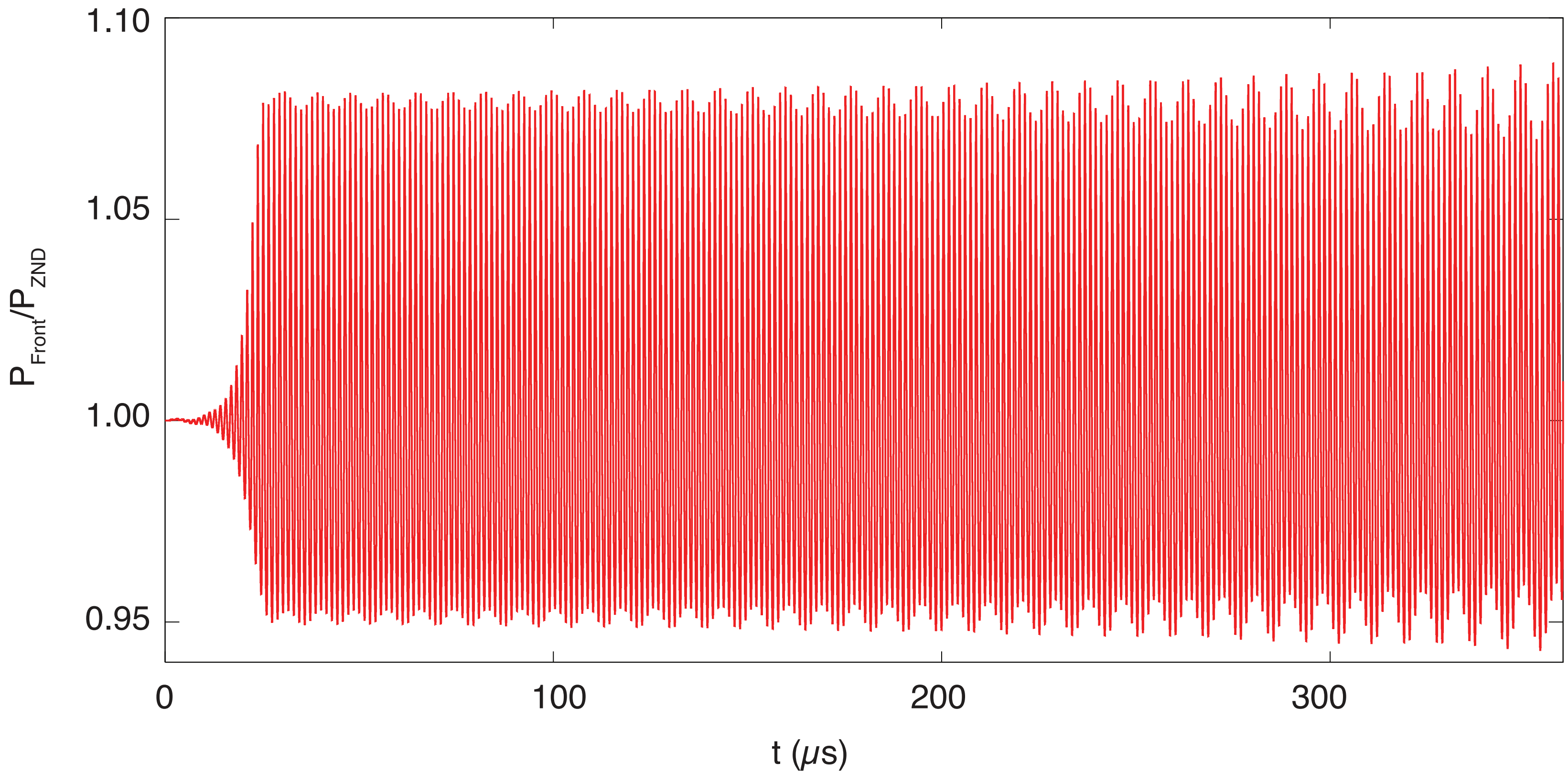
$f = 1.10$



The addition of viscosity has a stabilizing effect, decreasing the amplitude of the oscillations. The pulsation frequency relaxes to 0.97 MHz.

