The Influence of High-Frequency Instabilities on the Direct Initiation of Two-Dimensional Gaseous Detonations

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1 Introduction

In general, experiments in direct blast initiation of gaseous detonations show that the onset of detonation is represented by a rapid development of cellular structure to a fine multi-headed overdriven detonation which subsequently decays to the Chapman-Jouguet (CJ) detonation [1]. It is long suggested that the key mechanism of initiation is related to the ability of instabilities to develop cells in the shock-reaction zone complex during the blast wave decay, or to form the localized hot spots in the reaction zone. The effect of instabilities on the problem of direct initiation of one-dimensional (1-D) detonation has been previously studied by Mazheri [2] and later by Ng & Lee [3]. These studies show that by imposing different disturbances or hydrodynamic fluctuation to induce instability (either by introducing a density or chemical fluctuation), these local disturbances can get amplified and trigger the onset of detonation. A similar problem has also been studied by Chue et al. [4] where a density fluctuation in a sinusoidal form is used to trigger the transition from a 1-D quasi-steady deflagration to a pulsating detonation. Their study shows that the acceleration phase leading to the onset of detonation is dependent on the frequency of the applied, sinusoidal density perturbation. The applied periodic temperature perturbations help to stimulate transition and there exists an optimal frequency, of the order of the reaction time of the final detonation, that most facilitates transition.

More recently, the effect of cellular instability on the blast initiation of two-dimensional, weakly unstable detonations was investigated by Radulescu et al. [5]. In their two-dimensional (2-D) simulations using the reactive Euler equations with a single-step Arrhenius kinetic model, a perturbation is added in the distribution of the energy source to trigger a cellular front on the decaying reactive blast wave. In contrast to the 1-D results by Mazaheri [2] and Ng & Lee [3], their study shows that it is more difficult to initiate detonations in the presence of multi-dimensional perturbations and cellular instabilities. However, it is important to note that the wavelength of the perturbation used in their study is relatively large, corresponding to the natural cell size in the system. Such large perturbations may not reflect the reality where the direct initiation generally originates locally from very fine cells and that the strong frequency-selective nature of the formation of the self-propagating detonation may be a key parameter influencing the initiation process, as shown by Chue et al. [4].

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Furthermore, only one channel width with dimension of half of a cell size is studied and this may also have a significant effect on the direct initiation process with flow instabilities.

In this study, we focus on the effect of perturbation frequency and the channel width on the direct initiation of two-dimensional cellular detonations. High resolution simulations of a weakly unstable detonation are performed with the aid of GPU computing. We look at the effect of the channel size and the perturbation wavelength to trigger the fast growth of the instability within the reaction zone. The range of perturbation wavelengths extends down the scale of the half-reaction length. Following Radulescu et al. [5] we compare the critical source energies required for the establishment of 1-D and 2-D self-sustained cellular detonations with/without the perturbation.

2 Computational details

Numerical simulations of a cellular detonation are performed using the reactive Euler equations with the one-step Arrhenius kinetic model. The equations are non-dimensionalized using the unburned gas properties and the half reaction length $L_{1/2}$ (where half of the reactant is consumed) as the reference length scale, see [6]. The governing equations are discretized on a Cartesian uniform grid and solved with the MUSCL-Hancock scheme with first-order dimensional splitting. A hybrid HLLC-HLLE approximate solver is used for the Riemann problem [7]. A CFL number of 0.80 is considered for the simulation. To reduce the simulation runtime, the computation is performed using Graphic Processing Units (GPU). The numerical code is implemented using the CUDA programming language [8] and is structured to run on a NVIDIA Tesla C2075 GPU. This CUDA-enabled GPU device has 14 streaming multiprocessors or equivalently 448 CUDA cores with 6GB global memory. For the computation with the present CUDA algorithm, the solution for each cell is performed by a single thread, with threads being logically grouped into blocks of 64 threads which have capability for inter-thread communication. By executing multiple blocks at the same time, the GPU is able to "swap" between blocks in order to hide memory latency. With compute capability 2.0, concurrently 512 resident threads can be executed in parallel per streaming multiprocessor on this GPU [9]. Unless specified, a high grid resolution of 128 points per ZND half reaction zone length $L_{1/2}$ is used for the simulations. Indeed, simulations with lower resolutions were also performed to look at the "convergence" of the numerical results. For this chosen grid resolution, the simulation took about one day of runtime.

