The Dynamics of Detonation with WENO and Navier-Stokes Shock-Capturing

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Introduction

- 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, operator splitting, or turbulence modeling, all of which filter small scale physical dynamics?
- Do we really need WENO methods if the problem demands resolved diffusive length scales?

Introduction-Continued

- It is often argued that viscous forces and diffusion are small effects which 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.
- This suggests grid-dependent numerical viscosity may be problematic.

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 sub-microns to 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 chemical length scale is induced compared to the multiple scales of detailed kinetics.
- By choosing a one-step model, the effect of the interplay between chemistry and transport phenomena can more easily be studied.

Review

- In the one-dimensional inviscid limit, one step models have been studied extensively.
- Erpenbeck (*Phys. Fluids*, 1962) began the investigation into the linear stability almost fifty years ago.
- Lee & Stewart (*JFM*, 1990) developed a normal mode approach, using a shooting method to find unstable modes.
- Bourlioux *et al.* (*SIAM JAM*, 1991) studied the nonlinear development of instabilities.

Review-Continued

- Kasimov & Stewart (*Phys. Fluids*, 2004) used a first order shock-fitting technique to perform a numerical analysis.
- Ng *et al.* (*Comb. Theory and Mod.*, 2005) developed a coarse bifurcation diagram showing how the oscillatory behavior became progressively more complex as activation energy increased.
- Henrick *et al.* (*J. Comp. Phys.*, 2006) developed a more detailed bifurcation diagram using a fifth order mapped WENO method accompanied with shock-fitting.

One-Dimensional Unsteady Compressible Reactive Navier-Stokes Equations

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

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

Case Examined

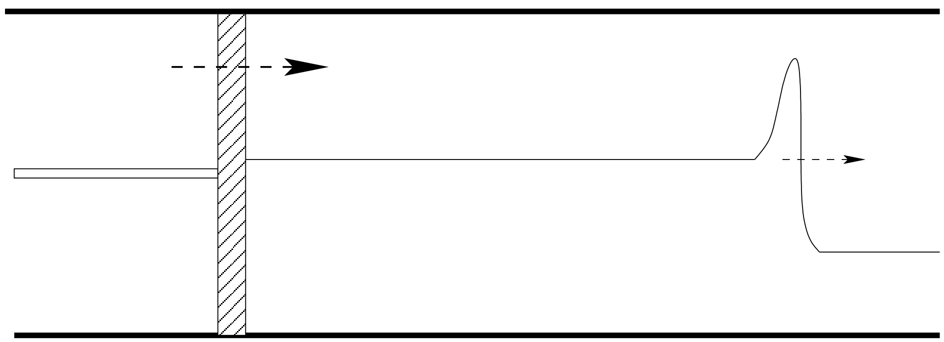
Let us examine this one-step kinetic model with:

- a fixed reaction length, $L_{1/2} = 10^{-6}\ m$, which is similar to the finest length scale of H_2-O_2 detonation.
- an ambient pressure, $P_o = 101325\ Pa$, ambient density, $\rho_o = 1\ kg/m^3$, heat release $q = 5066250\ m^2/s^2$, and $\gamma = 6/5$.
- a fixed the diffusion length, $L_\mu = 10^{-7}\ m$; mass, momentum, and energy diffusing at the same rate.
- a range of activation energies $(25 \leq E \leq 32)$ and thus a range for the collision frequency factor $(1.145 \times 10^{10}\ 1/s \leq a \leq 3.54 \times 10^{10}\ 1/s)$.