Low Frequency Mode Appearance - Inviscid

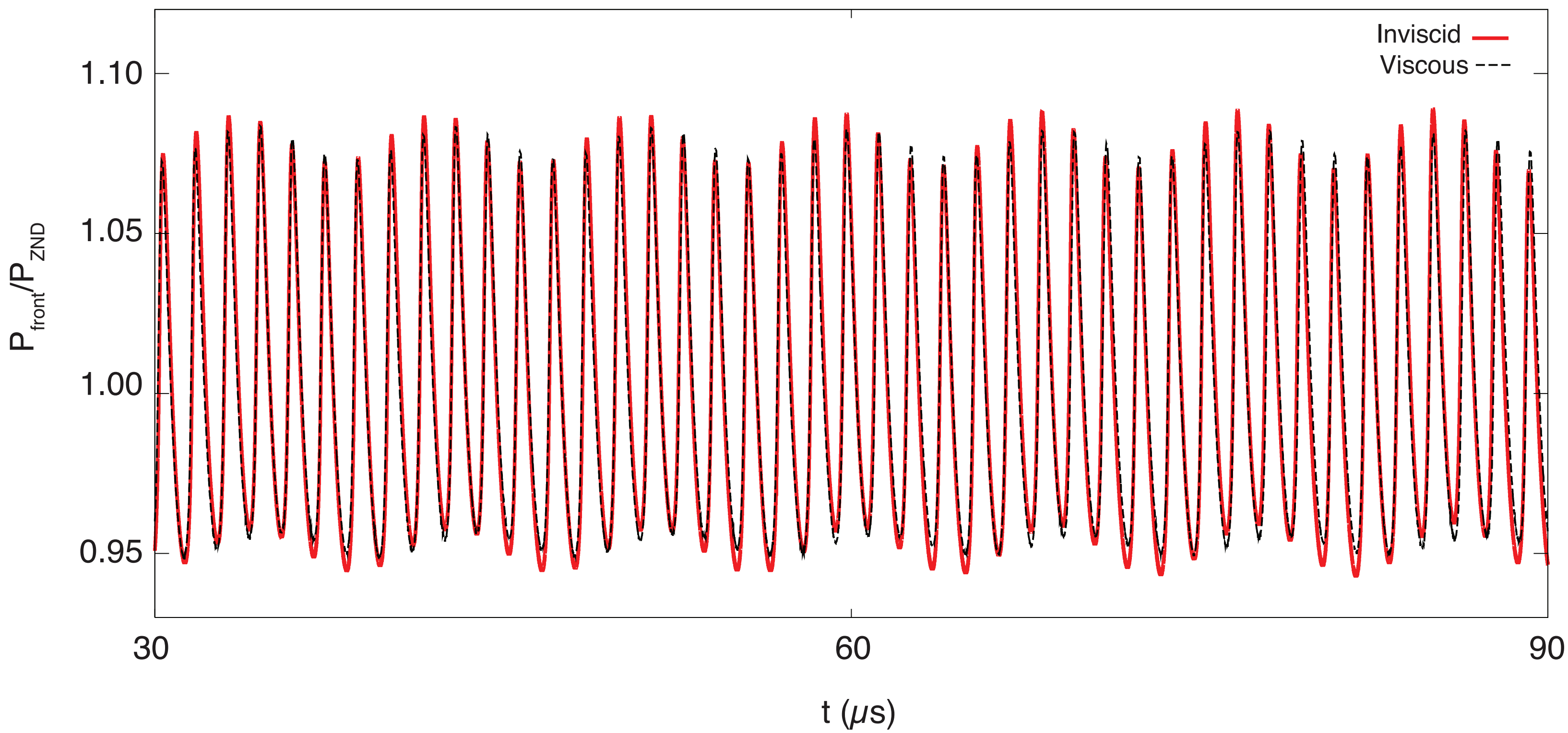
$f = 1.035$



As the overdrive is lowered, multiple frequencies appear, and the amplitude of the oscillations continues to grow. These multiple frequencies persist at long time.

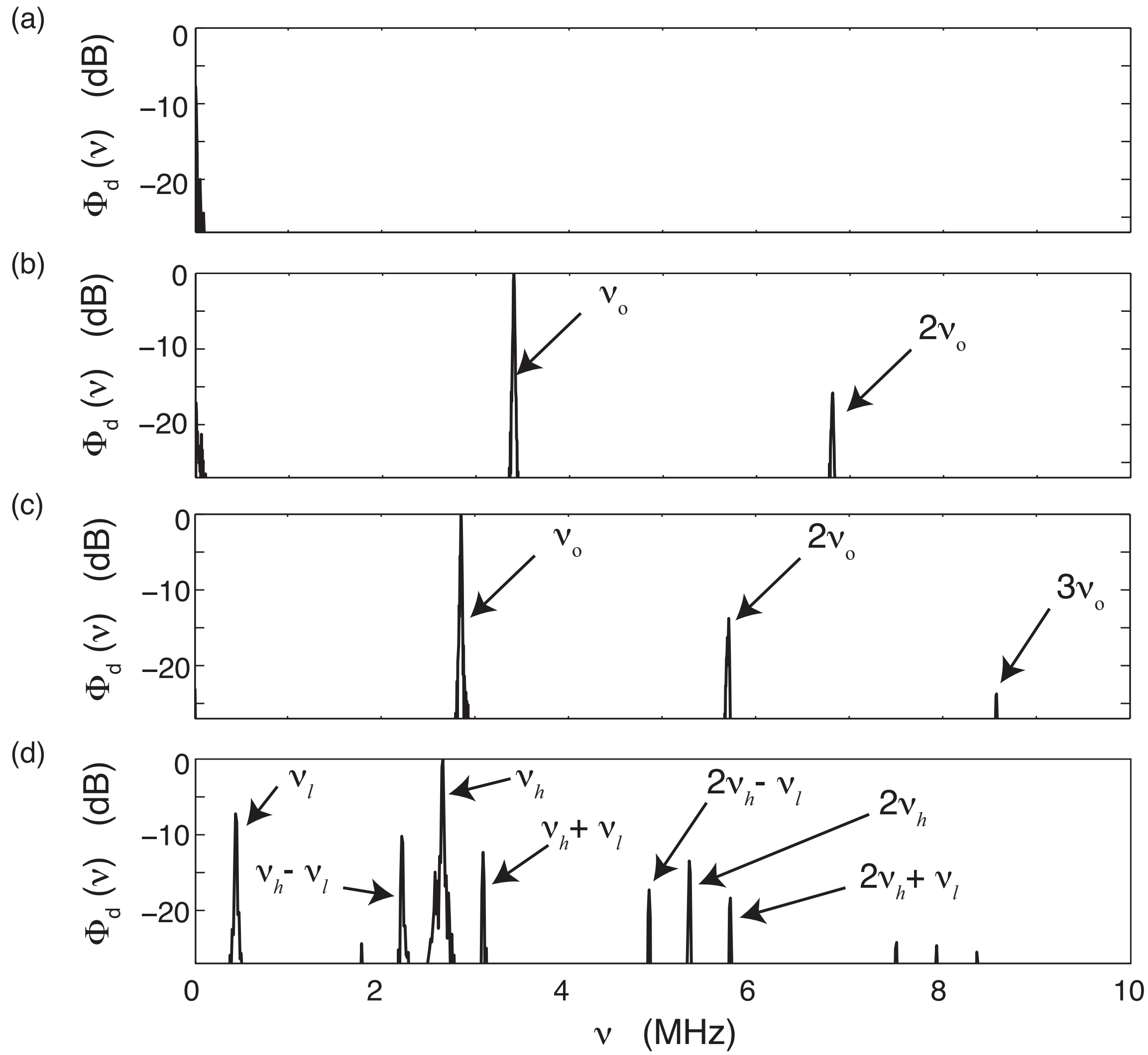
Low Frequency Mode Appearance - Viscous vs. Inviscid

