The Dynamics of Unsteady Detonation with Diffusion

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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 and turbulence modeling which filter small scale physical dynamics?

Introduction

- A common practice is to model detonations as inviscid; the stability and non-linear dynamics are well understood for one-dimensional, one-step kinetics (Bourlioux *et. al.*, *SIAM JAM*, 1991; Kasimov & Stewart, *Phys. Fluids*, 2004; Henrick *et. al.*, J. Comp. Phys., 2006).
- It is often argued that viscous forces & diffusion are small effects which do not affect detonation dynamics.
- However, numerical viscosity plays the role of physical viscosity in a way that is grid-dependent.

Introduction-Continued

- An alternative approach is to use the reactive Navier-Stokes equations.
  - Singh *et. al.* (*CTM*, 2001) studied NS with detailed kinetics and a wavelet method capturing all the fine length scales, with finite viscous shock thickness.
  - Powers & Paolucci (*AIAA J*, 2005) studied the reaction length scales of H_2-O_2 detonations and found the finest length scales on the order of sub-microns to microns.

Introduction-Continued

- Let us examine a simplier version which links one-step kinetics loosely to detailed kinetics.
  - Fix reaction length, $L_{1/2}$, to $10^{-6}\ m$, which is similar to finest H_2-O_2 length scale.
  - Fix the diffusion length, L_μ, to $10^{-7}\ m$.
  - have mass, momentum, and energy diffuse at the same rate
- All other parameters identical to widely studied classical inviscid one-step model

One-Dimensional Unsteady Compressible Reactive Navier-Stokes Equations

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

Equations were transformed to a moving reference frame.

Constitutive Relations

$$E = e + \frac{u^2}{2},$$

$$p = \rho R T,$$

$$e = c_v T - q Y_B = \frac{p}{\rho\,(\gamma - 1)} - q Y_B,$$

$$r = H(p - p_s) a\,(1 - Y_B)\, e^{-\frac{E_a}{p/\rho}},$$

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

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

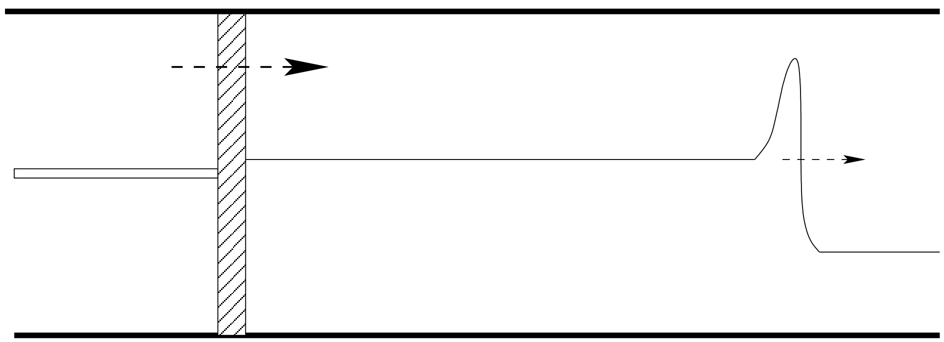
$$j^q = -k \frac{\partial T}{\partial x} + \rho \mathcal{D} q \frac{\partial Y_B}{\partial x}.$$

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 $\rho_o = 1\,\frac{kg}{m^3}$, $Le = Sc = Pr = 1.$

