Stability of Flame-Shock Coupling in Detonation Waves: 1D Dynamics

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1 Introduction

The study of detonation waves dates back to the late 19th century, where Chapman [1] and Jouguet [2] modeled detonations as a shock wave supported by the heat release of the combustible material in an infinitely thin zone, where all chemistry and diffusive transport takes place. Later Zel'dovich [3], von Neumann [4], and Doring [5] independently represented the detonation as a confluence of a shock wave moving at a detonation velocity, D, followed by a chemical reaction zone of finite length; this came to be known as the ZND model for a detonation wave. While the true structure of detonation waves inevitably calls for multi-dimensional effects, the simple 1D structure still provides a rich spectrum of dynamical features which are worthy of detailed exploration. This is especially important for the study of deflagration to detonation transitions [6] and sustained oscillating or galloping detonations [7, 8]. For a spark-induced detonation, as the detonation decays towards the self-sustaining Chapman-Jouguet mode from an over-driven mode, one obtains a sequence of physical oscillations between the flame and shock front. The numerical analysis of this effect has been explored by Cambier [9] using highly-resolved numerical simulations, albeit with only a 2nd-order shock capturing scheme. In the present study, we utilize high-order spatially accurate method in order to achieve grid convergence, reduce or eliminate numerical diffusion effects and provide detailed analysis of the non-linear dynamics involved in resolving detonations with complex reaction kinetics.

2 Numerical Methodology

2.1 Governing Equation

The governing equations used to simulate the inviscid, one-dimensional propagation of a detonation wave using a multi-step, reversible reaction mechanism are shown below:

$$\mathbf{Q}_t + \mathbf{F}(\mathbf{Q})_x = \mathbf{S}(\mathbf{Q}) \tag{1}$$

where the vectors represented by Q, F, and S are, respectively,

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$$\mathbf{Q} = \begin{pmatrix} \rho_s \\ \rho u \\ \hat{E} \end{pmatrix}, \mathbf{F} = \begin{pmatrix} \rho_s u \\ \rho u^2 + P \\ (\hat{E} + P)u \end{pmatrix}, \mathbf{S} = \begin{pmatrix} \omega_s \\ 0 \\ \sum_s \omega_s e_{0s} \end{pmatrix} \tag{2}$$

where the total mixture density $\rho = \sum_s \rho_s$, and the total energy $\hat{E}$ may be written

$$\hat{E} = \int c_p(T) dT + \frac{1}{2}\rho u^2 \tag{3}$$

In the governing equation, Eq. (2), ρ_s represents the density of species s, ω_s represents the net species production rate of the s^{th} species, and e_{0s} represents the formation energy of the s^{th} species. P and u represent pressure and velocity, respectively.

2.2 Numerical Scheme and Chemical Reaction Mechanism

In the present study, a fifth order accurate Monotonicity Preserving Scheme(MP5) as formulated by Suresh and Huynh [10] is principally used for high order interpolation of a system of governing equations. The MP schemes form a class of high order accurate, shock-capturing numerical algorithms especially equipped for solving non-linear hyperbolic systems of conservation law equations. MP has high accuracy (5^{th} order) in smooth regions of flow-field, while reducing to 1^{st} order near discontinuities in the flow, which is a condition for resolving discontinuities without introducing spurious oscillations. This makes MP schemes well suited for resolving flow-fields where shocks and flame fronts are present. The MP scheme interpolates the value of the conserved variables at the cell interface. The interface flux is then solved utilizing the Roe Flux (RF) building block with the Harten, Lax, van Leer, and Einfeldt [11] entropy fix applied to the eigenvalues. The RF scheme is slightly more computationally expensive than one of its popular variants, Local Lax Friedrich(LLF), but the RF scheme is less dissipative, making it optimal for studying stability and resolving high frequency wave structures. A third order Total Variation Diminishing(TVD) Runge-Kutta time integration scheme is used in conjunction with MP5. Since complex chemical reaction mechanisms are simulated, operator splitting is implemented to facilitate the concurrent implementation of point-implicit backwards Euler kinetics solver with the MP scheme.

As in [9], the chemical kinetics of a diluted hydrogen-oxygen mixture are solved. The chemistry includes eight reacting species, H_2, O_2, H, O, OH, HO_2, H_2O_2, H_2O, and the non-reacting diluent N_2. Thirty eight elementary reactions are used in this mechanism and the backward rates are computed from equilibrium constants.

3 Detonation Phenomena

Direct initiation of the detonation is obtained in a chamber filled with a stoichiometric mixture of H_2 and air (temperature 300K and pressure 1 atm) by setting a region adjacent to an end-wall of the simulated shock tube at high pressure (40 atm) and temperature (1500K), as a simulated spark. Requirements to achieve detonation ignition with the MP5 scheme include sufficient spatial resolution (with grid cell size Δx = 50 μm and a sufficiently distributed simulated spark of length 0.25 to 0.5 cm). Figure 1(a) illustrates the pressure contours of a spark ignited mixture which does not achieve detonation, while Figure 1(b) illustrates contours of the same mixture and grid resolution with a higher spark pressure that achieves detonation.