$f = 1.035$

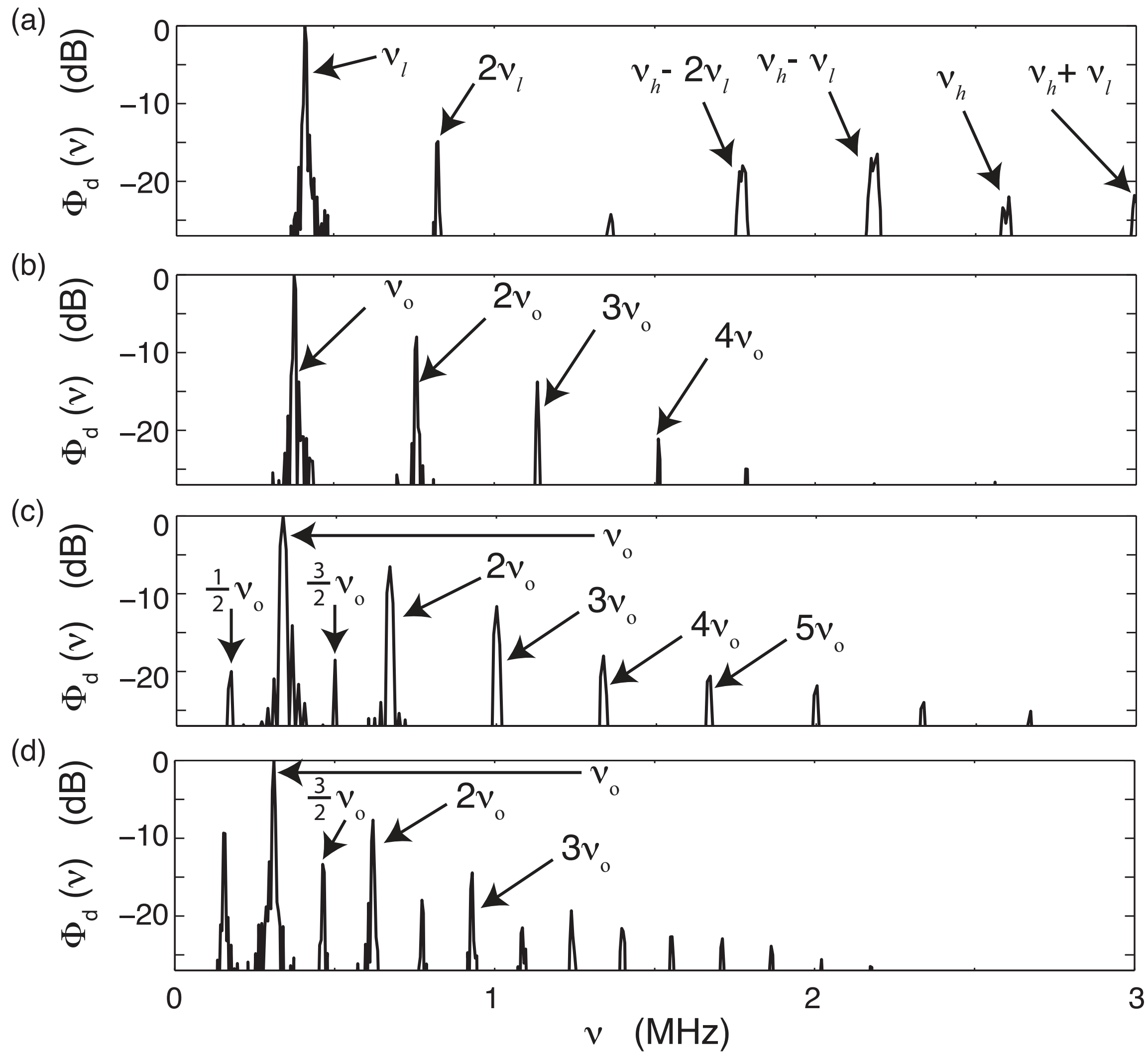


Viscosity still decreases the amplitude of oscillation, though the effect is reduced compared to higher overdrives.

