On the Resolution Necessary to Capture Dynamics of Unsteady 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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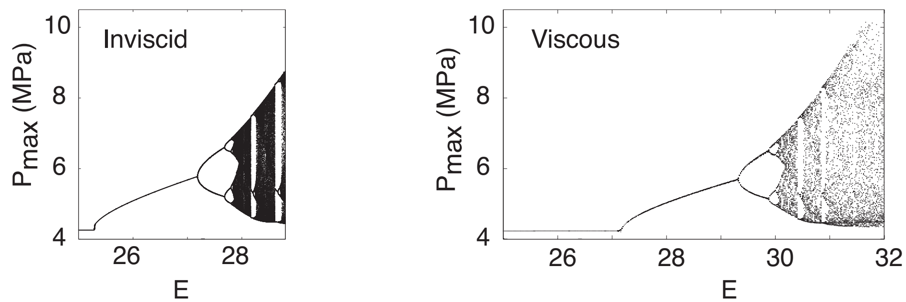
Motivation

- 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.



- Mazaheri *et al.* (*Comb. and Flame*, 2012) also found diffusion plays a critical role in regions of high resolution using one-step kinetics in their two-dimensional studies.
- Here, we will consider detonation dynamics with inviscid, shock-fitting and shock-capturing, and Navier-Stokes models for H_2-air detonations.
- New harmonic analysis presented here reveals the multi-modal nature of oscillatory detonations in H_2-air.

Unsteady, Compressible, Reactive Navier-Stokes Equations

$$
\begin{aligned}
&\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \\
&\frac{\partial}{\partial t} (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u}\mathbf{u} + p\mathbf{I} - \boldsymbol{\tau}) = \mathbf{0}, \\
&\frac{\partial}{\partial t} \left(\rho \left(e + \frac{\mathbf{u}\cdot\mathbf{u}}{2}\right)\right) + \nabla \cdot \left(\rho \mathbf{u} \left(e + \frac{\mathbf{u}\cdot\mathbf{u}}{2}\right) + (p\mathbf{I} - \boldsymbol{\tau}) \cdot \mathbf{u} + \mathbf{q}\right) = 0, \\
&\frac{\partial}{\partial t} (\rho Y_i) + \nabla \cdot (\rho \mathbf{u} Y_i + \mathbf{j}_i) = \overline{M_i}\, \dot{\omega}_i ,
\end{aligned}
$$

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

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

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

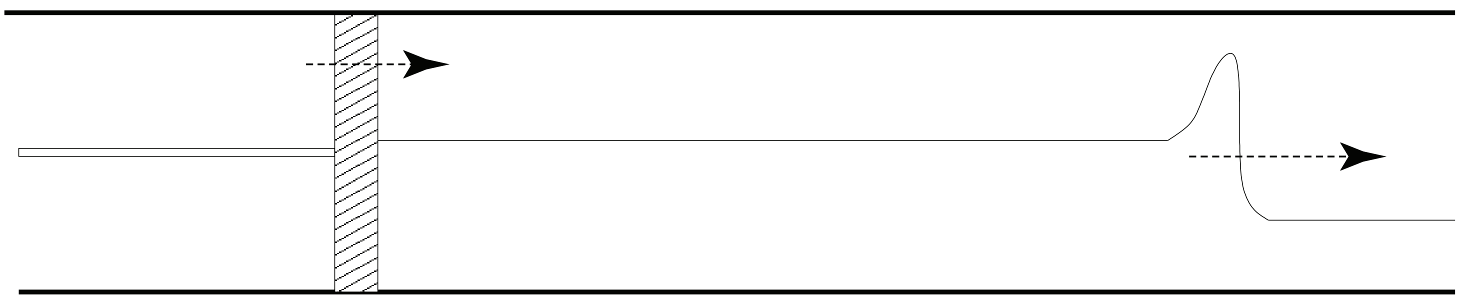
$$
\mathbf{q} = -k \nabla T + \sum_{i=1}^{N} \mathbf{j}_i h_i - \mathcal{R} T \sum_{i=1}^{N} \frac{D_i^T}{\overline{M_i}} \left(\frac{\nabla \overline{y}_i}{\overline{y}_i} + \left(1 - \frac{\overline{M_i}}{\overline{M}}\right) \frac{\nabla p}{p} \right).
$$

Computational Methods

- Inviscid
  - Shock-fitting : Fifth order algorithm adapted from Henrick *et al.* (*J. Comp. Phys.*, 2006)
  - Shock-capturing : Second order min-mod algorithm
- Viscous
  - Wavelet method (WAMR), developed by Vasilyev and Paolucci (*J. Comp. Phys.*, 1996 & 1997)
  - User-defined threshold parameter controls error
- All methods used a fifth order Runge-Kutta scheme for time integration

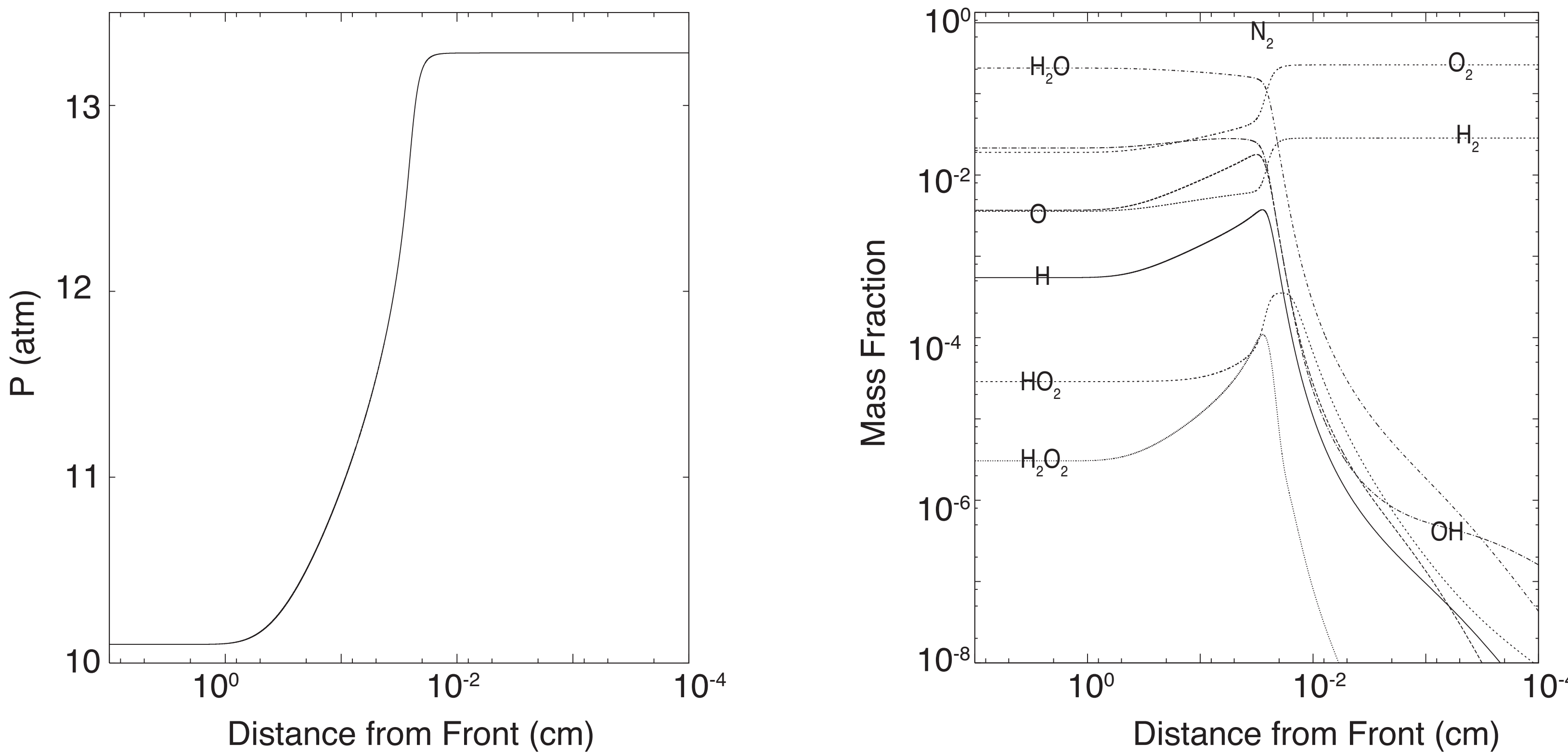
Case Examined

- 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 $1.018 < f < 1.150$ were examined