Numerical Method

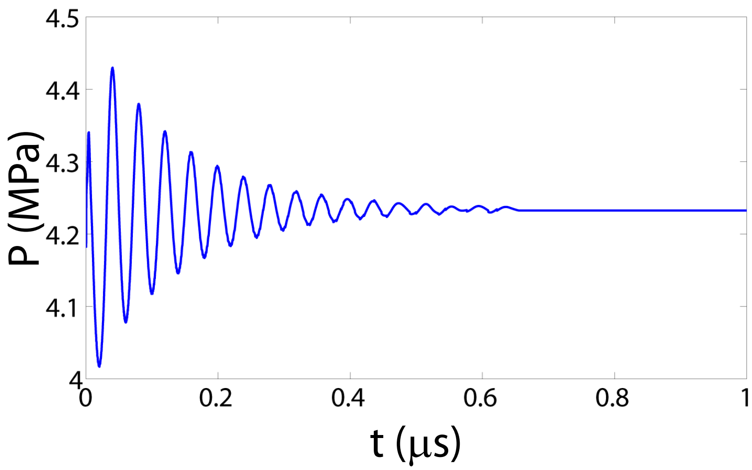
- Finite difference, uniform grid $\left(\Delta x = 2.50 \times 10^{-8} m, N = 8001, L = 0.2\, mm\right)$.
- Computation time = 192 hours for $10\ \mu s$ on an AMD $2.4\, GHz$ with $512\, kB$ cache.
- Advective terms were calculated using a combination of fifth order WENO and Lax-Friedrichs.
- Sixth order central differences were used for the diffusive terms.
- Temporal integration was accomplished using a third order Runge-Kutta scheme.
- Method of Manufactured Solutions confirms convergence at 5th & 3rd order in space and time.