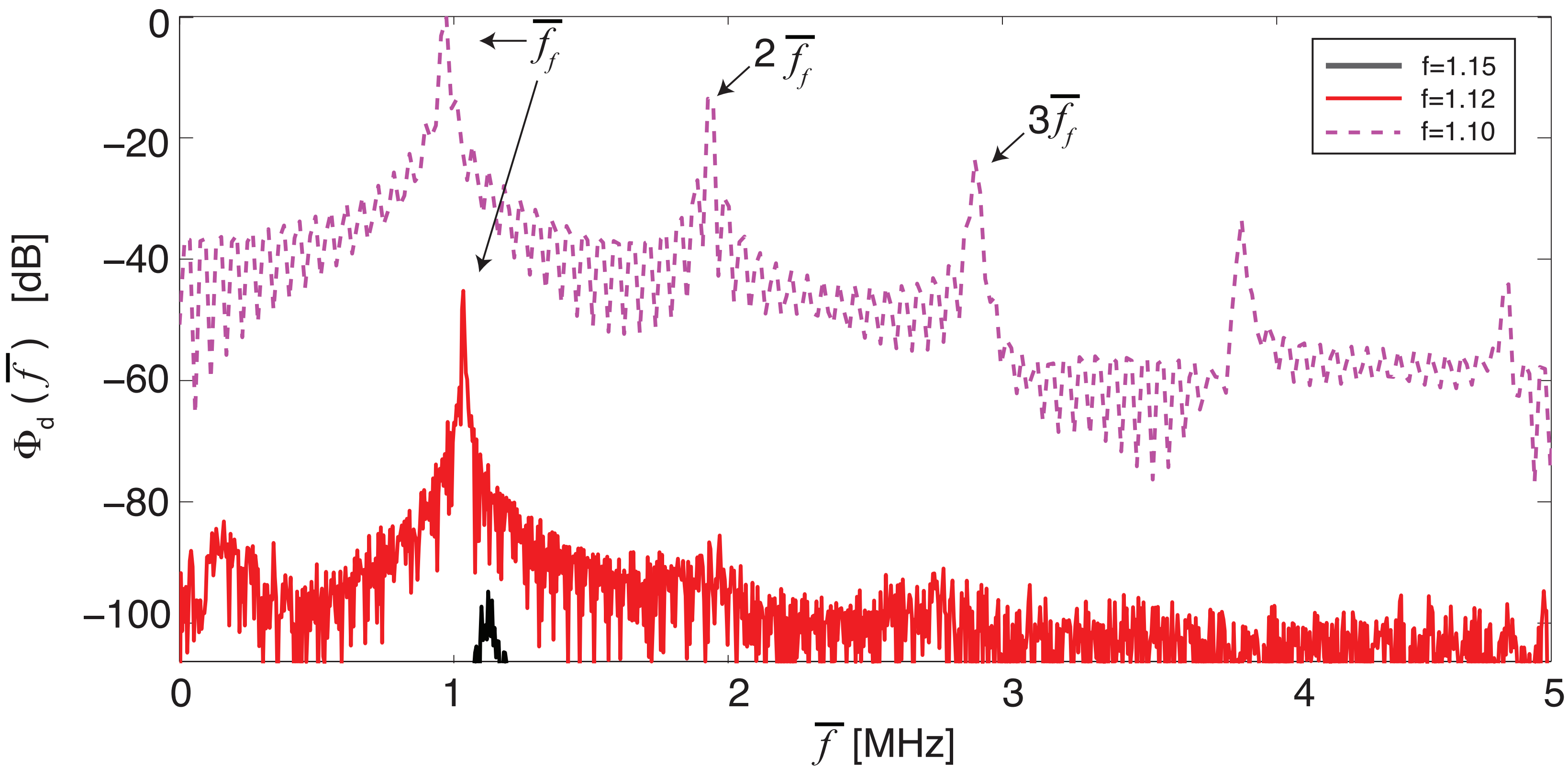
Viscous H_2-Air Harmonics: Effect of Overdrive



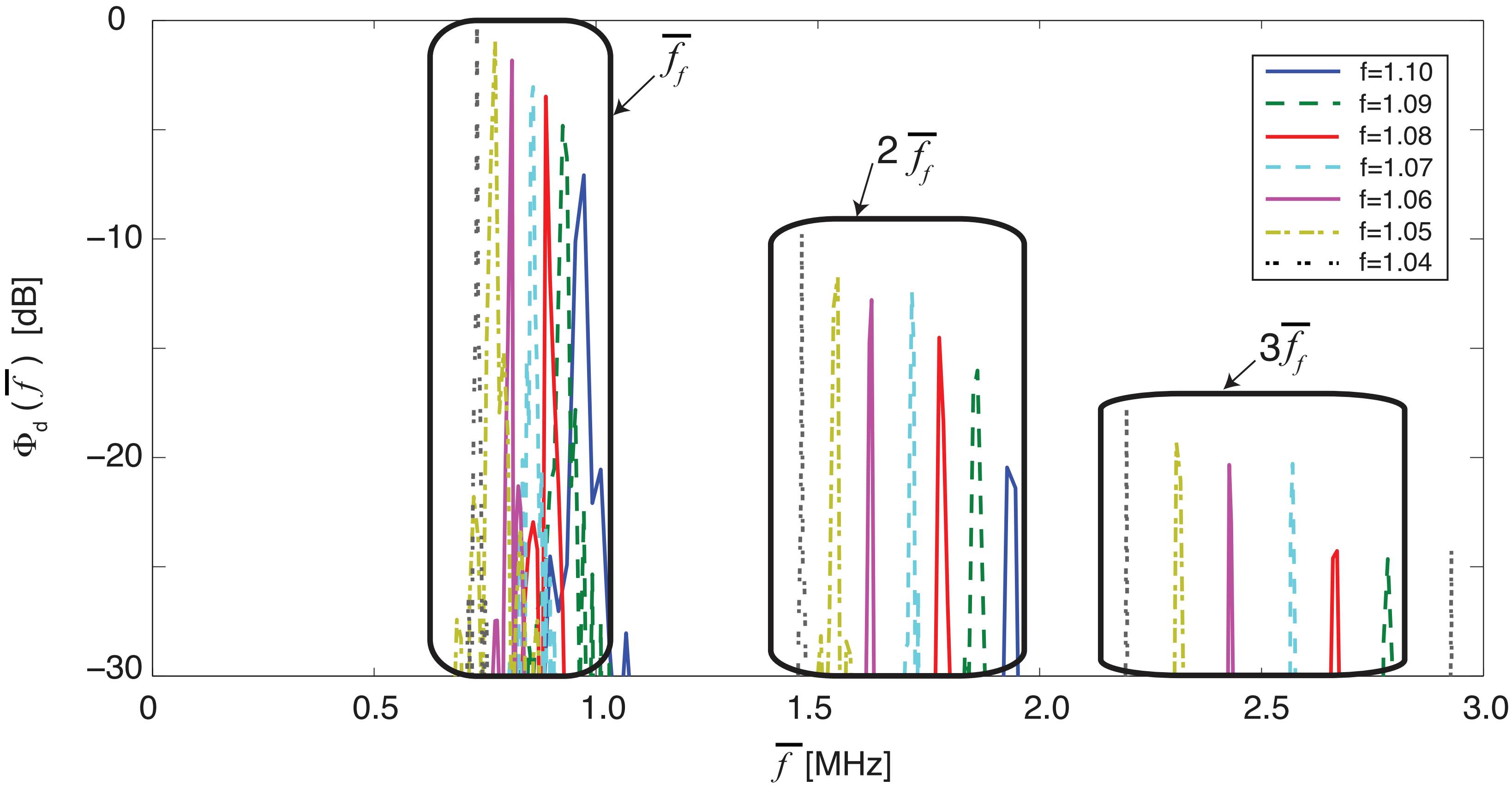
Viscous H_2-Air Harmonics: Effect of Overdrive