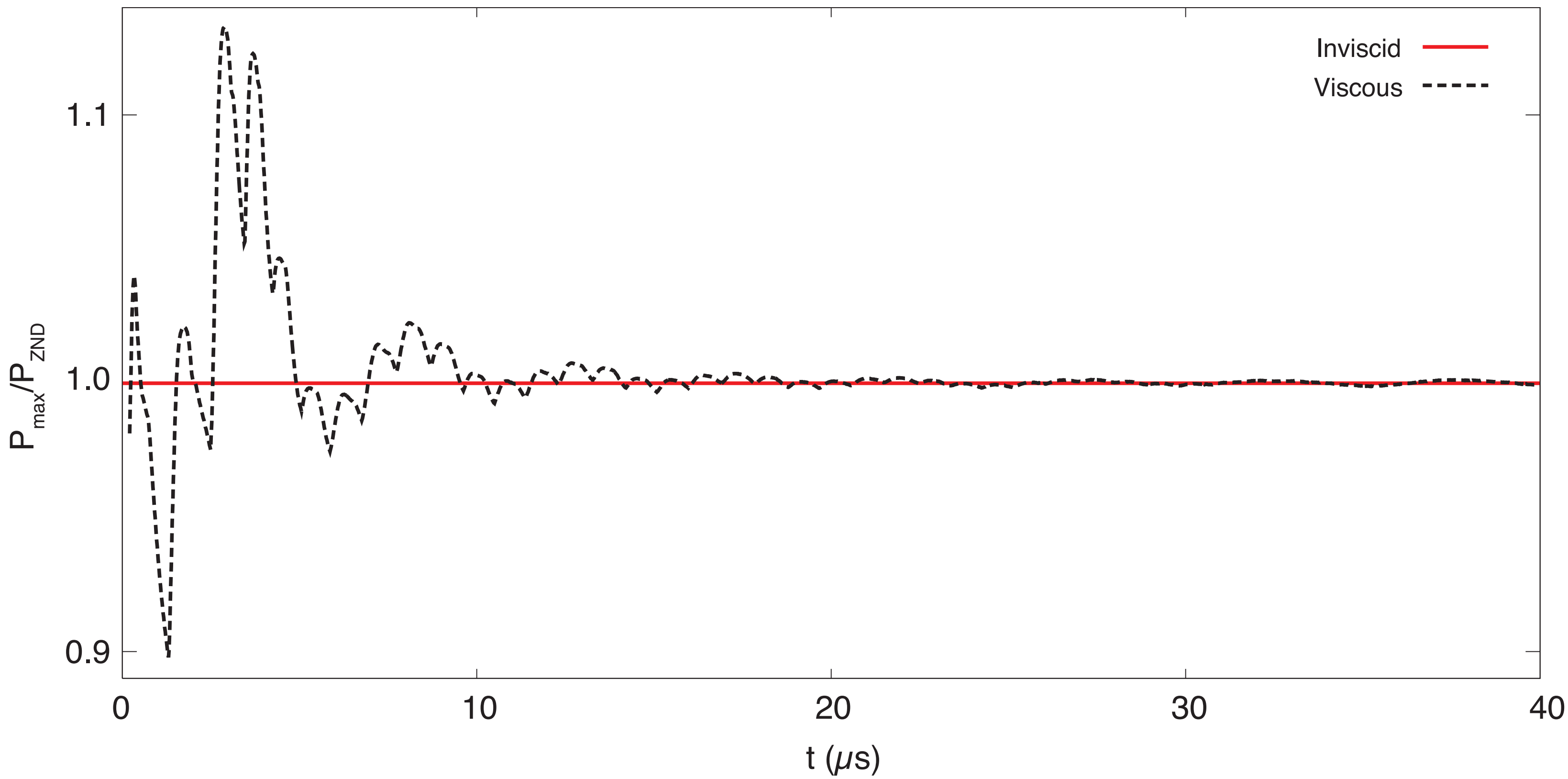
Typical ZND Profile

$f = 1.15$



Stable Detonation

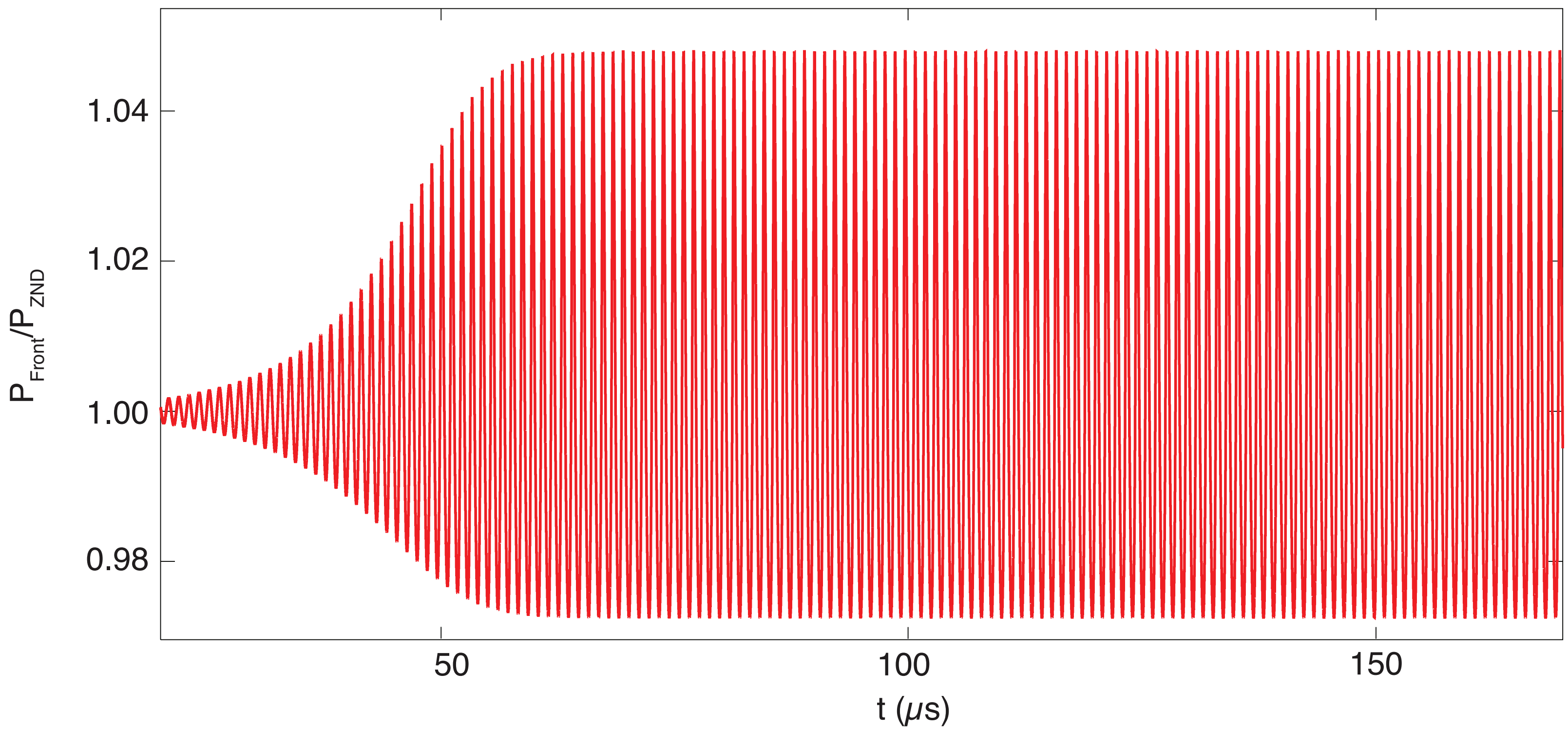
$f = 1.15$



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

High Frequency Mode - Inviscid

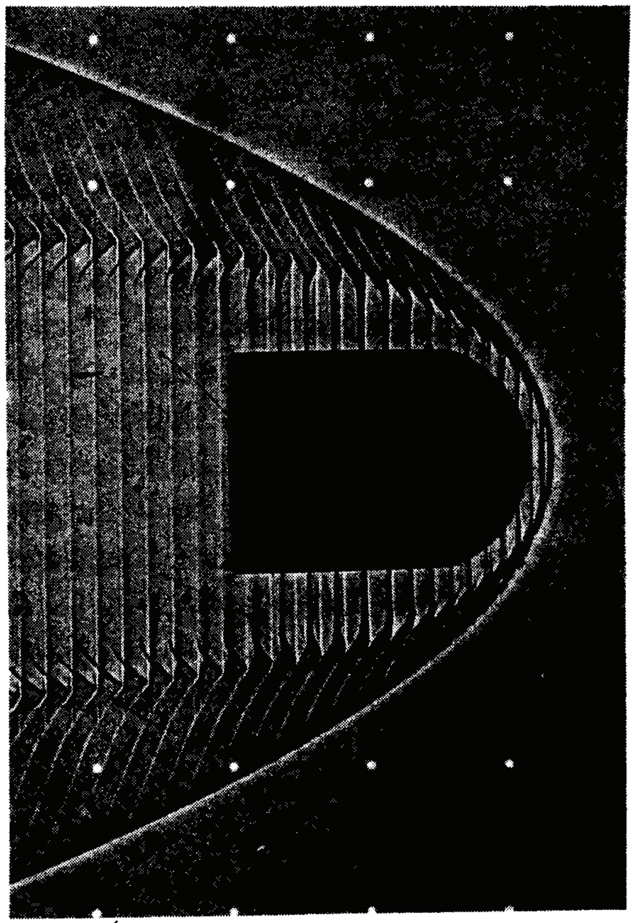
$f = 1.10$



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).

Lehr's High Frequency Instability

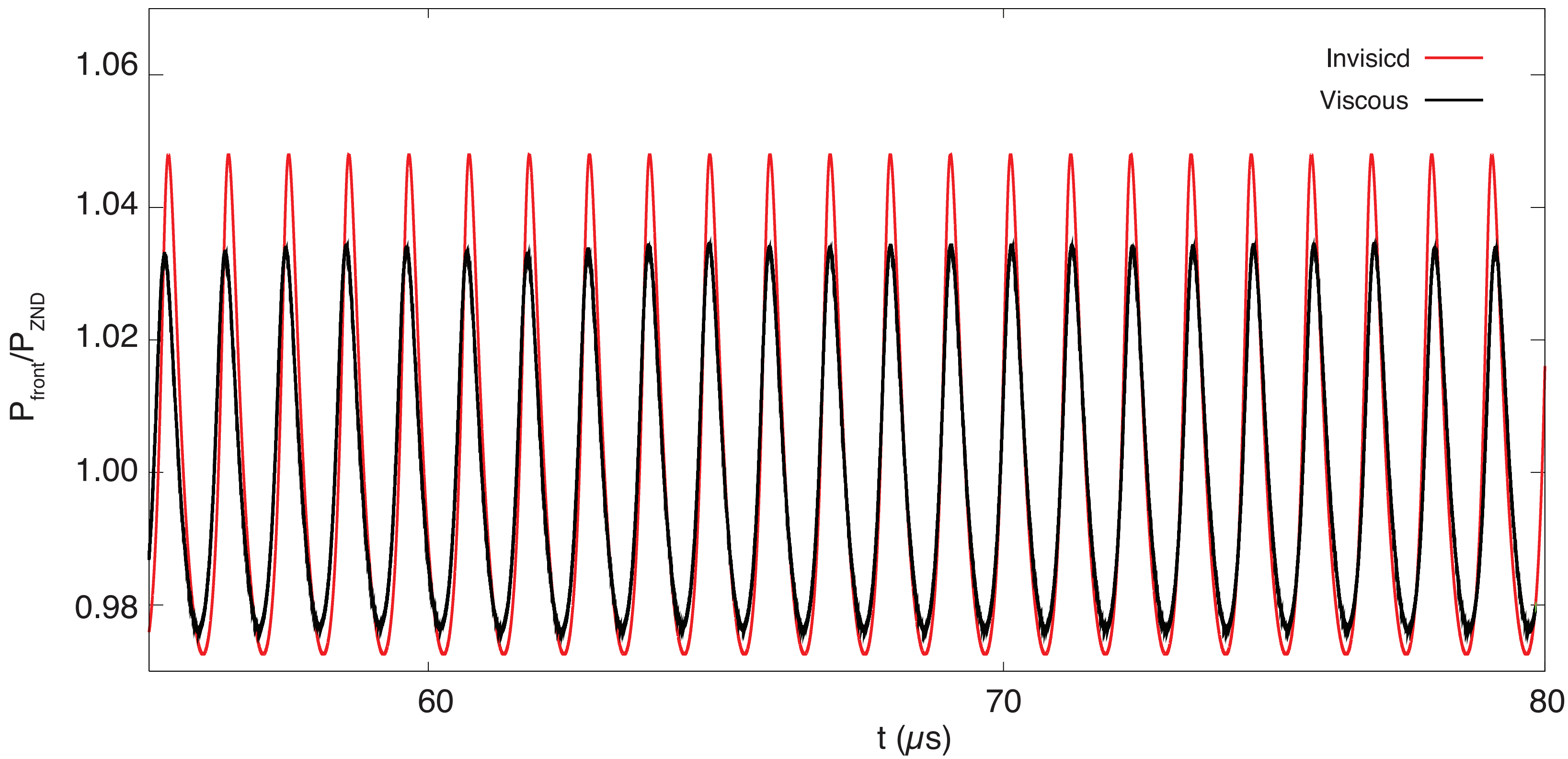


(*Astro. Acta*, 1972)