For comparison, we used the same chemical parameters from Radulescu et al. [5]. These are: γ = 1.2, heat release Q = 50 and activation energy E_a = 27 typical of weakly unstable cellular detonations. The initial conditions, as used in [5], consist of a thin region of high pressure gas (with density equal to the unburned gas) placed at the left wall. The thickness Δ of this energy source is equal to the half reaction length of the steady wave. The energy per surface area of the source is hence given by the internal energy of the high-pressure gas. Using the unburned gas properties for non-dimensionalization and the half reaction length $L_{1/2}$ as the reference length scale, the initiation energy can be expressed as: $E_s = p/D_{CJ}^{\ 2}(\gamma\text{-}1)$. Only one type of perturbation is studied in this work to generate instabilities. A sinusoidal perturbation with amplitude a is introduced on the surface of the high energy slab in the y-direction. Different values of wavelength, Ω, are chosen to modulate different size of instabilities while the average energy per surface area of the total source energy E_s is kept constant.

3 Result and discussion

Figure 1 first shows temperature contour plots illustrating the wave evolution for the case with channel width w = 10, amplitude a = 1.0 and wavelength Ω = 20 of the perturbation, as used similarly in [5]. It is worth noting again that the wavelength of the applied perturbation corresponds to the natural cell size in the system. According to [5], the critical energy E_s required for initiation of a 1-D detonation is bracketed between 27 and 27.5, and the energy required for the establishment of a detonation from a perturbed blast wave resulted from the imposed disturbance is between 35-40. In agreement with [5],

Fig. 1 corresponding to the result with E_s = 30 indicates a failure to successfully initiate a detonation with the perturbed energy source with large wavelength and amplitude. For this case, the temperature contours show large unburned gas pockets resulting from the cellular instability induced by the original perturbation. These unburned regions further cause the reaction zone to decouple from the decaying blast and no onset of detonation occurs.