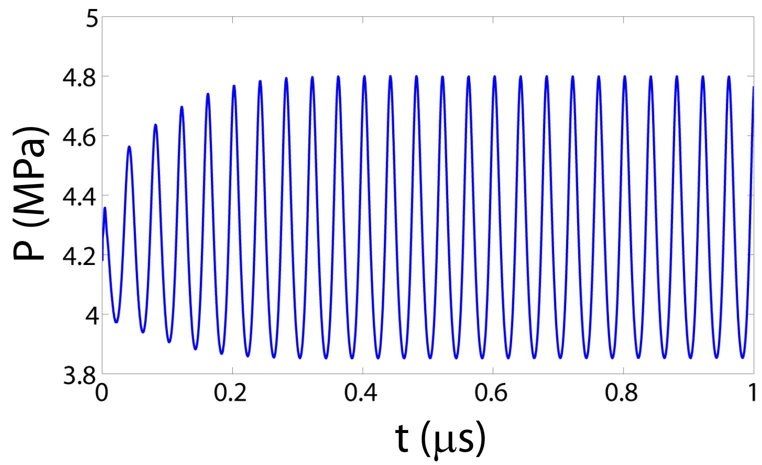
Method



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

Results

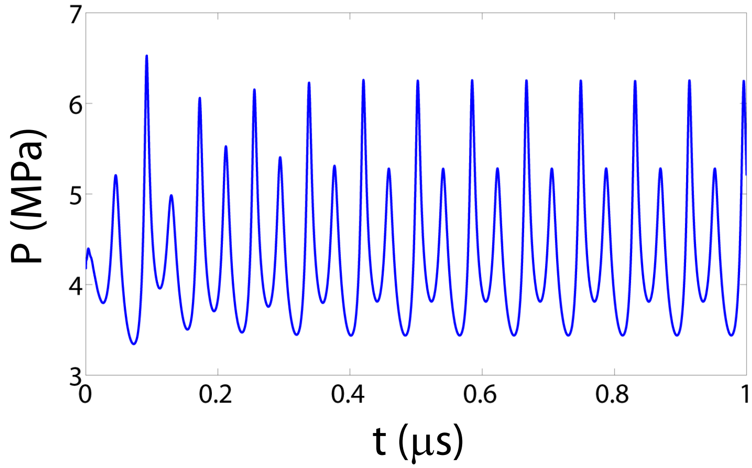


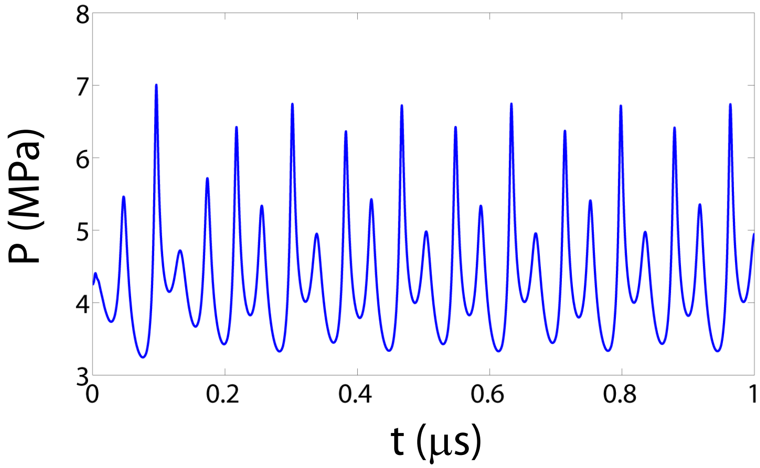


E_a=26.6469

E_a=27.6339

Period Doubling Phenomena

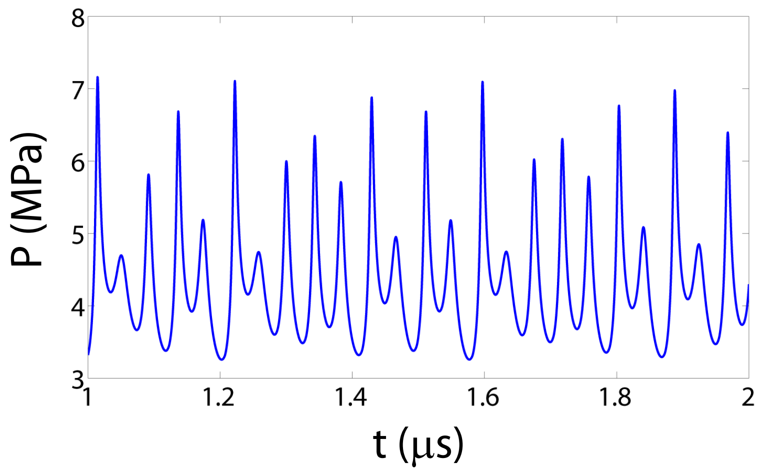


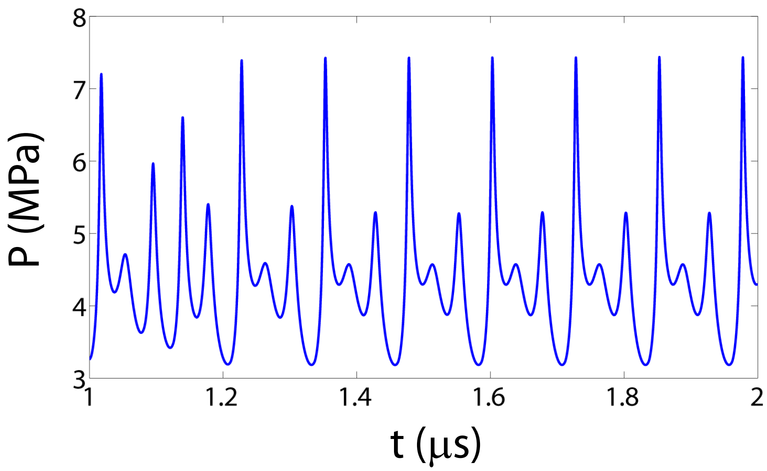


E_a=29.6077

E_a=30.0025

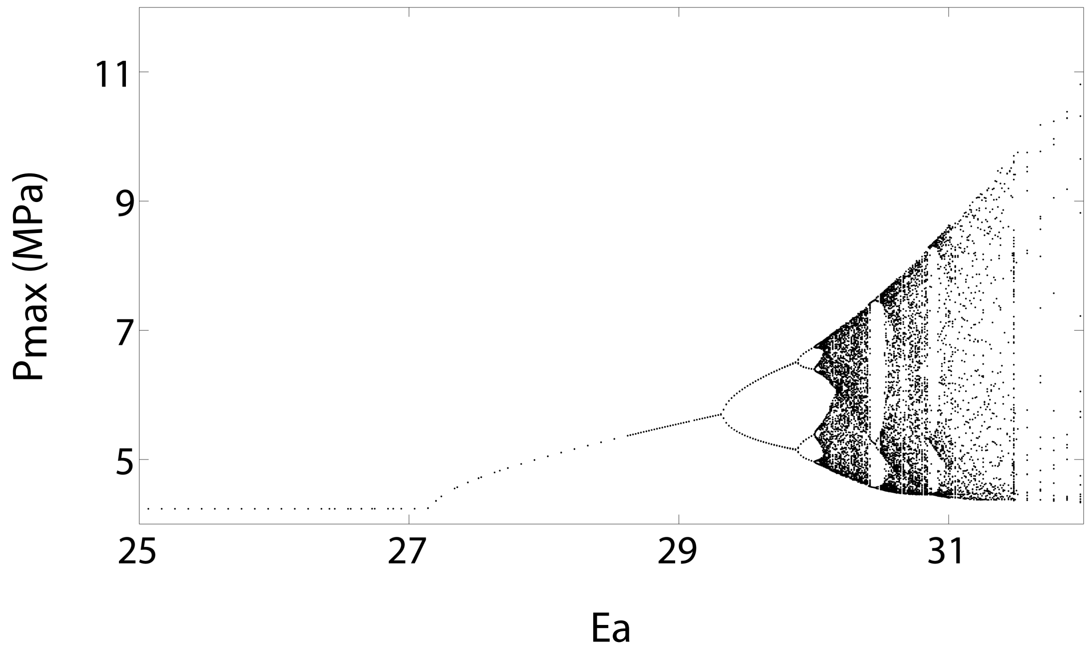
Chaos & Period 3





$E_a=30.2985$ $E_a=30.4268$

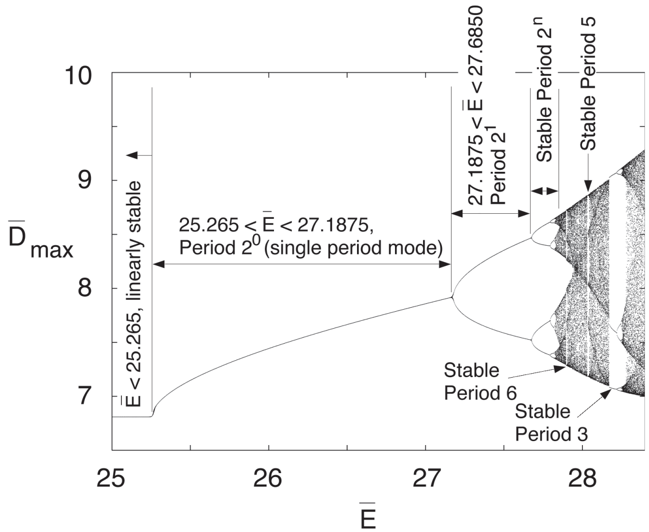
Bifurication Diagram