- 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 $f \approx 1.10$
- 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

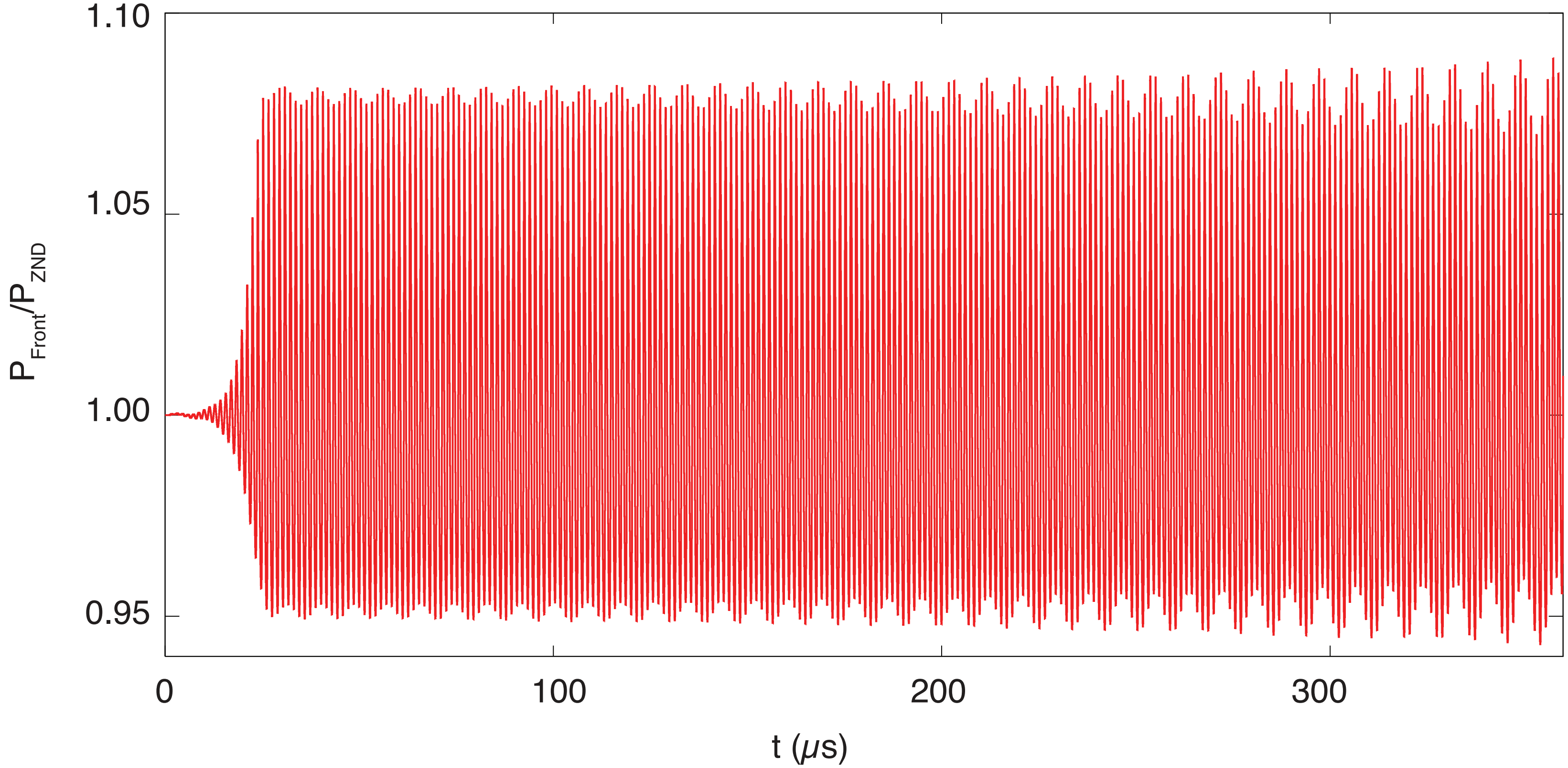
$f = 1.10$



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

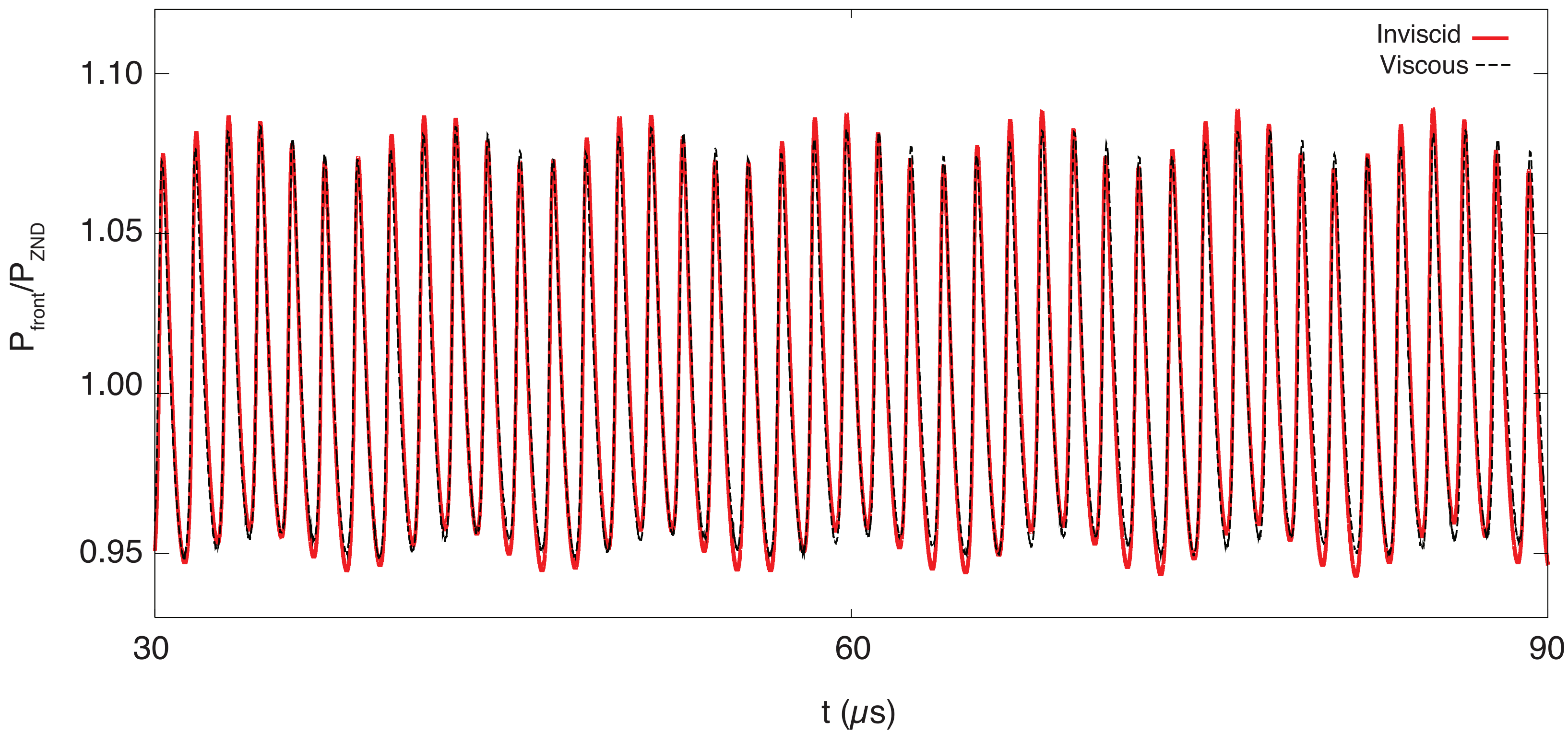
$f = 1.035$



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. Longer times need further investigation.

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

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

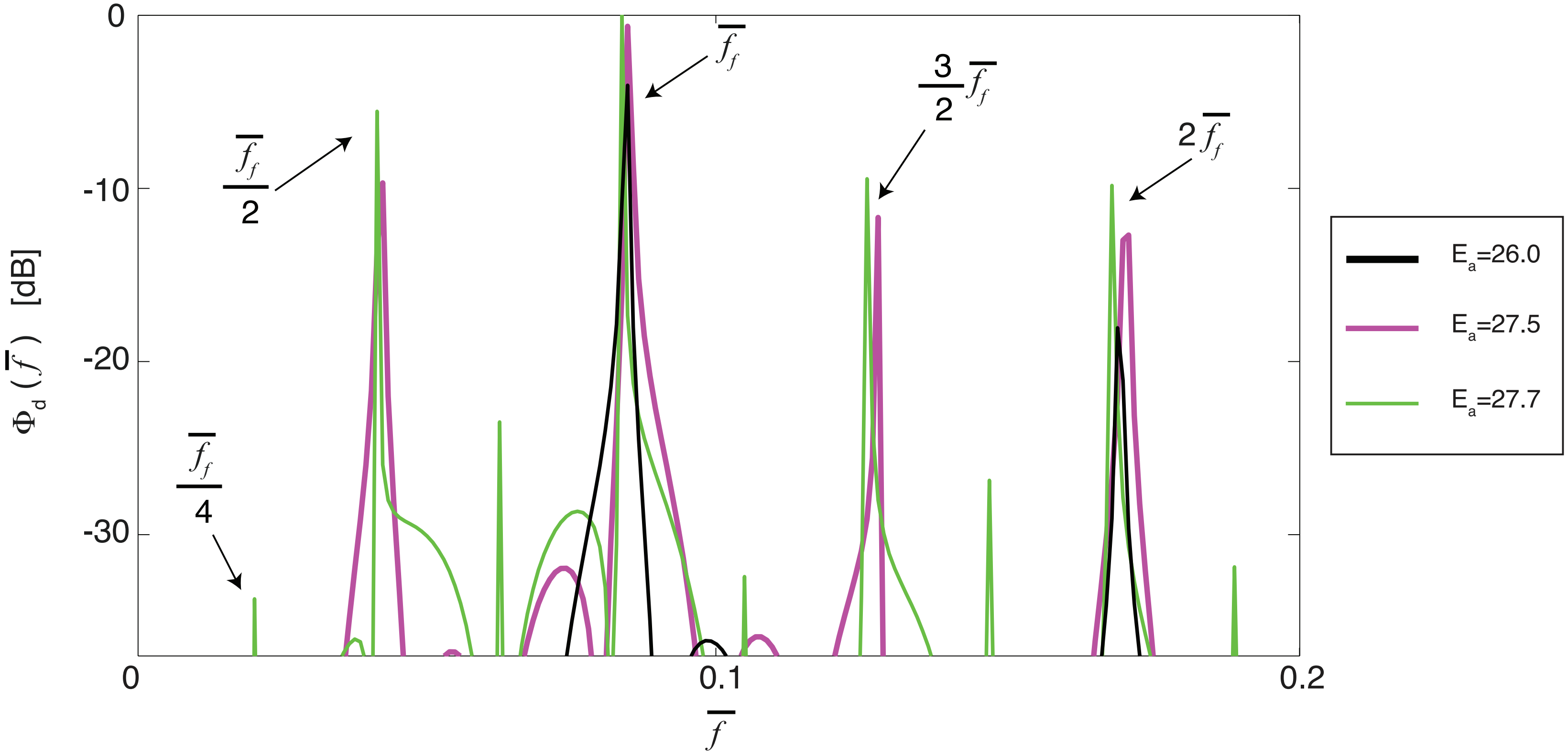
$$\Phi_d(\bar{f}_k) = \frac{2}{N^2}|P_k|^2, \qquad k = 1, 2, \ldots, (N/2-1),$$