For successful detonation, at time $t = 0^+$, a shock propagates into the unburned medium, which is rapidly heated and ignites after an induction time delay. The induction time may be characterized by an induction length, ℓ, in the reference frame of the shock. The flame is initially strongly coupled to the shock ($\ell \rightarrow 0$) and the wave is over-driven, i.e., its speed exceeds that of the Chapman-Jouget (CJ) detonation. As the degree of overdrive decays and the detonation approaches the CJ limit, instabilities begin to appear. These fluctuations in key properties (e.g. species concentration, temperature, and pressure) of the fluid at the flame are described by Oran and Boris [12] as 'hot spots'. In the present study, we have found that these 'hot spots' contribute to an initial stage of the flame dynamics.

Earlier findings [9] as well as recent studies [13] have shown that a detonation at the CJ limit has two distinct instability modes. The first is a high frequency mode, which marks the transition from a 'stable' CJ detonation. In this regime, the induction length is very small ($\ell << \ell_{CJ}$), and acoustic waves generated by the perturbed chemistry are rapidly transmitted to the shock. Because there is a very limited amount of fluid that can participate in the fluctuation of the heat release, only low-amplitude perturbations of the CJ peak pressure appear. As these acoustic waves reach the leading shock and strengthen it, their frequency can be measured as that of the fluctuations of the peak pressure. Eventually the average induction length continues to increase and a second mode can be seen, which directly couples the flame speed with the shock, resulting in fluctuations with lower frequency but much higher amplitude.

The present spark-ignited detonations utilizing high order schemes demonstrate these different modes. Figure 2 illustrates the peak pressure of a spark-ignited detonation with two different grid sizes. At a time of the order of $30\mu s$, there appears to be a transition into a high frequency mode, shown in detail in Figure 3, after which the detonation transitions into the low frequency, high amplitude mode, shown in more detail in Figure 4. There are clearly differences in the specific dynamical features of these instabilities, e.g., in the time of initiation of the high frequency behavior and in the temporal waveforms of the instabilities. Yet fast Fourier transform analysis indicates that dominant high and low frequencies for the instabilities are nearly the same, generally independent of grid size, when Δx is smaller than about 10 μm. It is clear that the location and approach to the onset of the instability also may not be exactly reproducible, i.e., they may have a very high sensitivity to the past history of the wave formation. This is characteristic of non-linear systems at the onset of chaos, which brings the interesting question of whether a truly chaotic mode can be observed computationally. Further studies will examine these sensitivities.

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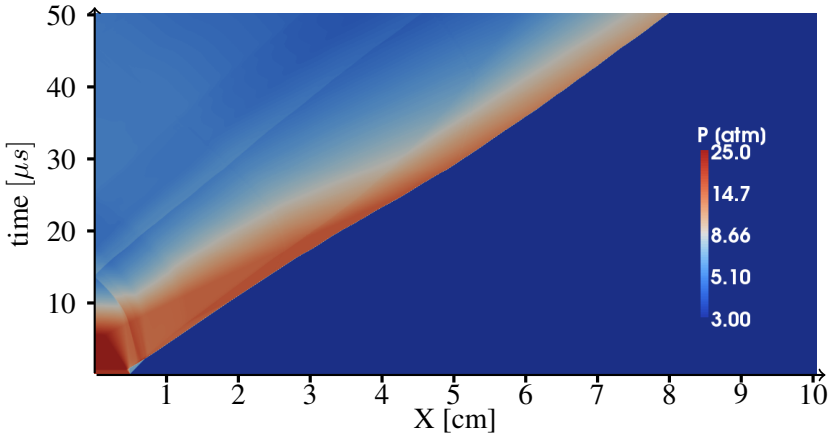
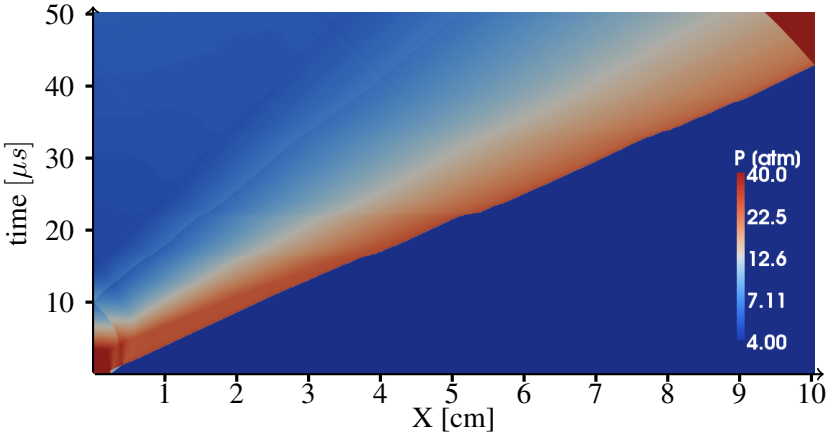
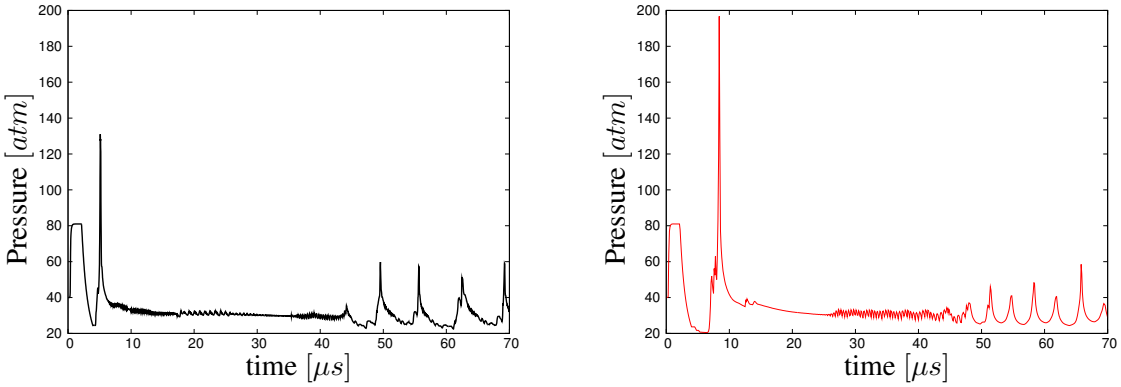