H_2-Air: Near Neutral Stability



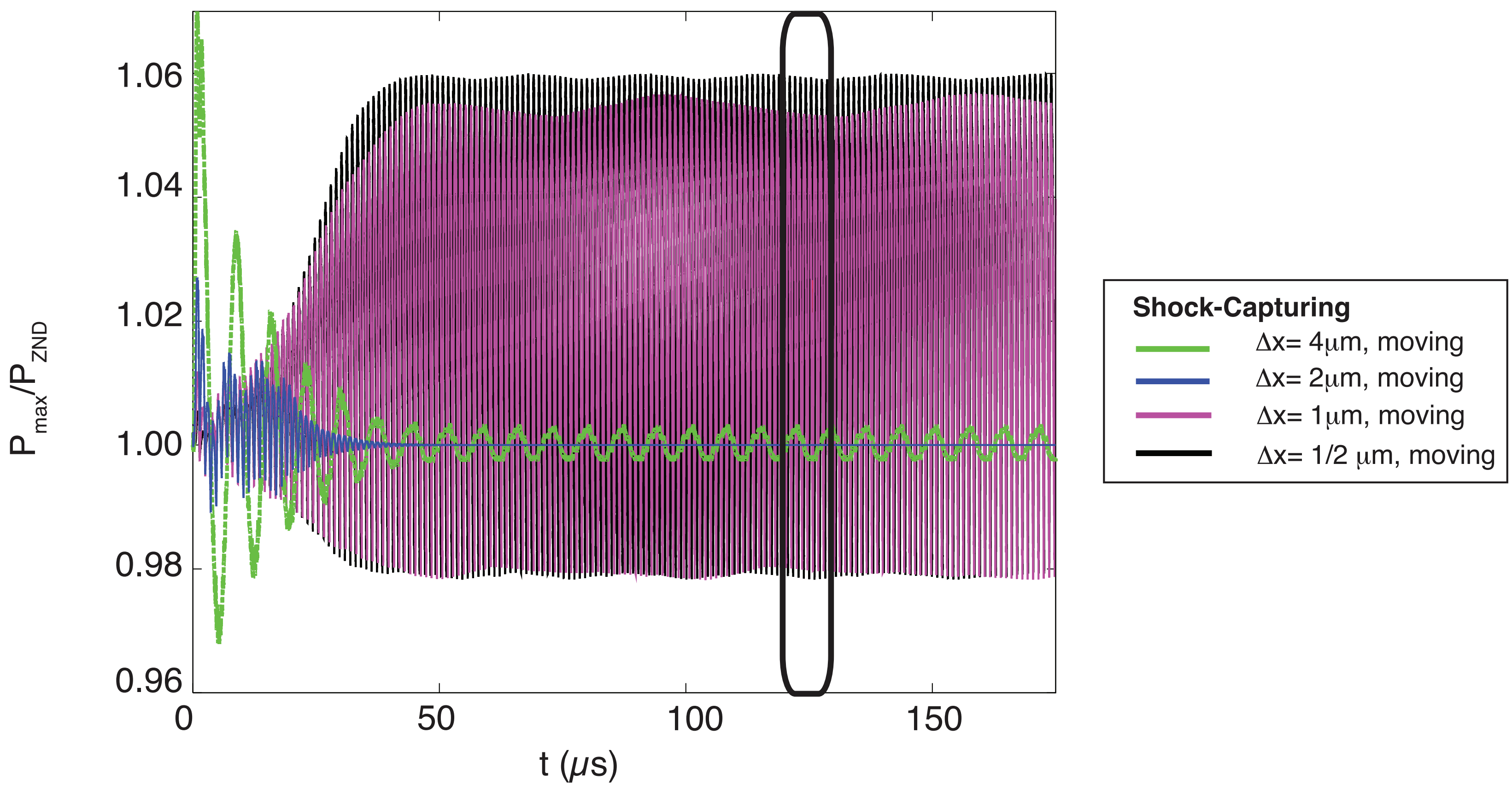
H_2-Air: High Frequency Shift



The amplitude of the oscillations continues grow as the overdrive is lowered. There appears to be a near power-law decay in the amount of energy carried by the higher harmonics.