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

where P_k is the standard discrete Fourier Transform of p,

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

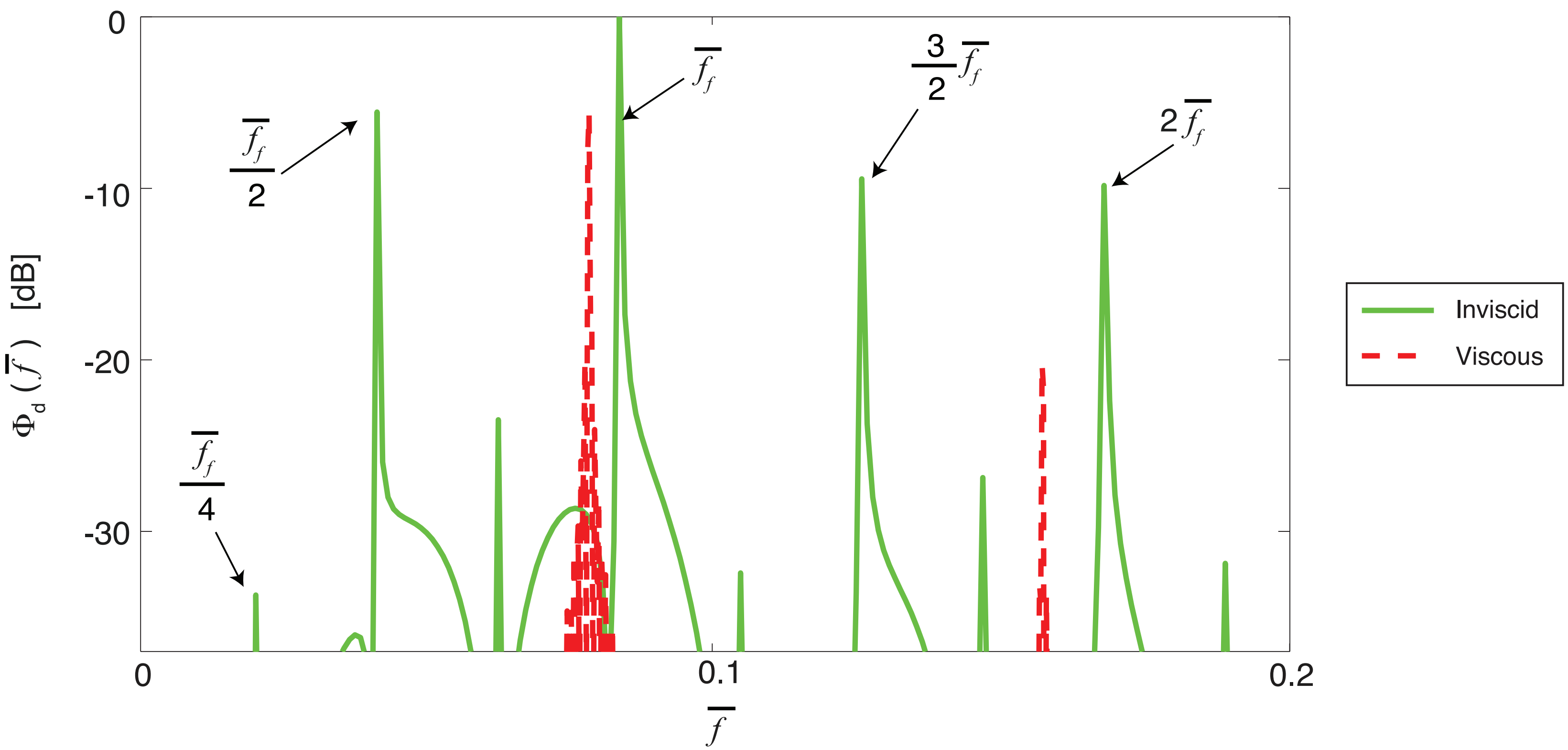
One Step Kinetics - Inviscid



As the activation energy is increased, the one-step kinetics' fundamental frequency shifts to a lower frequency, and its amplitude grows. Period-doubling and higher order harmonics are clearly visible. Non-linear effects alter the predicted fundamental frequency from linear theory by $3.4\%, 6.2\%,$ and 6.8%.