Numerical Method

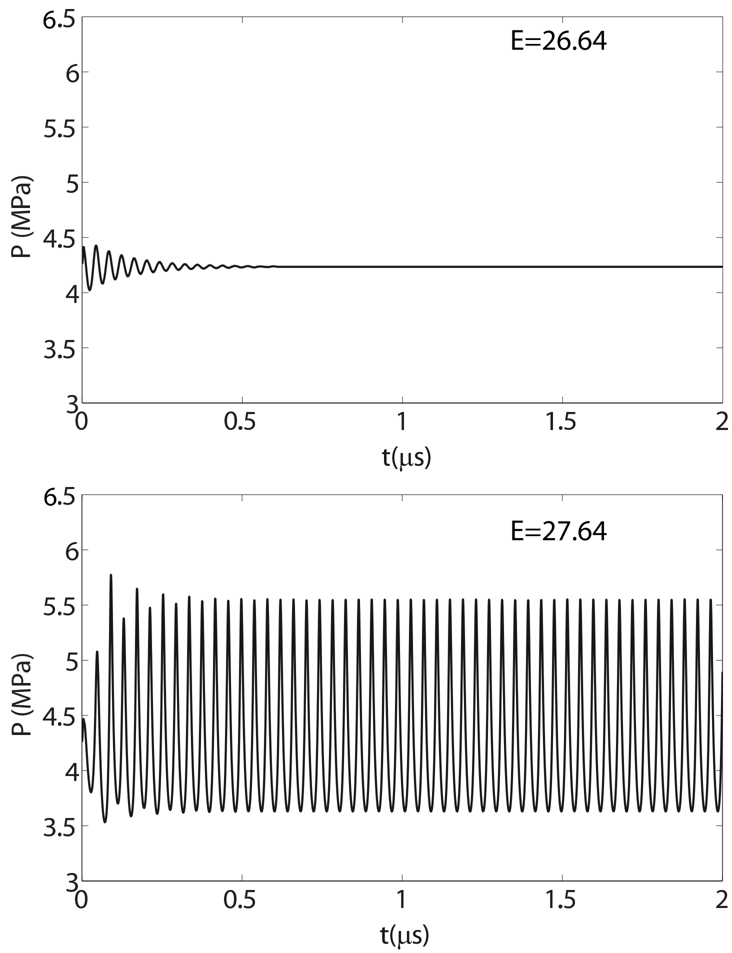
- Finite difference, uniform grid $\left(\Delta x = 2.50 \times 10^{-8} m, N = 8001, L = 0.2\, mm\right)$.
- Computation time = 192 hours for $10\ \mu s$ on an AMD $2.4\ GHz$ with $512\ kB$ cache.
- A point-wise method of lines aproach was used.
- Advective terms were calculated using a combination of 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.

Method



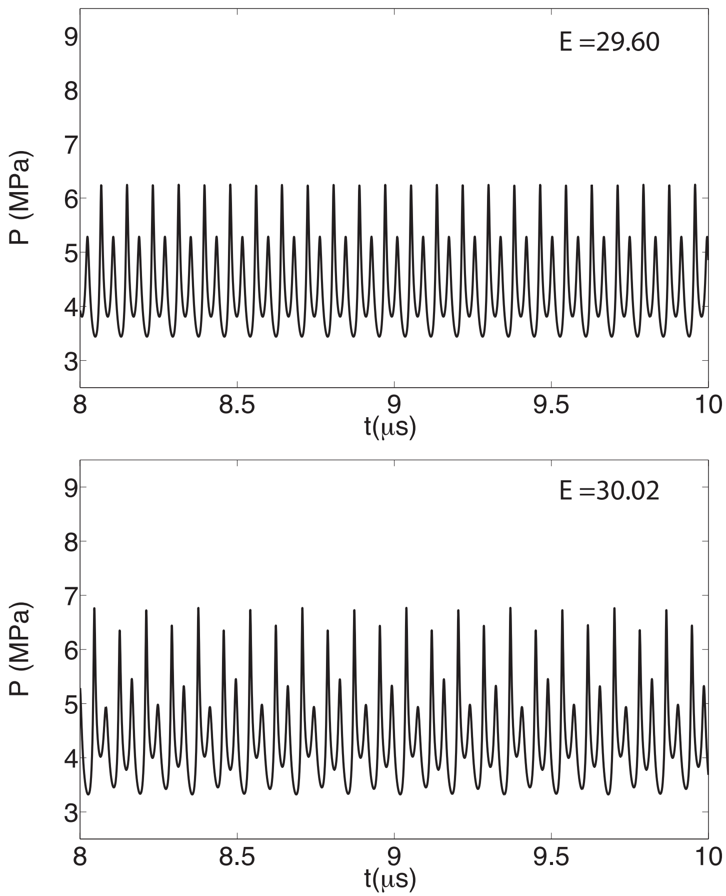
- Initialized with inviscid ZND solution.
- Moving frame travels at the CJ velocity.
- Integrated in time for long time behavior.