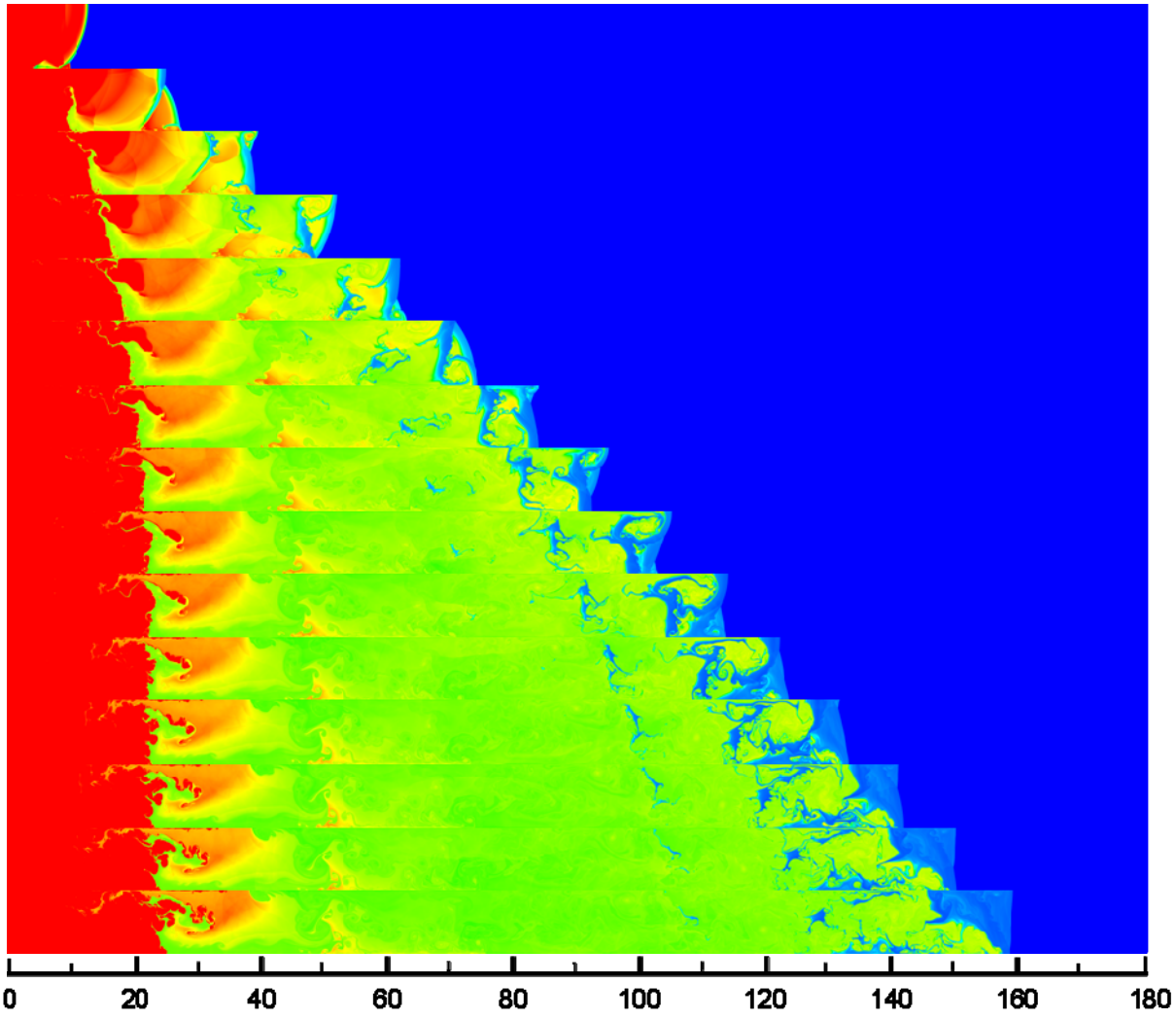

Figure 1. Temperature contours showing the failure of initiation for E_s = 30, a = 1.0 and Ω = 20.

To investigate the effect of perturbation frequency on the initiation of detonation, Fig. 2 shows the temperature field evolution for a case with a much smaller perturbation wavelength of the order of the reaction zone length scale (Ω = 1.25), and a relatively smaller amplitude a = 0.1. For this computational case, it is found that the critical energy required to stimulate detonation initiation is very close to the value for the 1-D case. With E_s = 27 used here, a 1-D detonation fails to initiate [5] while in the perturbed 2-D case the detonation can be established. Hence, it appears that the formation of detonation waves is strongly dependent on the frequency of the flow perturbations exciting it. Smaller, cold pockets can be seen initially possibly due to the fragmentation caused by the high frequency fluctuation of the imposed perturbation. The high frequency fluctuations appear to prevent the wave from decaying rapidly and stimulate the onset of the detonation.