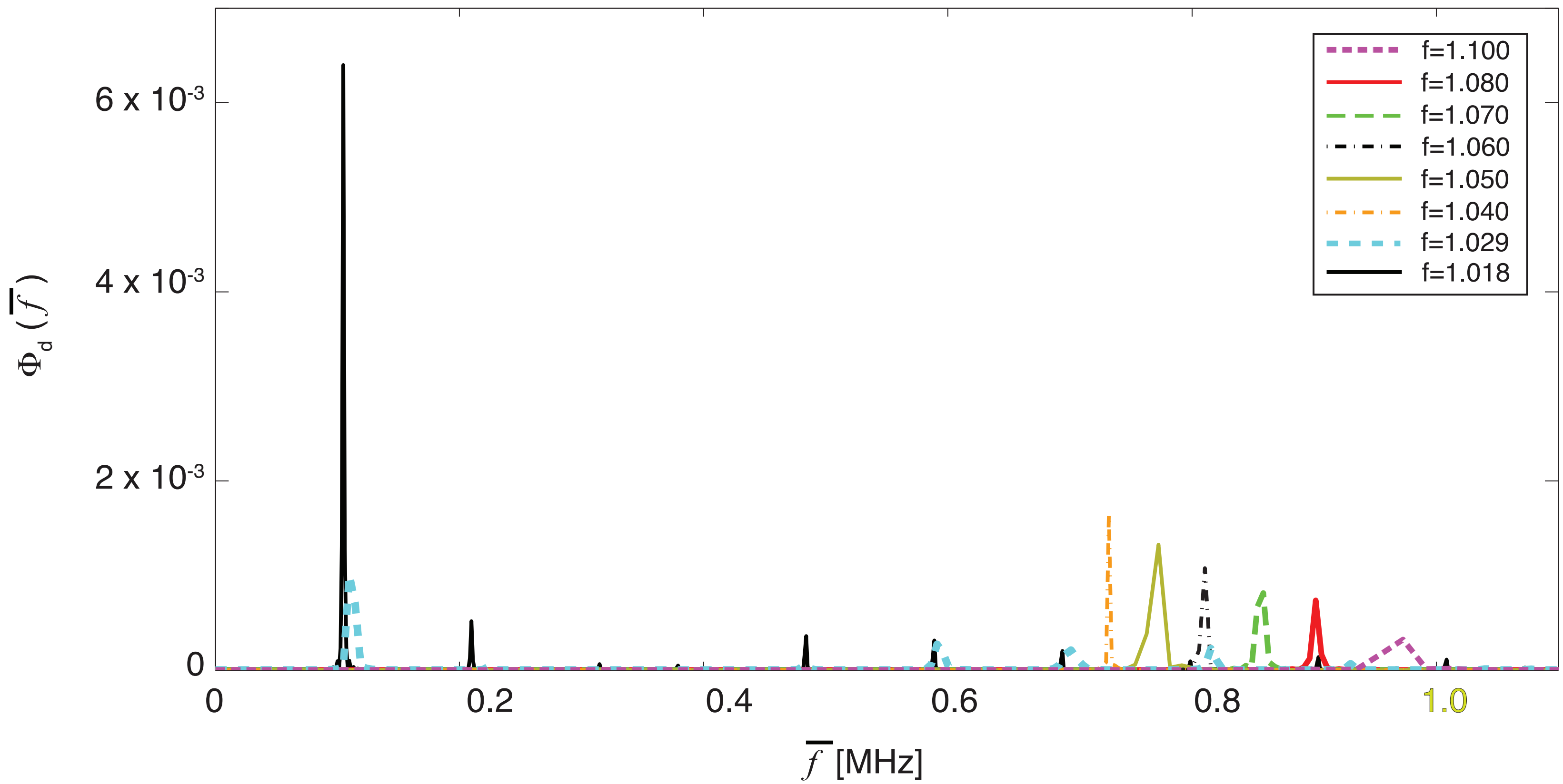
One Step Kinetics - Viscous Modulation

$E_a = 27.7$



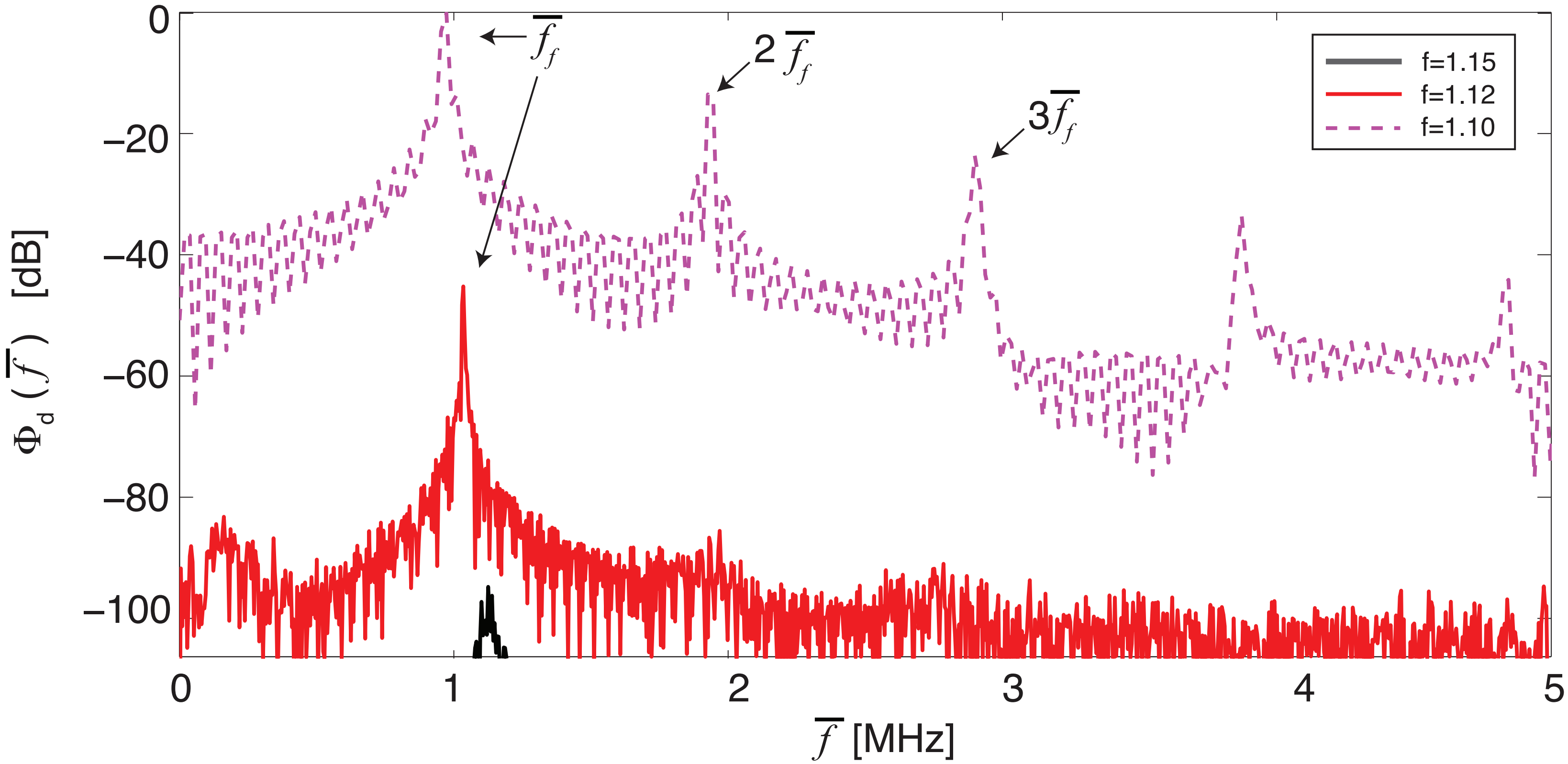
Viscous effects significantly reduce the amplitude of oscillations and alter the predicted behavior from a period-4 to period-1 detonation. Additionally, the predicted fundamental frequency is also altered; it is shifted from 0.0839 to 0.0787.

Hydrogen-Air: Overview



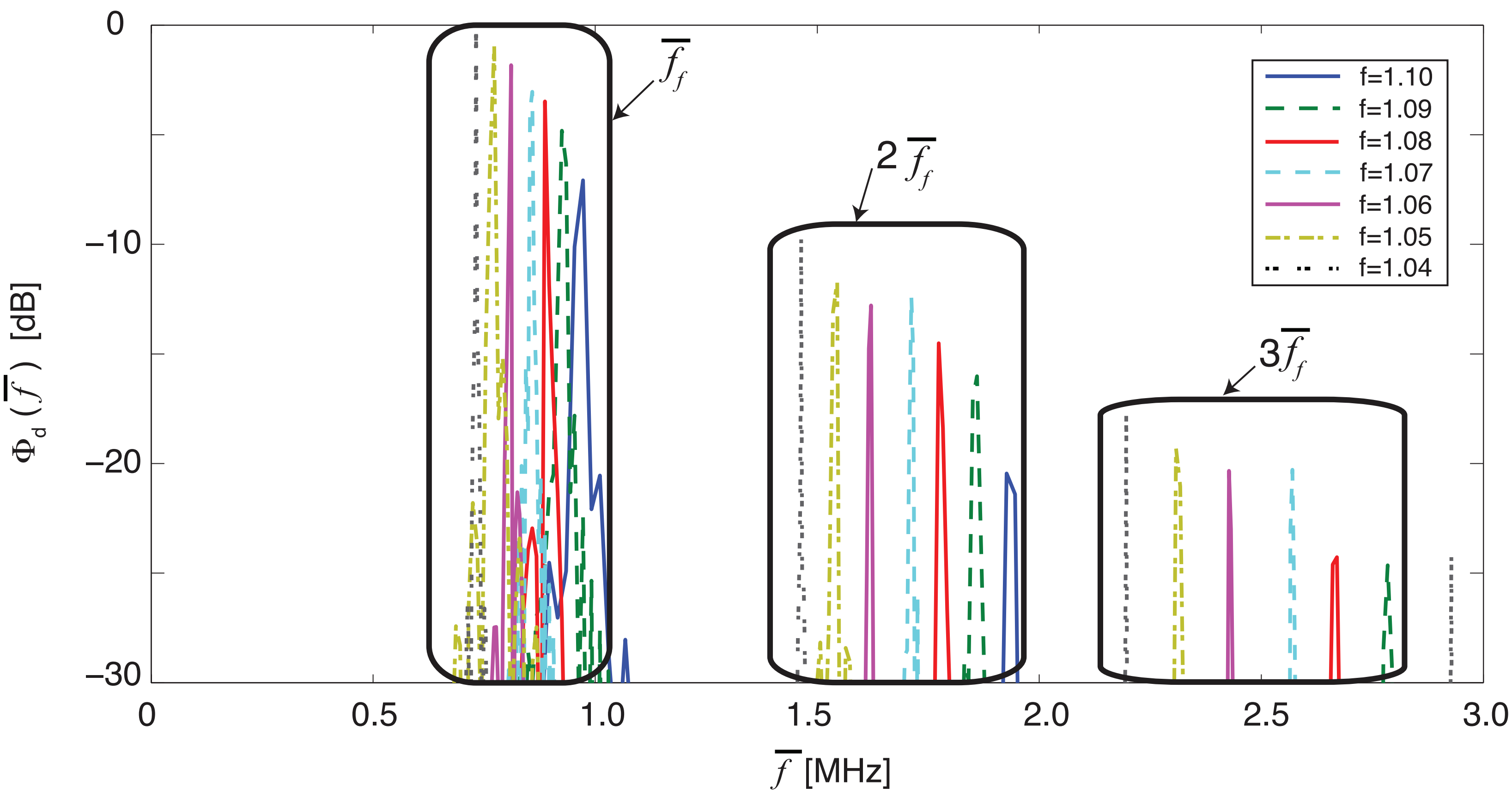
Unlike one-step kinetics, hydrogen-air detonations do not go through a period-doubling phenomena at these conditions. However, there is an appearance of a lower frequency as the overdrive is lowered.

Hydrogen-Air: Near Neutral Stability



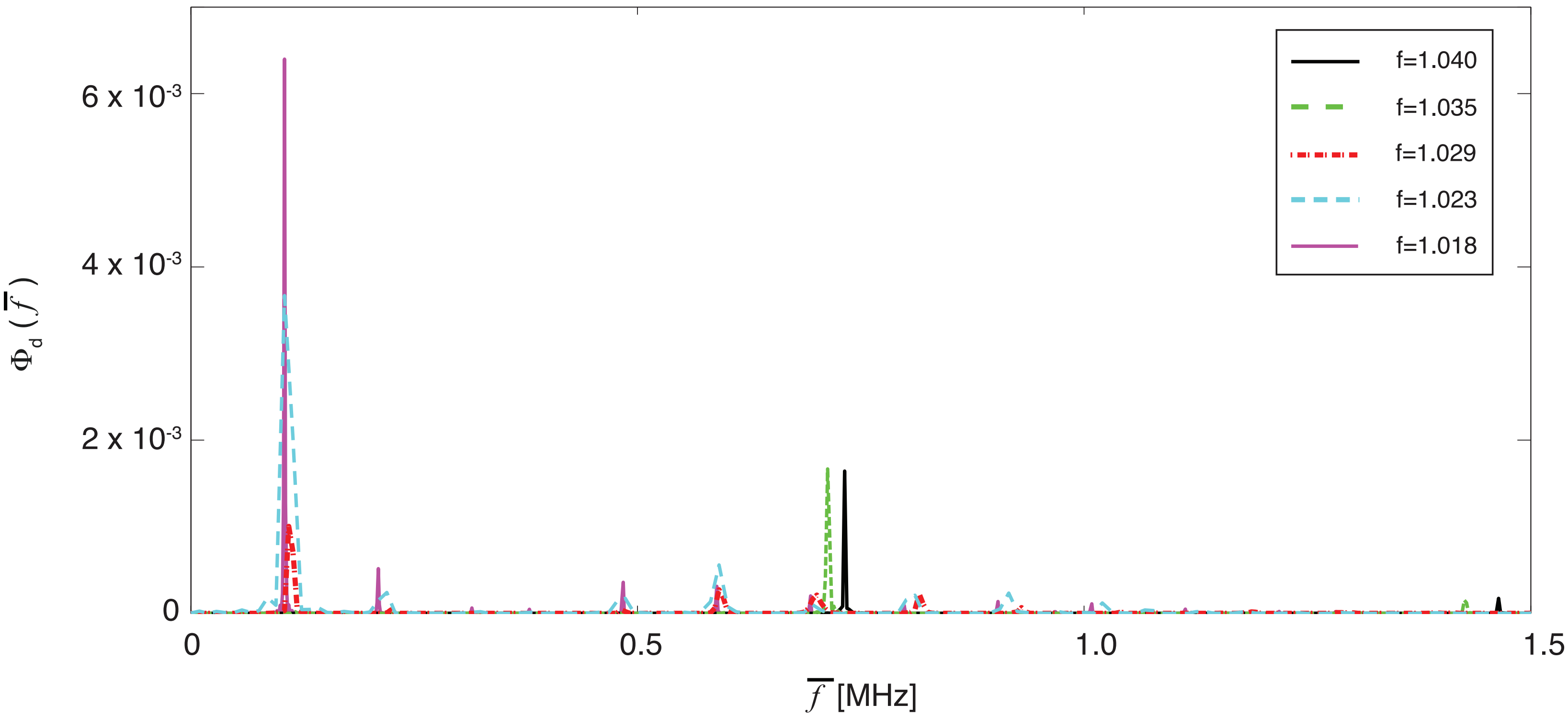
Significant growth of the amplitude of oscillations occurs as one passes through the neutral stability point.