Effect of Diffusion on Limit Cycle Behavior



- For the inviscid case, the stability limit was found at $E_0 = 25.26$ (Lee & Stewart, Henrick *et al.*)
- In the viscous case $E = 26.64$ is still stable; however, above $E_0 \approx 27.14$ a period-1 limit cycle can be realized.

Period-Doubling Phenomena: Viscous Case



- 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 $E_1 \approx 29.32.$

Effect of Diffusion on 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 $E_\infty \approx 30.0327$.
- For $E > 30.0327$, 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

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

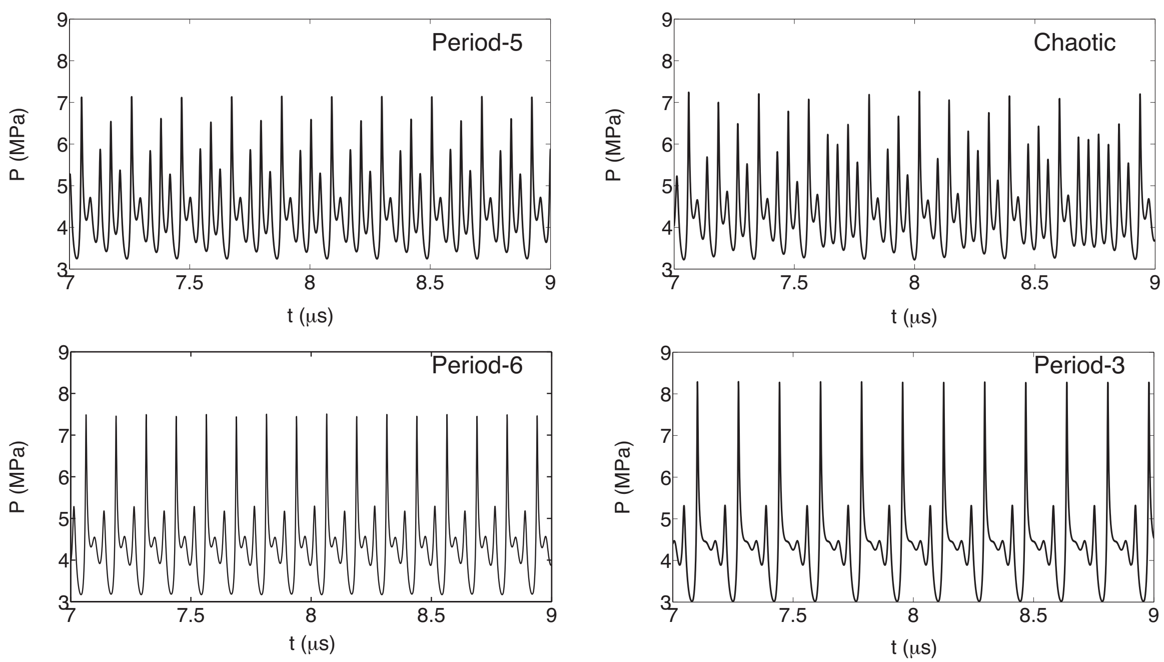
Feigenbaum predicted $\delta_\infty \approx 4.669201.$

	Inviscid	Inviscid	Viscous	Viscous
n	E_n	δ_n	E_n	δ_n
0	25.2650	-	27.14	-
1	27.1875	3.86	29.32	3.89
2	27.6850	4.26	29.88	4.67
3	27.8017	4.66	30.00	-
4	27.82675	-	-	-