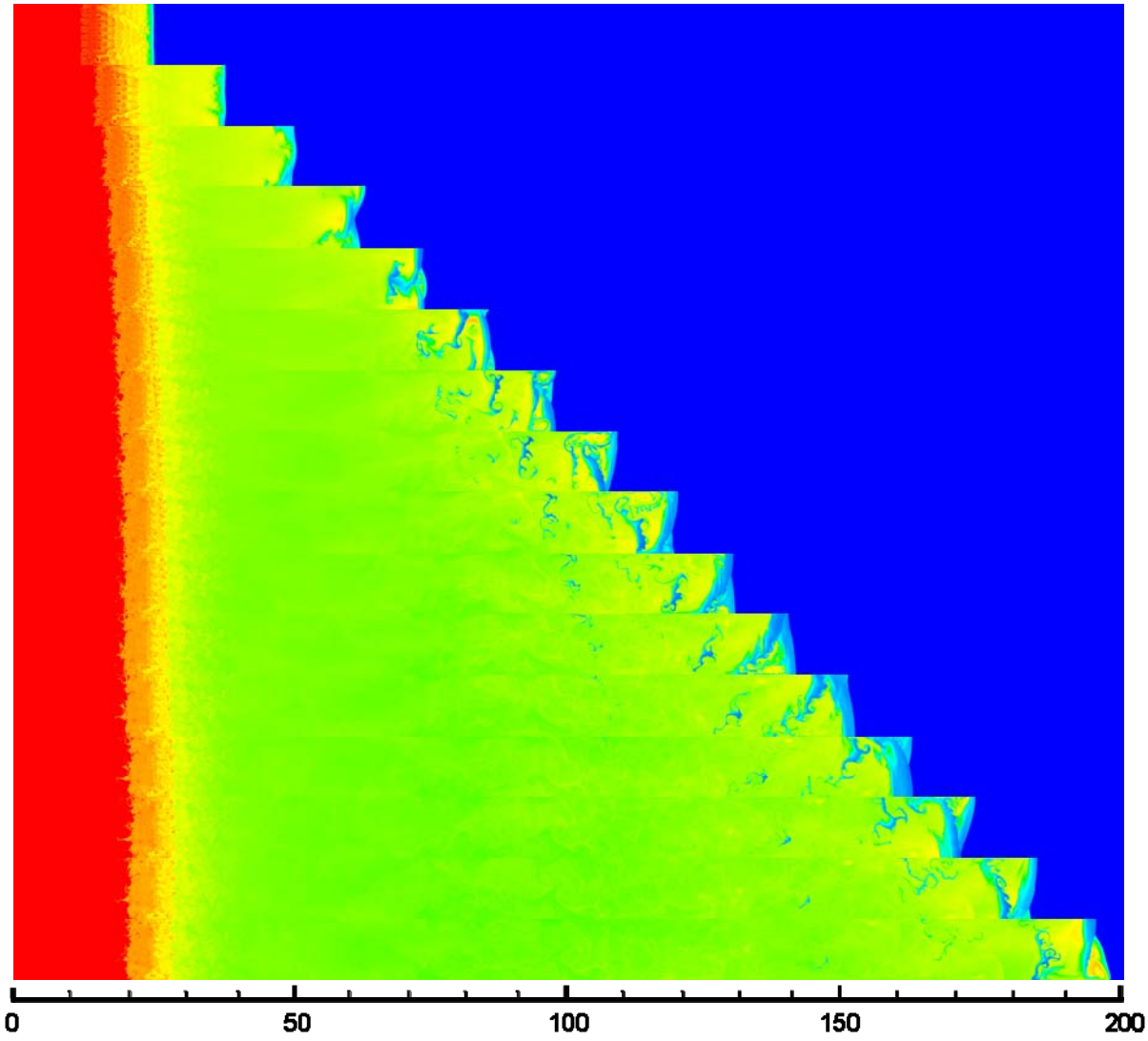

Figure 2. Temperature contours showing the successful initiation for E_s = 27, a = 0.1 and Ω = 1.25.

For the results shown in Figs. 1 and 2 as well as those reported in [5], only one channel width w is considered which corresponds to half of the natural cell size (λ = 20). In such cases, the boundary can contribute primarily to the cause of initiation failure and the influence of the imposed perturbation on the development of the cellular instabilities cannot be fully understood. In Fig. 3, the result for the case of w = 20, with high frequency and small amplitude perturbation (a = 0.1 and Ω = 1.25) is presented. The initiation energy is E_s = 26 distinctly below the 1-D limit and a successful initiation is observed in this case.

3.1 Implication on the initiation Mechanism

There remains a controversial debate as to whether cellular instabilities play a role in enhancing the initiation or detonability of gaseous detonations. A number of studies attempt to answer this fundamental question using high-resolution numerical simulations. Unlike the work carried out by Radulescu et al. [5], the present study performs a parametric study with different amplitudes and wavelengths of the perturbation, and shows that the frequency of the perturbation plays an important role in either facilitating or suppressing the initiation. Evidently, from experiments, detonation

initiation often originates from local hot spots where instabilities manifest. The present results indicate a similar, qualitative trend to [4], i.e., that flow perturbations with high frequency seem to be optimal for stimulating the initiation or transition process, and that the modeling of initiation with perturbed wavelengths of the order of the reaction zone length may appear to be more appropriate. As shown in Fig. 3, with such applied instabilities, direct initiation can be favored with less initiation energy compared to the unperturbed case.