Hydrogen-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.

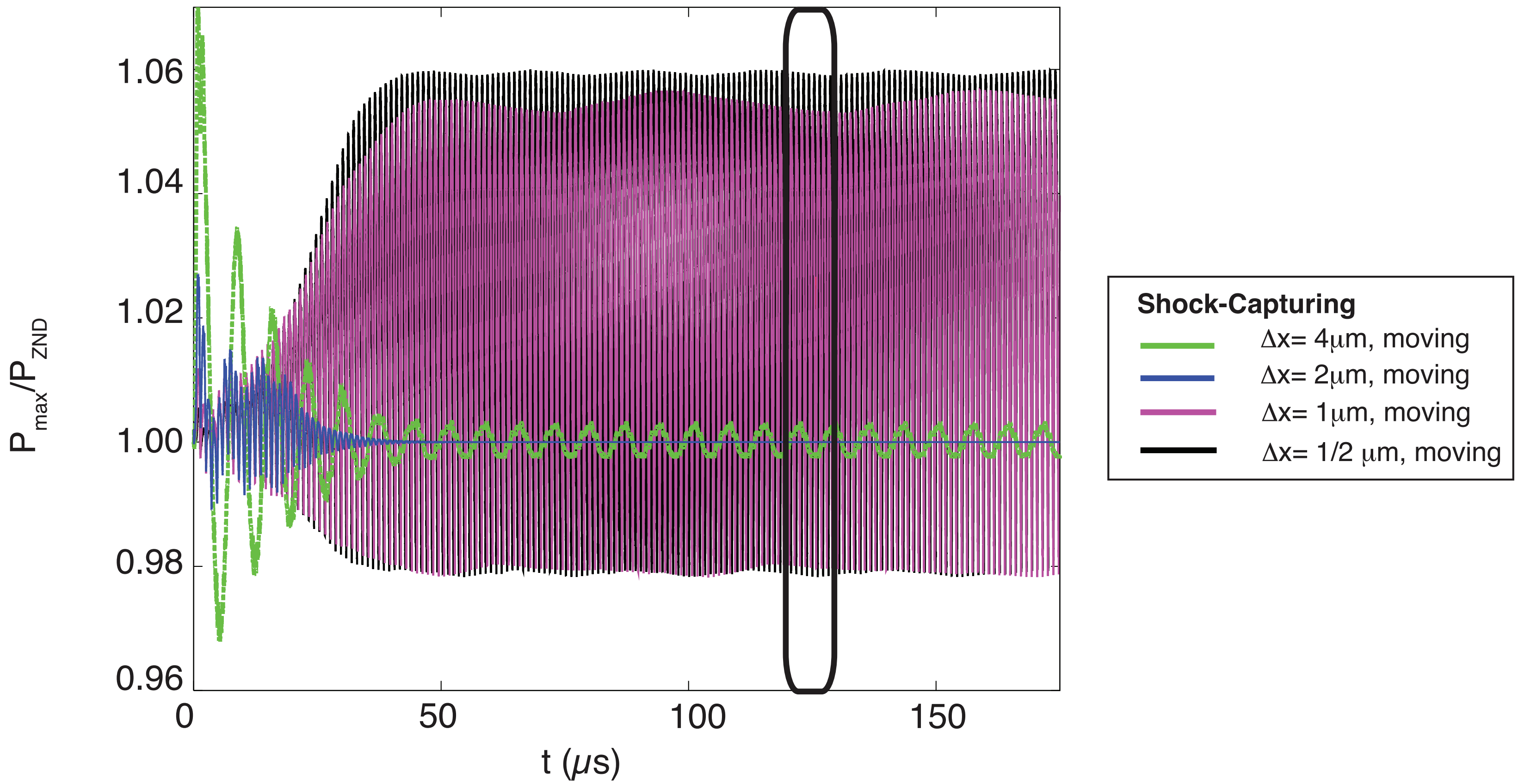
Hydrogen-Air: High-to-Low Frequency Transition



A transition of the dominant mode from the high-frequency mode, $(0.7\ MHz)$ to the low-frequency mode, $(0.1\ MHz)$, occurs at $f = 1.029$. Furthermore, in this transition region the second harmonic of the low-frequency contains less energy than a higher frequency near $0.6\ MHz$, until the overdrive reaches $f = 1.018$.

Capturing vs. Fitting - High Frequency Mode

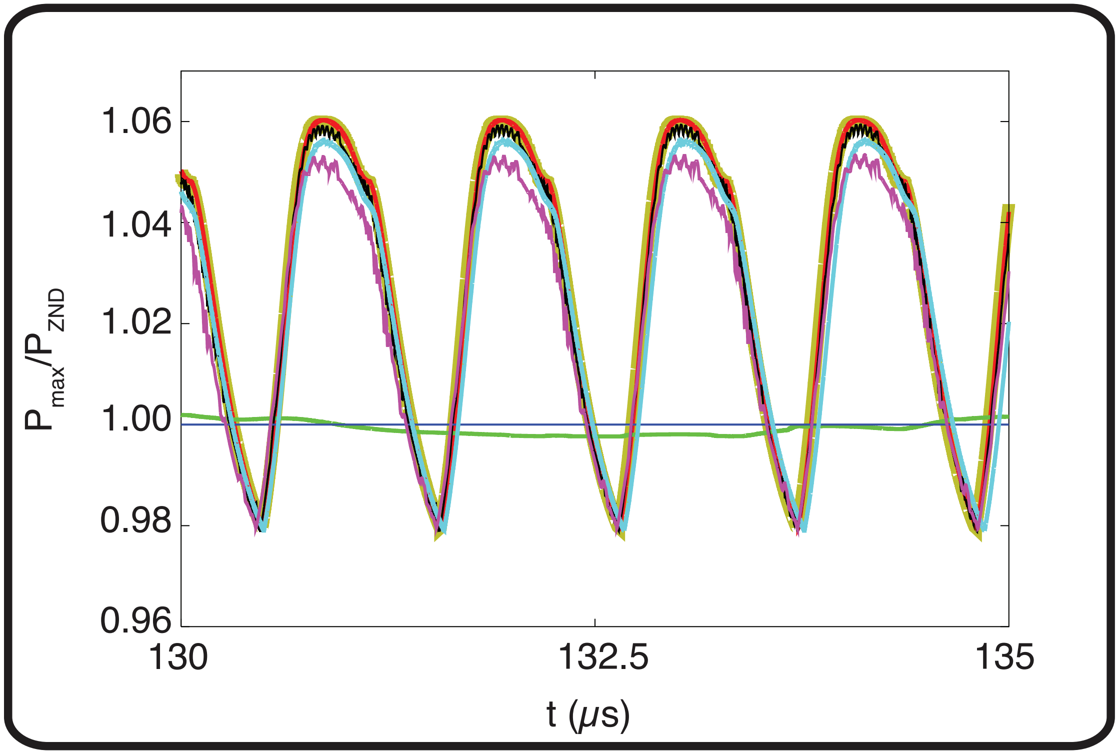
$f = 1.10$

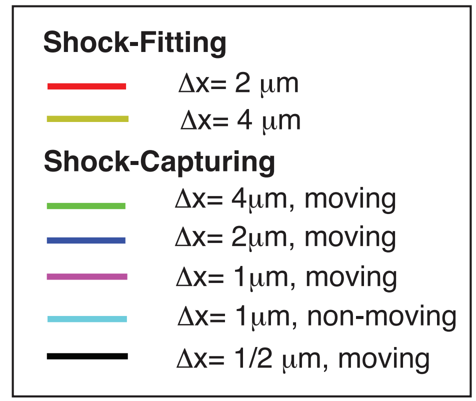


Using the same grid size as shock-fitting $(\Delta x = 4\ \mu m)$, shock-capturing misses the essential dynamics.

Capturing vs. Fitting - High Frequency Mode

$f = 1.10$

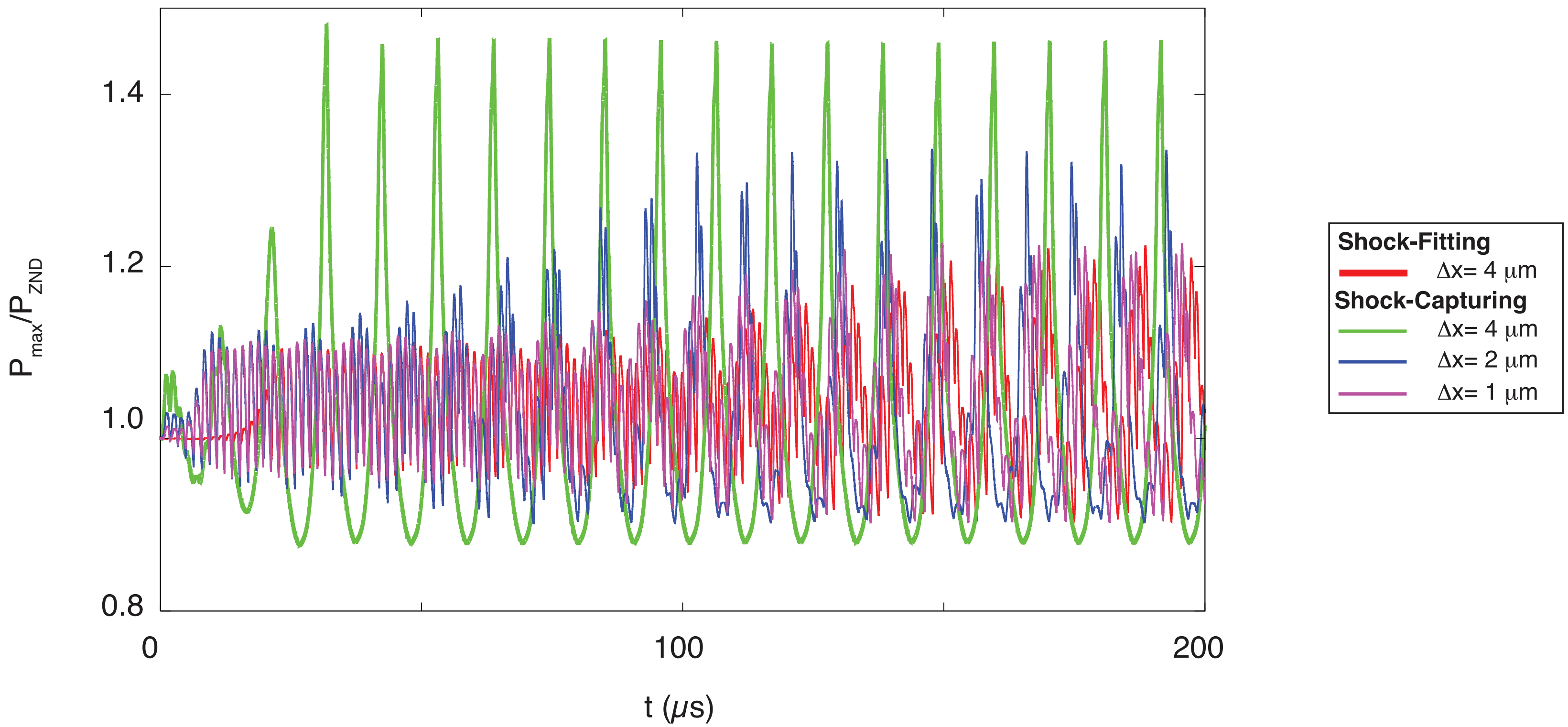




Using a four times finer grid with shock-capturing than shock-fitting allows the pulsations to be captured. However, both much higher and lower frequency spurious oscillations are predicted as well.