(a) $P_{spark} = 20atm$ with $0.25cm$ spark length where detonation is not achieved



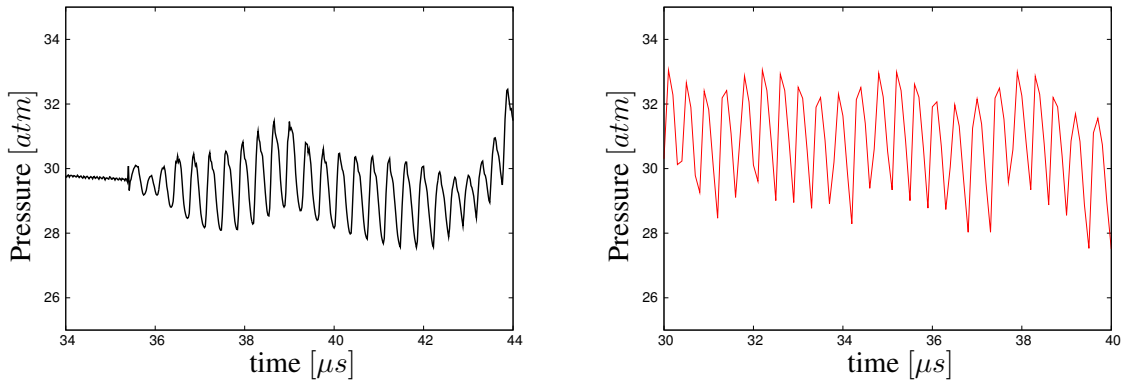
(b) $P_{spark} = 50atm$ with $0.5cm$ spark length where detonation is achieved

Figure 1: Pressure contour of a spark ignited H_2-Air mixture with $\Delta x = 50\mu m$.



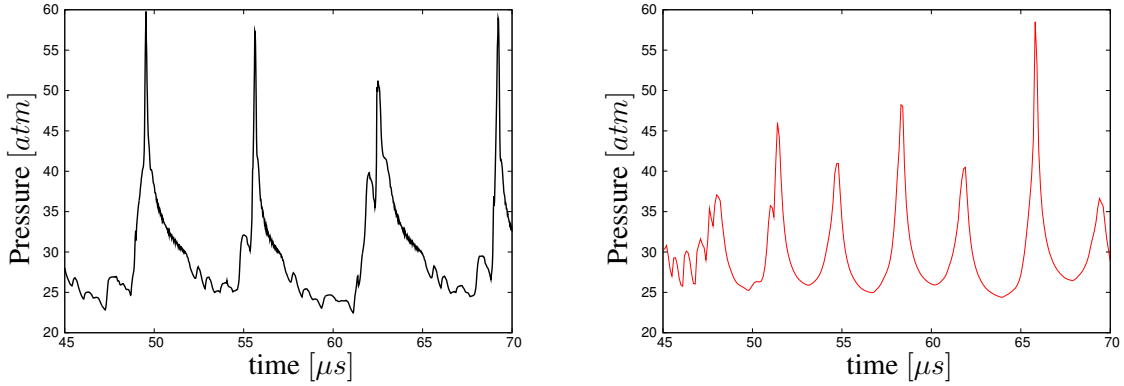
(a) $\Delta x = 12.5\ \mu m$ (b) $\Delta x = 2.5\ \mu m$

Figure 2: Peak pressure time history of a spark-ignited H_2-air mixture simulated with two different grid cell sizes Δx.



(a) $\Delta x = 12.5\ \mu m$ (b) $\Delta x = 2.5\ \mu m$

Figure 3: High frequency portion of peak pressure time history as in Fig. 2, simulated with two different grid cell sizes Δx.



(a) $\Delta x = 12.5\ \mu m$ (b) $\Delta x = 2.5\ \mu m$

Figure 4: High amplitude portion of peak pressure time history as in Fig. 2, simulated with two different grid cell sizes Δx.