Fine Grids Required for Accurate Shock-Capturing

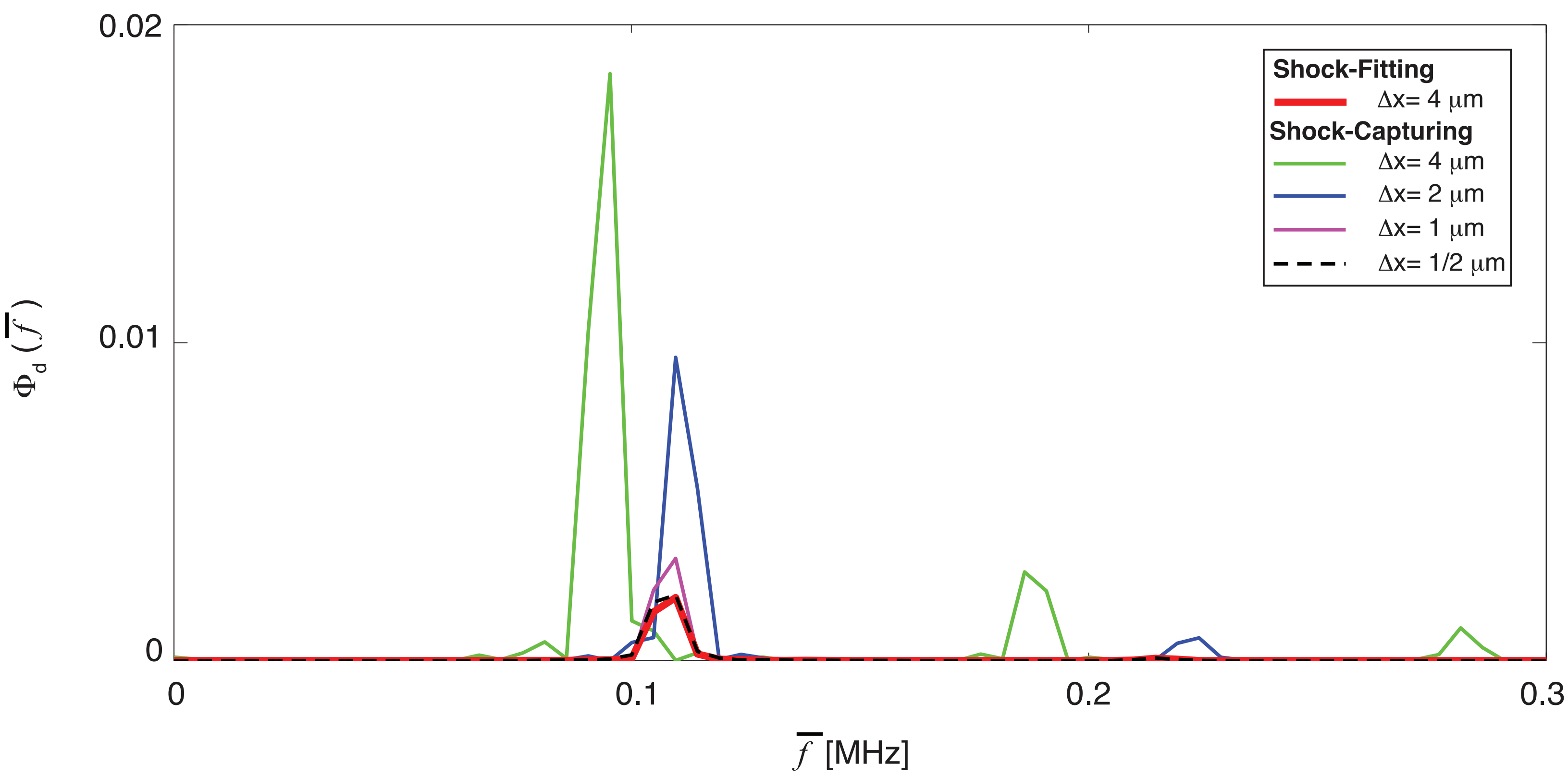
$f = 1.10$



Using the same grid size as shock-fitting $(\Delta x = 4\ \mu\text{m})$, shock-capturing misses the essential dynamics.

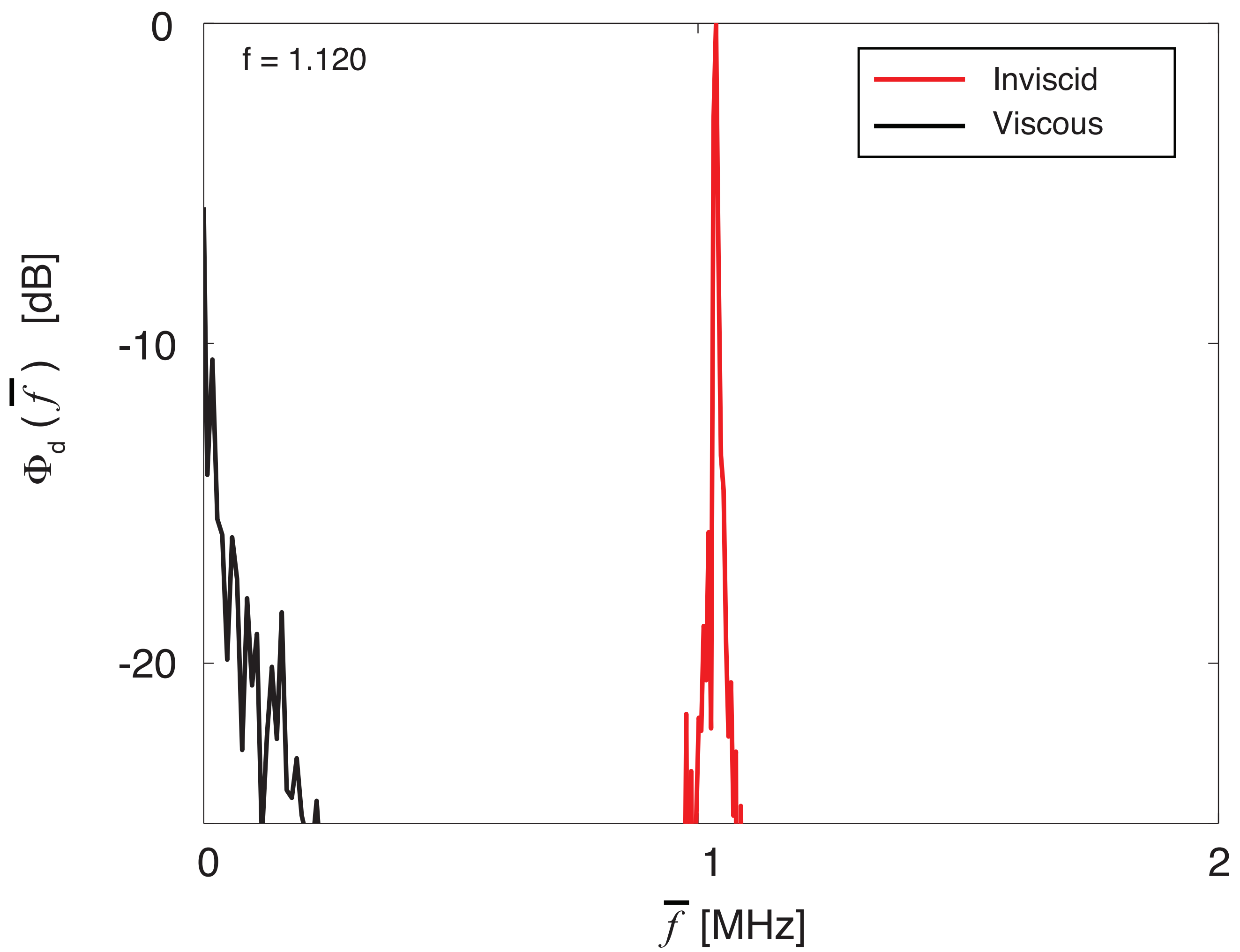
Fine Grids Required for Accurate Shock-Capturing