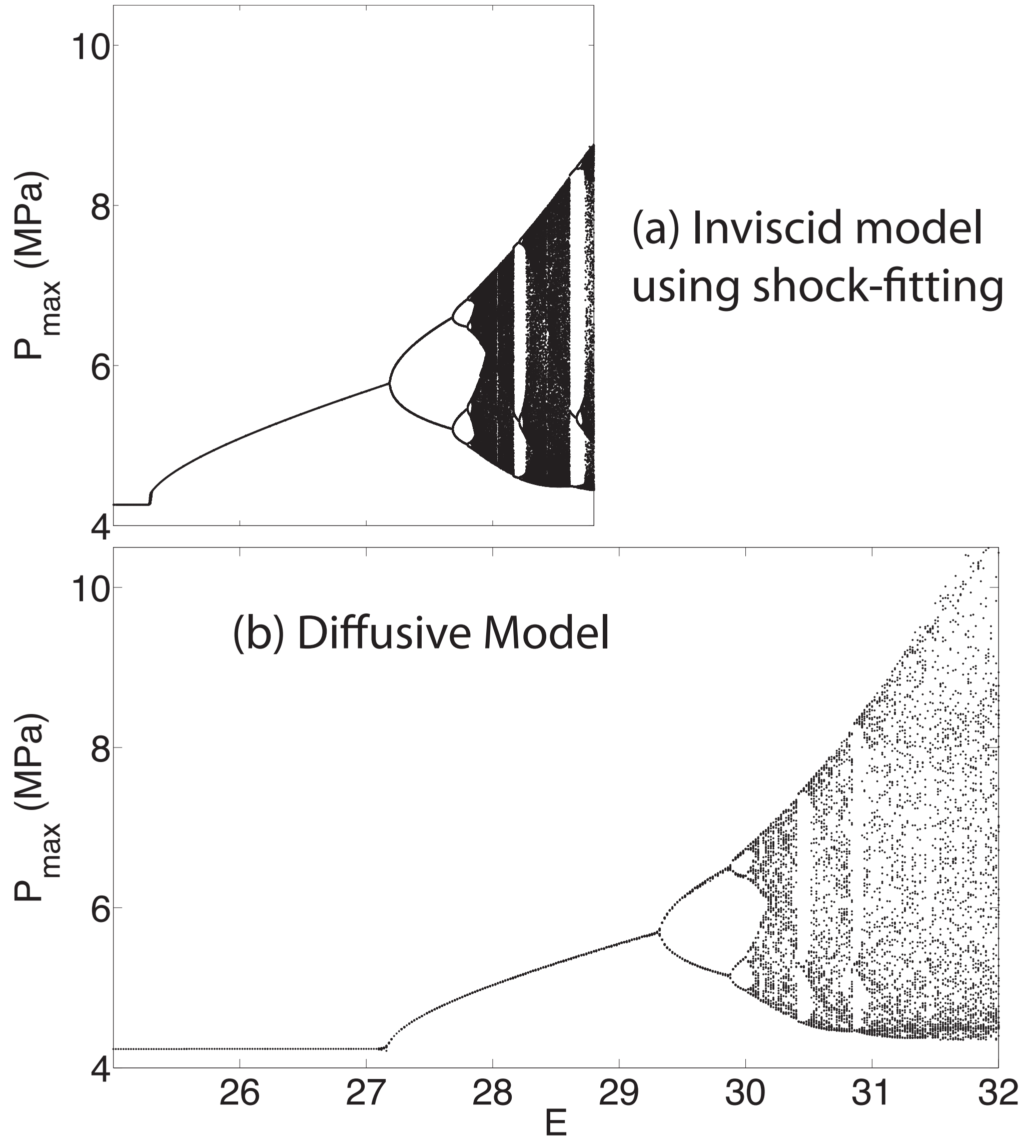
Chaos and Order: Viscous Case

- The period-doubling behavior and transition to chaos predicted in the inviscid limit is also observed in the diffusive case.
- Within this chaotic region, there exist pockets of order with periods of 5, 6, and 3 present.

Viscous Detonations:

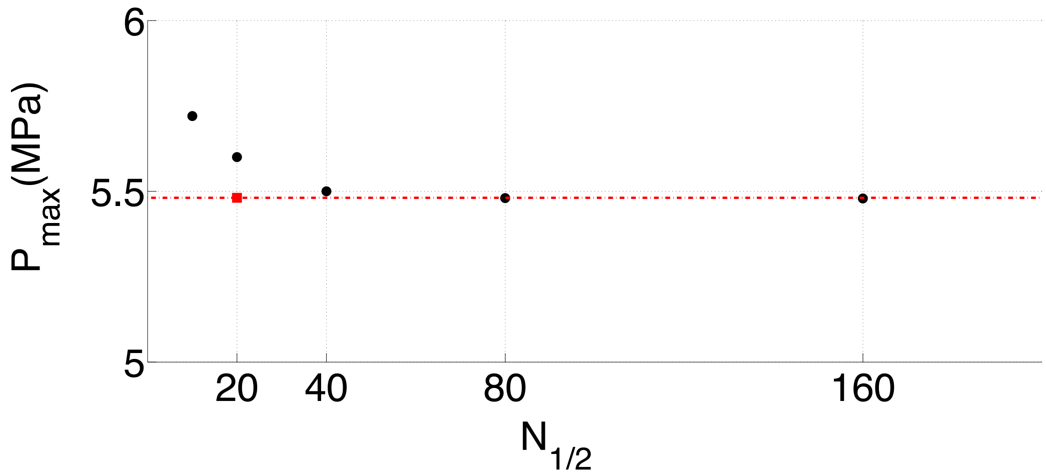


Bifurcation Diagram

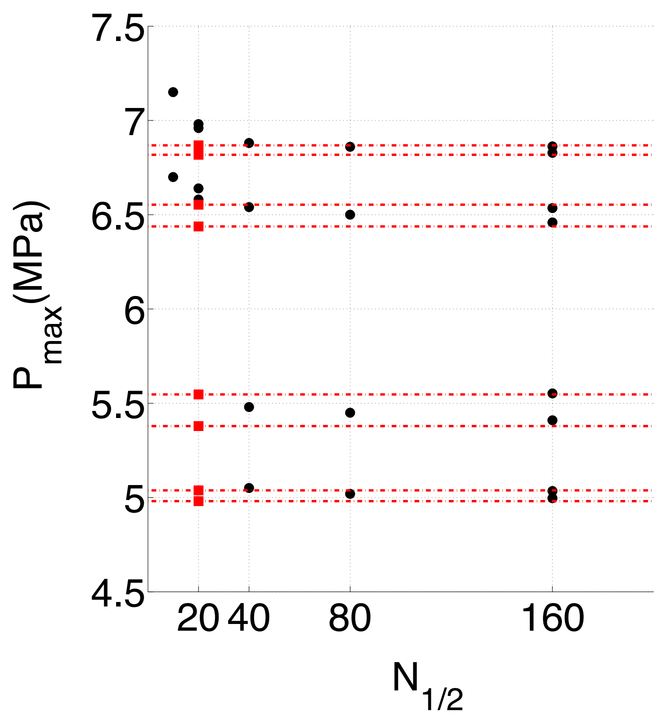


WENO5M Shock-Capturing: Inviscid Case

- For an inviscid model, at lower activation energies shock-capturing compares well with shock-fitting with similar resolutions.
- At $E = 26.64$, shock-fitting predicts a period-1 oscillating detonation $(P_{max} = 5.48\ MPa)$.
- Shock-capturing using $N_{1/2} = 20$, yields a relative difference of 2.1%; using $N_{1/2} = 40$ this relative difference is reduced to 0.34%