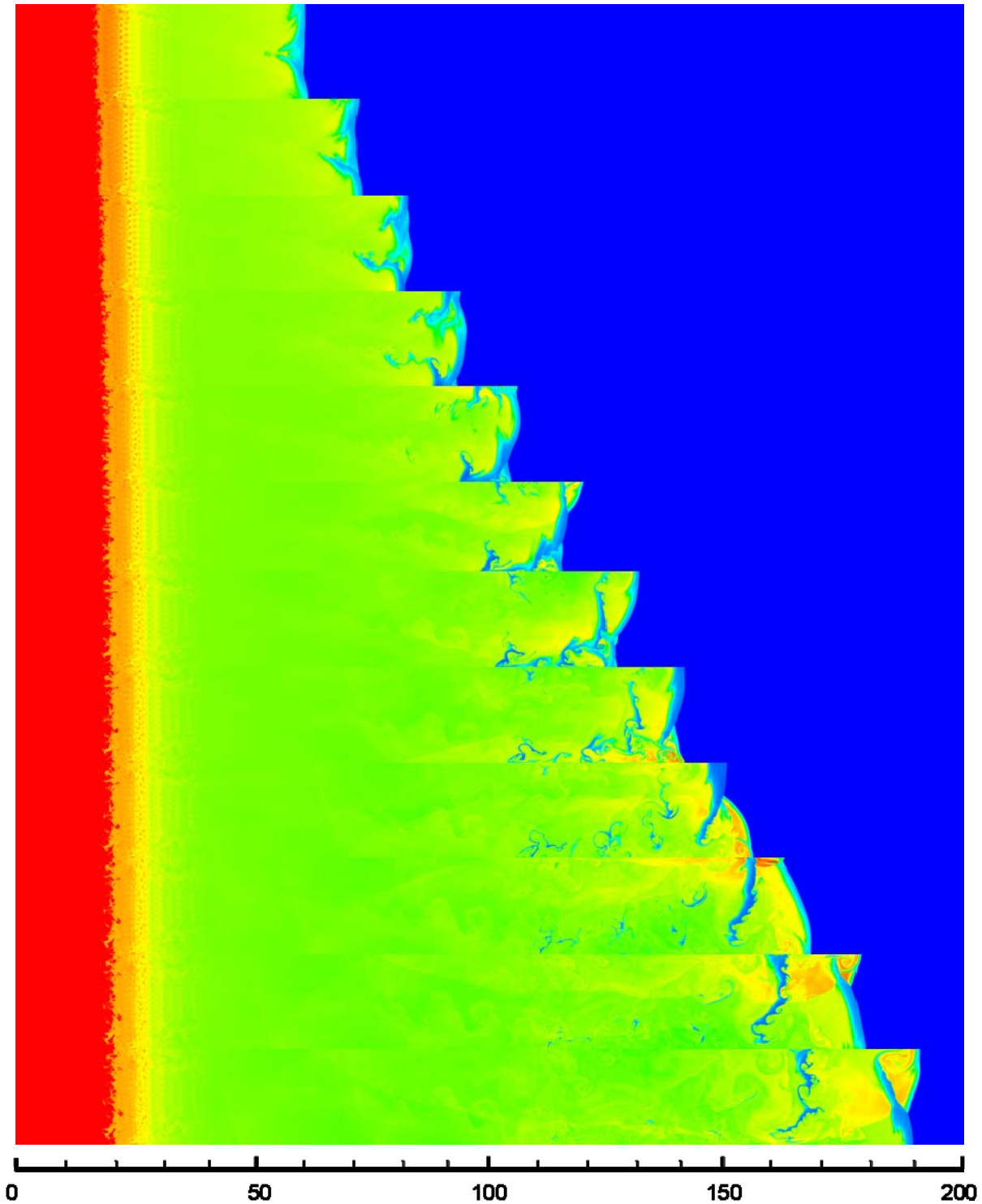

Figure 3. Temperature contours showing the successful initiation for E_s = 26, a = 0.1 and Ω = 1.25 with w = 20.

4 Conclusion

The present results show that the effect of perturbations on the direct initiation of detonations is frequency-selective. Unlike what is found in [5], it appears that fine scale instabilities generated by high frequency, small amplitude perturbations have a prominent role in accelerating the heat-release rate and tend to promote the onset of detonation. We caution that care must be exercised when choosing the channel width to analyze the effect of cellular instabilities as its ability to suppress the spatial development of instabilities may lead to a different conclusion.

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