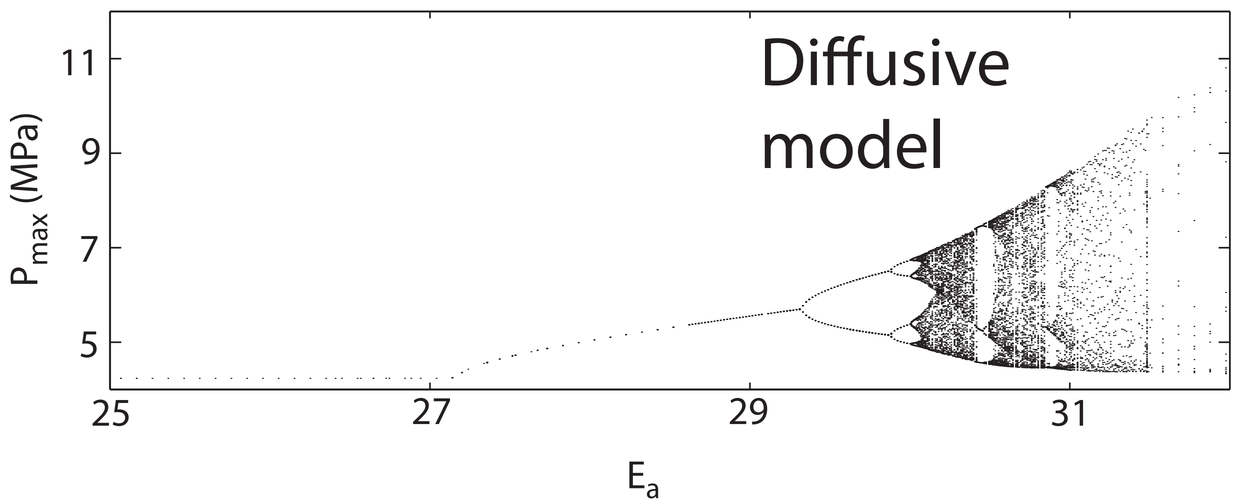
Feigenbaum's constant,

$$\delta = \frac{E_{a_3} - E_{a_4}}{E_{a_4} - E_{a_5}} = \frac{29.8840 - 30.0074}{30.0074 - 30.0339} = 4.656$$

Comparsion with Inviscid

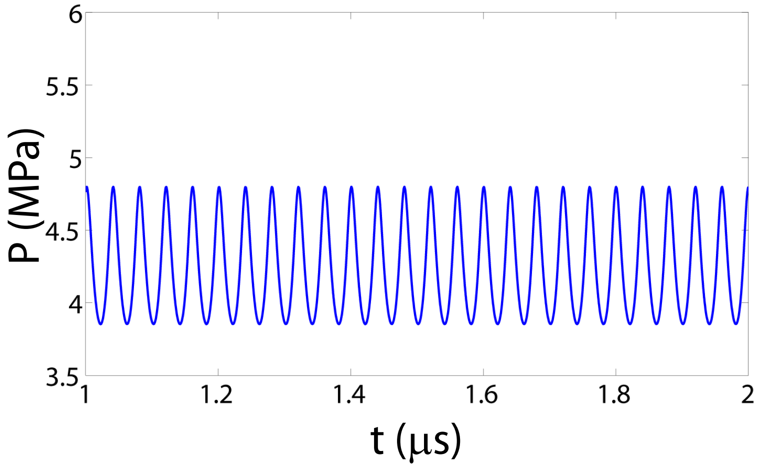


Inviscid model with shock fitting algorithm

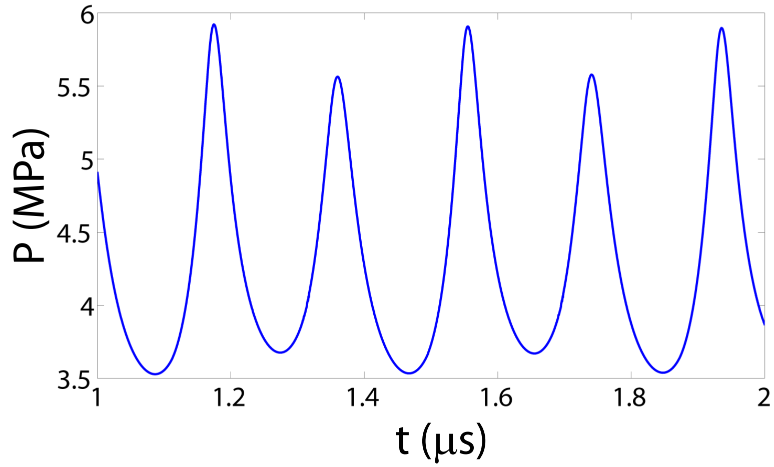


Diffusive model

Effect of Diminshed Viscosity ($E_a = 27.6339$)



$L_{1/2}/L_\mu = 10$



$L_{1/2}/L_\mu = 50$

The amplitude increases, the frequency decreases, and period 2 is realized instead of period 1.

Conclusions

- Dynamics of one-dimensional detonations are influenced significantly by diffusion in the region of instability.
- In general, the effect of diffusion is stabilizing, but it can also be destabilizing.
- In order to capture the dynamics correctly, physical viscosity must dominate numerical viscosity.
- Results will likely carry forward to detailed kinetic systems.
- Likely that detonation cell pattern formation will be influenced by the magnitude of the physical diffusion (Powers, *JPP*, 2006).