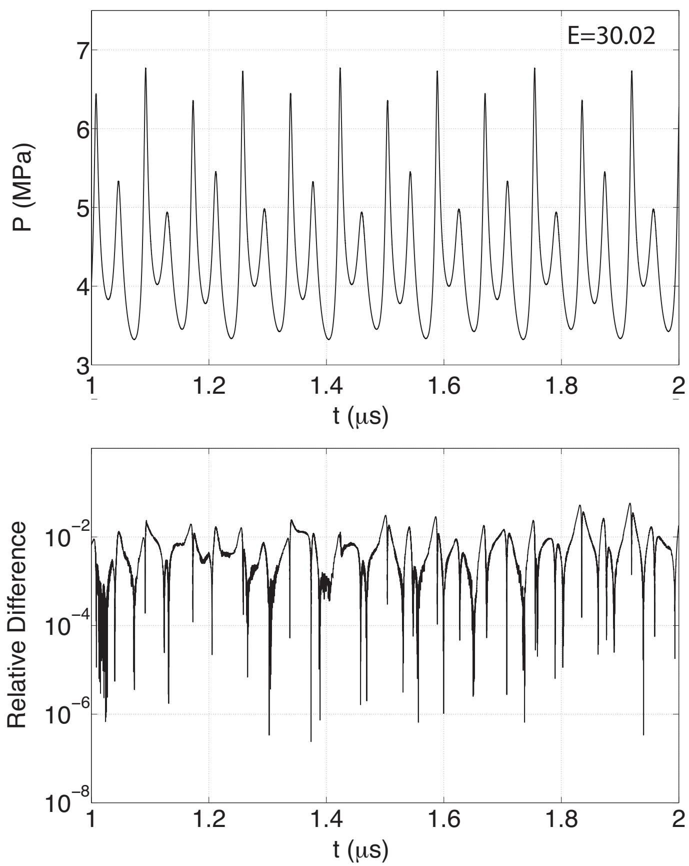


WENO5M Shock-Capturing: Inviscid Case



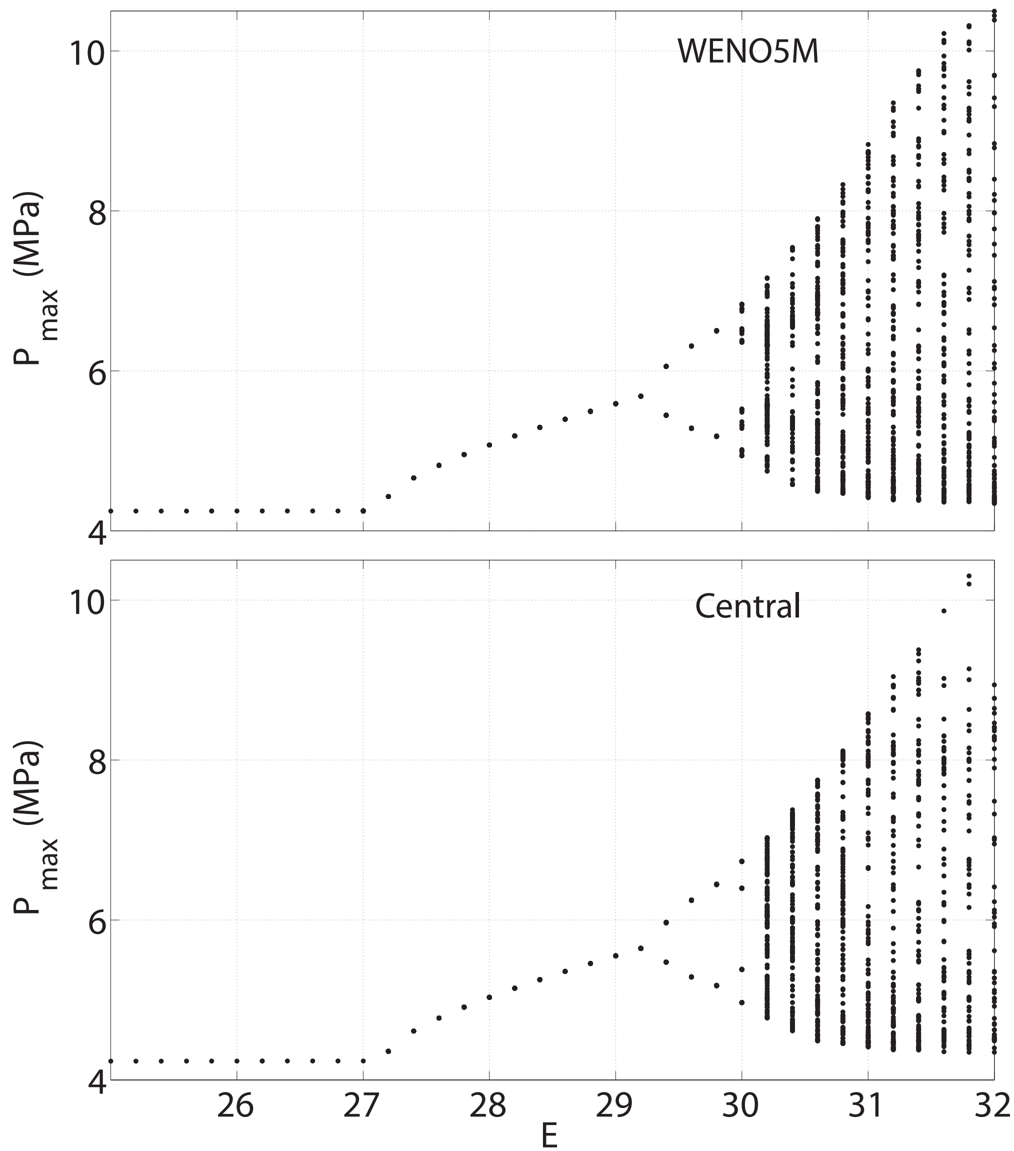
- At a higher activation energy, $(E = 27.82)$, shock-fitting predicts a period-8 detonation, whereas shock-capturing using $N_{1/2} = 40$ predicts a period-4 detonation. To reconcile this difference, the resolution of the shock-capturing technique must be increased to $N_{1/2} \approx 160$.
- Numerical diffusion is playing an important role in determining the behavior of the system. Let's add physical diffusion and see how that affects the behavior of the system.