Capturing vs. Fitting - Low Frequency Mode

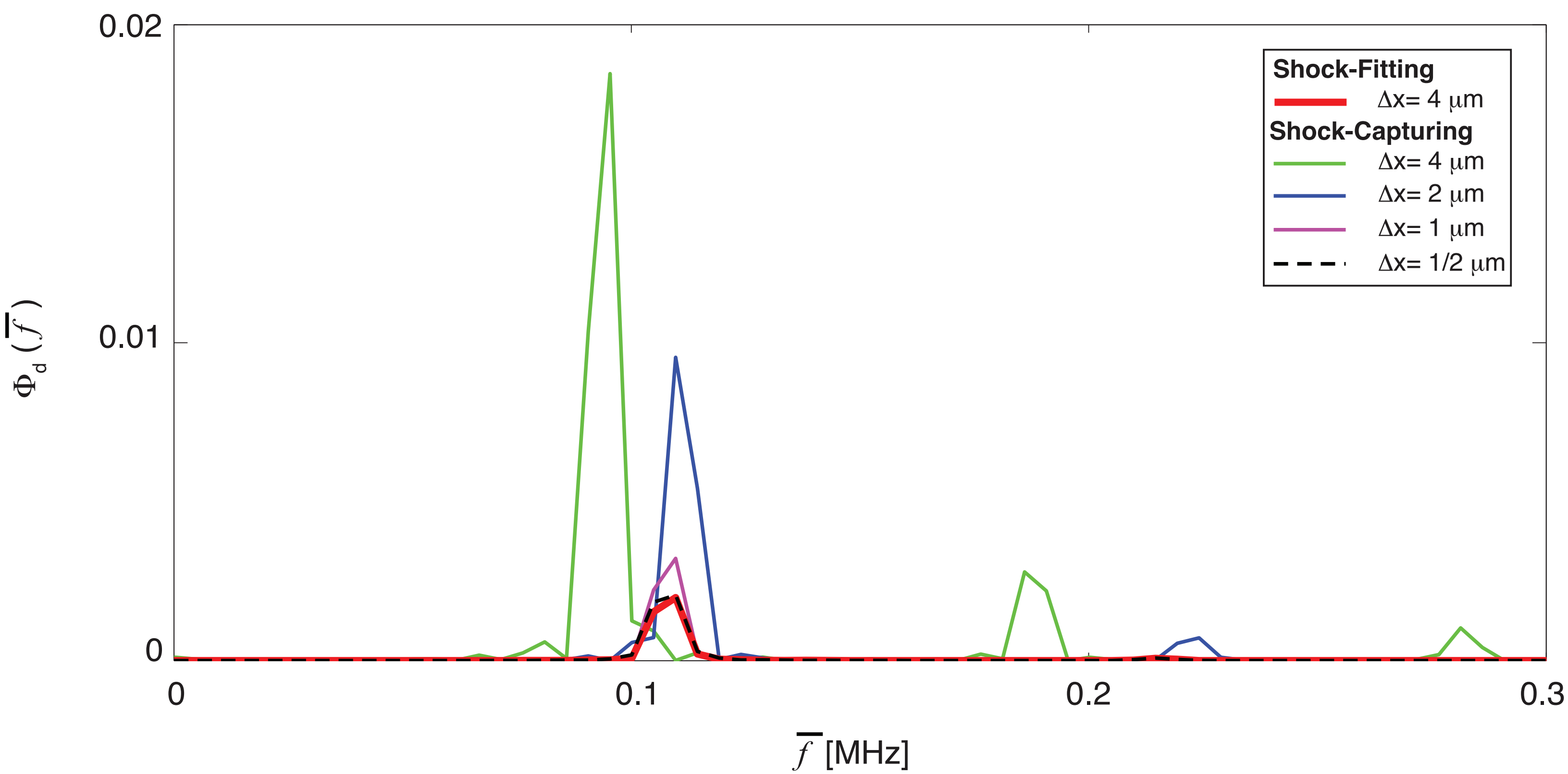
$f = 1.023$



Using the same grid size $(\Delta x = 4\ \mu m)$ as shock-fitting, shock-capturing dramatically over-predicts the pulsation amplitude. In shock-capturing, a resolution of $\Delta x = 1\ \mu m$ is needed to begin capturing the essential dynamics at long time.

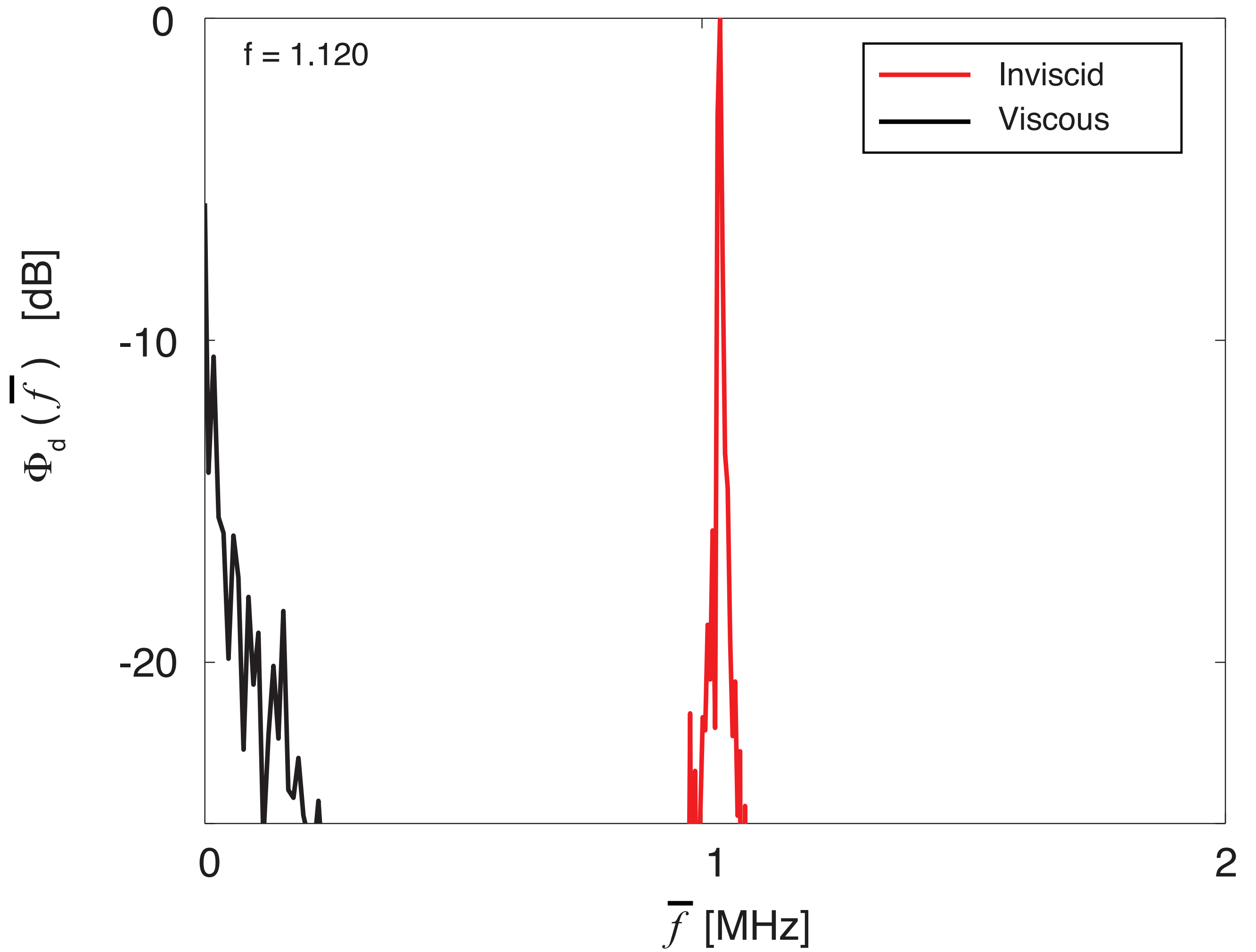
Capturing vs. Fitting - Low Frequency Mode