$f = 1.023$

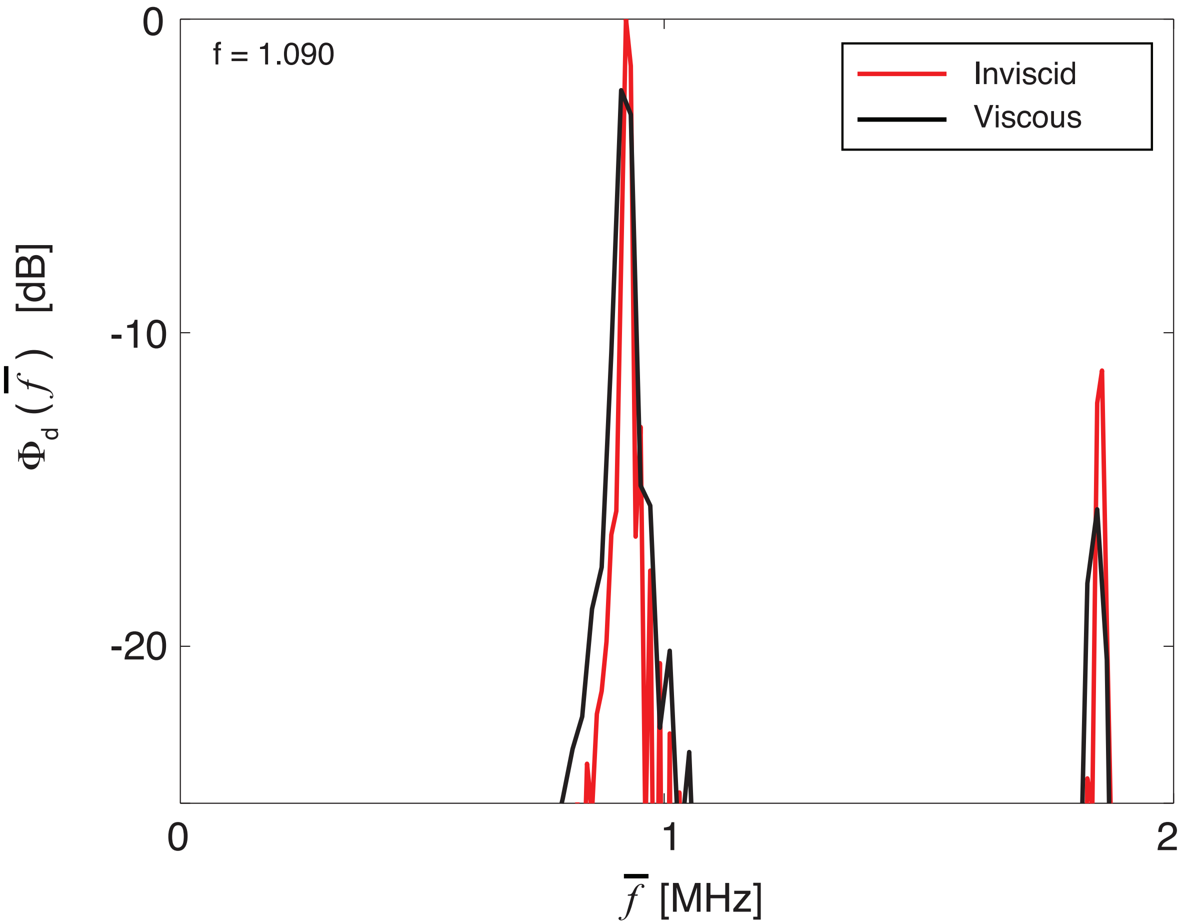


Only when $\Delta x = 1/2\ \mu$m is used does the PSD of shock-capturing become nearly indistinguishable with that of shock-fitting.