WENO5M vs. Central Differencing: Viscous Case

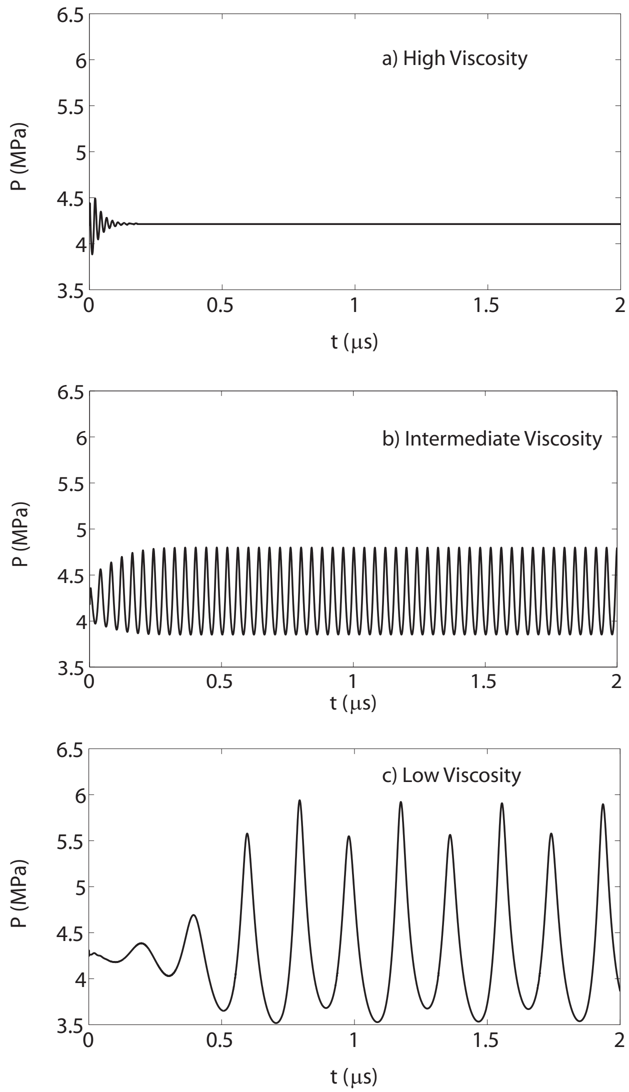


- Increase to $E = 30.02$, where a period-8 viscous detonation is realized.
- Study viscous WENO5M vs. generic 6th order central differencing.
- Results are essentially identical.
- The values of the detonation pressures match minus a time-shift which orginates at the initialization.

WENO5M vs. Central Differencing: Viscous Case



Effect of Diminshing Viscosity $(E = 27.64)$



- 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.

Conclusions

- When physical diffusion is captured with an appropriately fine grid, a central difference of advective terms works as well as a WENO method in capturing the detonation dynamics.
- Dynamics of one-dimensional detonations are influenced significantly by mass, momentum, energy diffusion in the region of instability.
- In general, the effect of diffusion is stabilizing.
- Bifurcation and transition to chaos show similarities to the logistic map.

Conclusions-Continued

- For physically motivated reaction and diffusion length scales not unlike those for H_2-air detonations, the addition of diffusion delays the onset of instability.
- As physical diffusion is reduced, the behavior of the system tends towards the inviscid limit.
- If the dynamics of marginally stable or unstable detonations are to be captured, physical diffusion needs to be included and dominate numerical diffusion or an LES filter.
- Results will likely extend to detailed kinetic systems.
- Detonation cell pattern formation will also likely be influenced by the magnitude of the physical diffusion.