$f = 1.023$



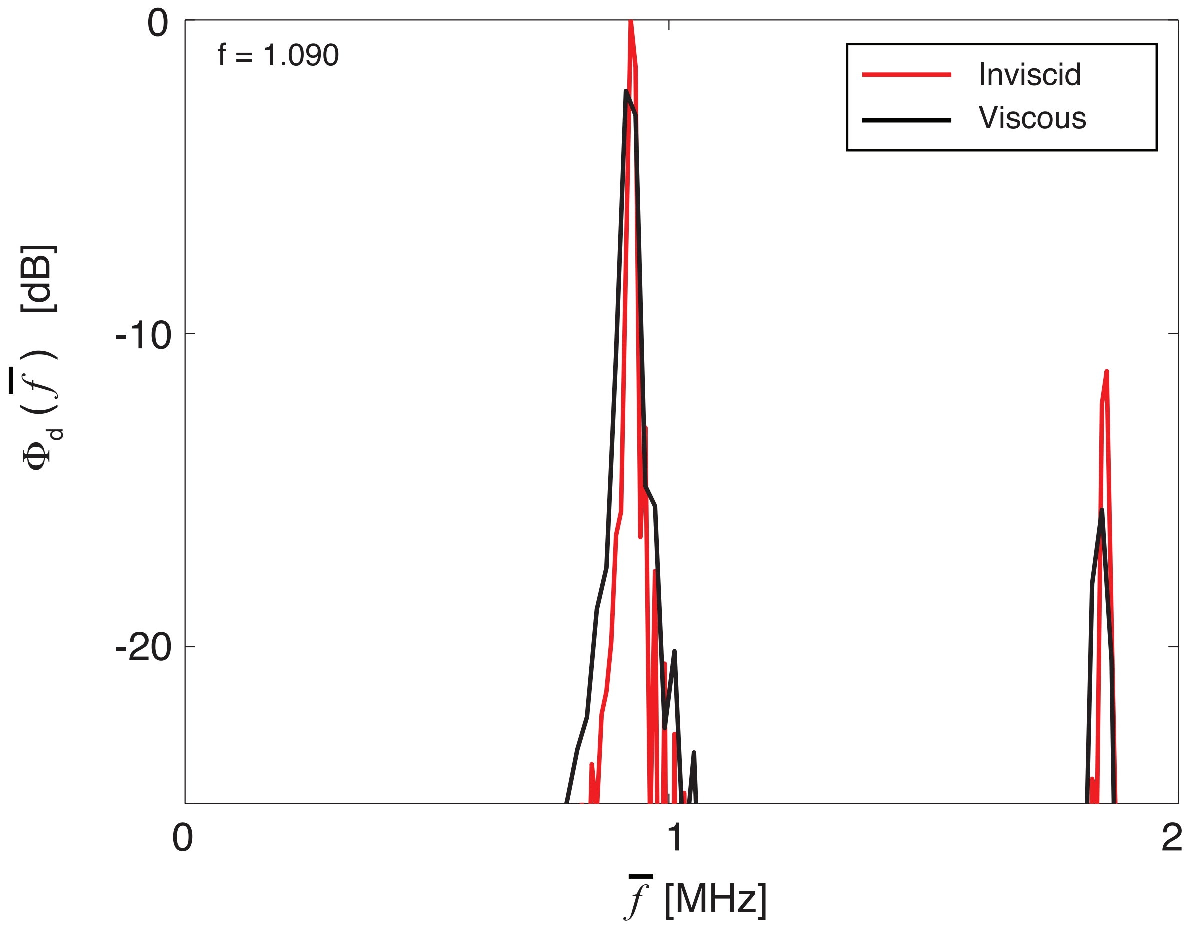
Only when $\Delta x = 1/2\ \mu m$ is used does the PSD of shock-capturing become nearly indistinguishable with that of shock-fitting.

Effect of Physical Viscosity



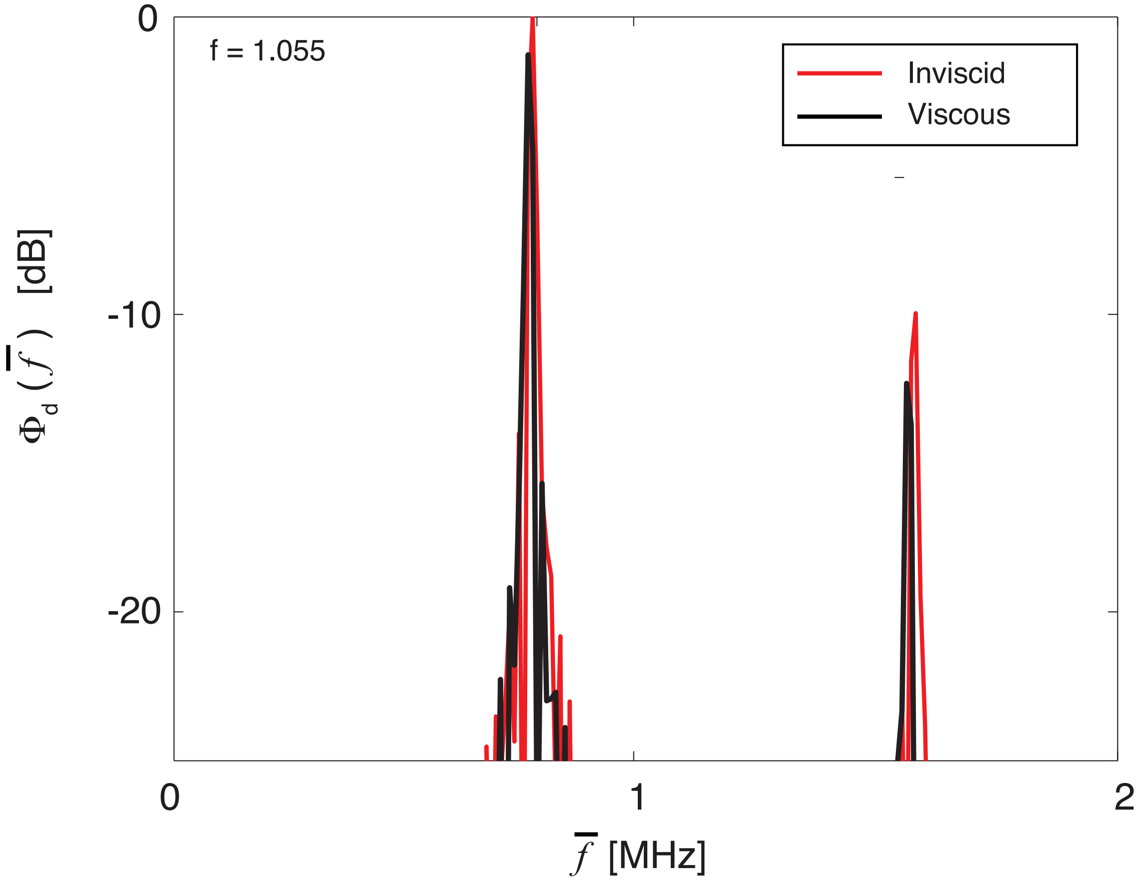
Near the neutral stability boundary, viscosity damps the small amplitude oscillations.

Effect of Physical Viscosity



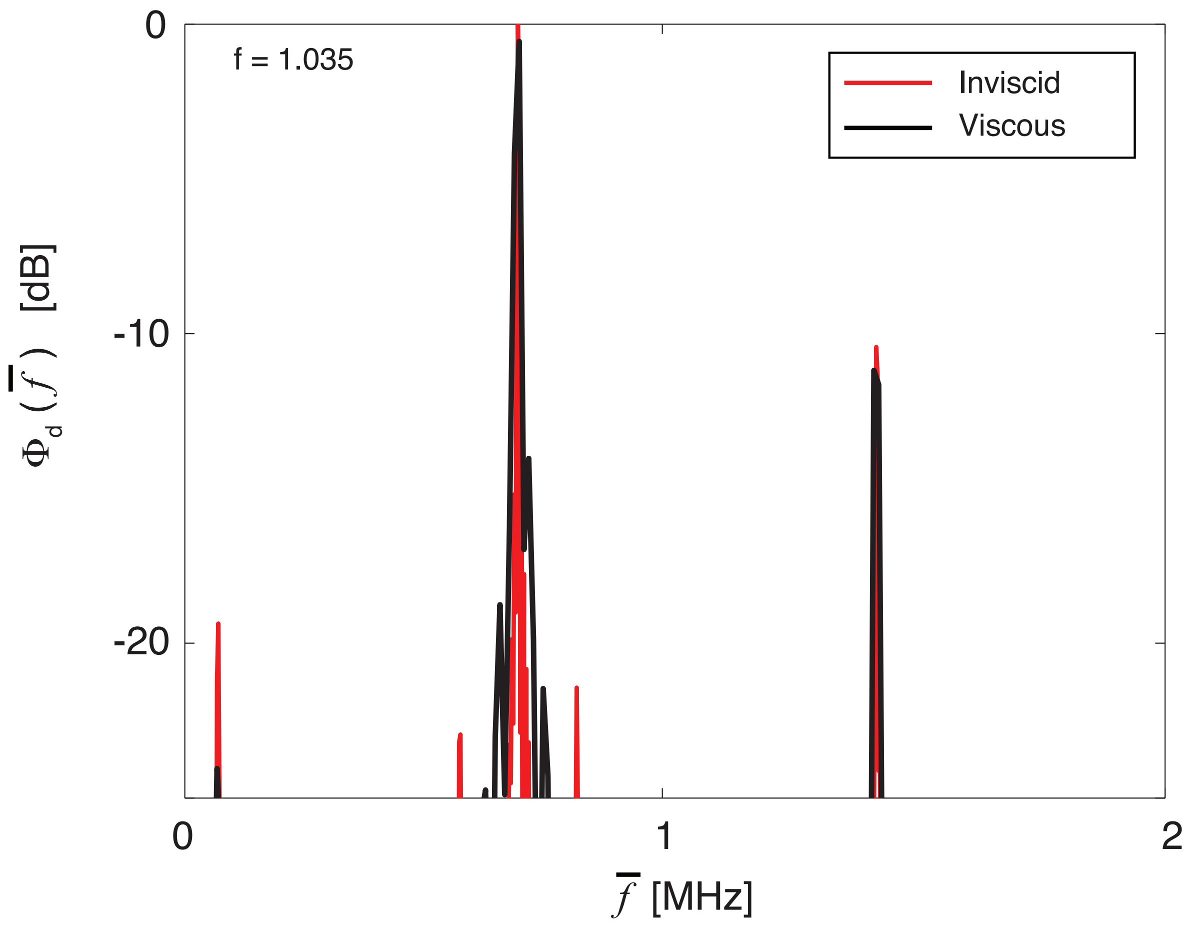
Viscosity effects reduce the magnitude of the peaks at the first and higher harmonics.

Effect of Physical Viscosity



As the overdrive is lowered, the viscous PSD looks increasingly like that of the shock-fitted inviscid case.

Effect of Physical Viscosity



The fundamental frequency’s peak is barely reduced; however, the lower frequency’s peak in the inviscid case is nearly removed in the viscous analog.

Conclusions

- Long time behavior of a hydrogen-air detonation becomes more complex as the overdrive is decreased; three phemonona are predicted:
  - a stable detonation,
  - a single dominant high frequency mode oscillatory detonation,
  - a dual mode oscillatory detonation, dominated by the low frequency mode.
- Harmonic analysis has revealed the first harmonic frequency moderately lowers as the overdrive is lowered in the high frequency mode.
- At the second bifurcation there is a drastic shift in the fundamental frequency from $0.71\ MHz$ to $0.11\ MHz$.
- Shock-capturing requires a four times finer grid to predict the essential dynamics of an inviscid detonation than the minimal artificial viscosity shock-fitting scheme.
- Physical diffusion causes a amplitude reduction in all cases examined; further investigation is needed at longer times near the bifurcation limits.