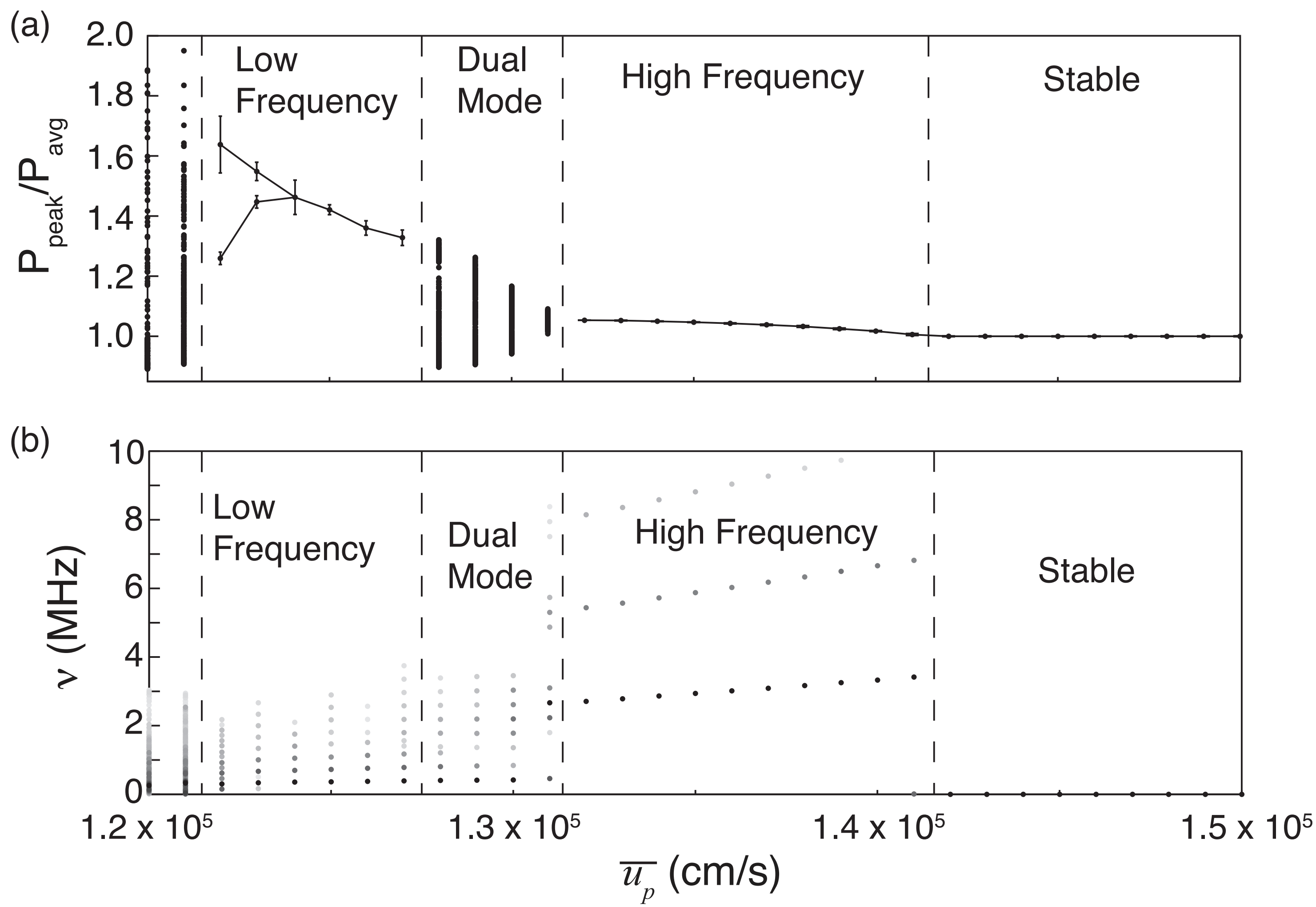
Near the Neutral Stability Boundary, Diffusion Damps the Small Oscillations



Diffusion Reduces the Magnitude of the First and Second Harmonics



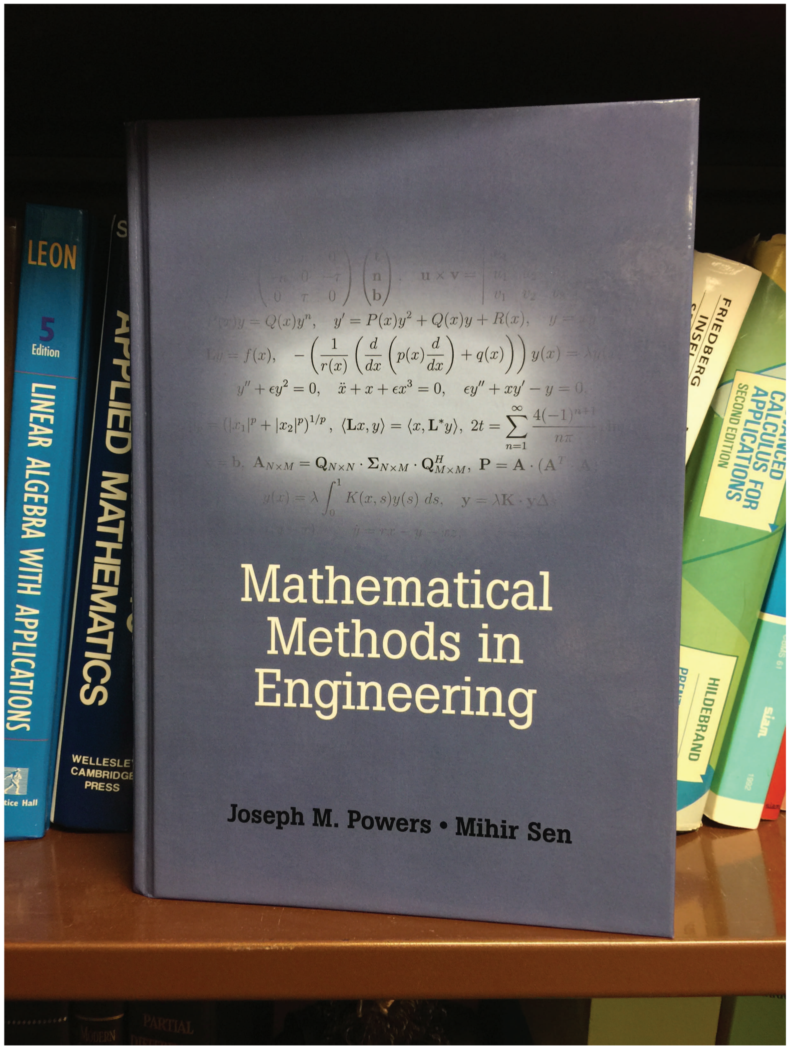
Bifurcation Diagram for Hydrogen-Air Detonation



Conclusions

- Predictions of complex hydrogen-air detonations can be verified and validated.
- WAMR gives automatic verification; other methods have been verified by selection of sufficiently fine grids.
- Long time behavior of a hydrogen-air detonation becomes more complex as the overdrive is decreased.
- Advection and reaction effects *usually* dominate those of diffusion.
- Physical diffusion causes an amplitude reduction and phase shift; it is more important near bifurcation points.
- Filtering (shock-capturing, numerical viscosity, WENO, and by inference LES, implicit time-stepping, kinetic reduction, etc.) alters detonation dynamics.
- Like Bach's baroque harmonies, those of real detonations are complex; a Mozartian classicism is still needed to strip away the intricate excess and capture, in a validated way, the essential character of detonation.

A New Book



- Powers & Sen, *Mathematical Methods in Engineering*, Cambridge U. Press, 2015.
- Foundation of AME 60611, taught for over twenty-five years.