Eulerian and Lagrangian Statistics in Weakly Two-dimensional Detonations

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1 Introduction

Typical detonations are unstable with a complex three-dimensional lead front and associated transverse waves [1, 2]. The variation in the lead shock strength changes substantially the reaction rates of the shocked gases which in turn affect the lead shock. In spite of the large variation in the lead shock strength, the ideal Zel'dovich–Neumann–Döring (ZND) model [3] predicts accurately the average detonation speed for mixtures well within the detonability limits. In the ideal ZND model the transverse waves are neglected, the flow is considered as inviscid and the shock propagates at the Chapman-Jouguet (CJ) speed in a constant area flow. Despite its earlier success in predicting the detonation speed, the ideal ZND model can not predict accurately the dynamic detonation parameters such as the critical initiation energy, critical tube diameter, or detonation limits.

One of the ultimate goal in detonation research is the development of a simplified model that can accurately predict the dynamic parameters. The model should account for the important dynamic futures involved in the detonation reaction zone at least in a statistical sense. This has been the main motivation of the hydrodynamic thickness approach of cellular detonations [4, 5]. The hydrodynamic approach is built on the existence of a mean sonic surface behind the lead shock separating the flow of the reaction zone structure from the unsteady expansions.

There are two perspectives to consider the dynamics of a fluid flow: Eulerian and Lagrangian. Detonation studies primarily focused on the Eulerian formalism because of its simplicity. The Lagrangian formalism, however, is more appropriate for instance to study the transport and mixing of scalar quantities. To date, very little if any attention has been given to the Lagrangian perspective. The main motivation of this work is to revisit the hydrodynamic thickness approach using a Lagrangian formalism.

2 Numerical experiment

Two dimensional Euler computations were performed employing the MG code [6, 7], which uses a second-order-accurate exact Godunov solver with adaptive mesh refinement [8]. To describe the chemical kinetic rate processes, a two-step chain-branching kinetic was chosen [9]. The thermochemical

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parameters were chosen to represent two mixtures. A mixture of $2H_2$+O_2+12Ar, at an initial pressure of $p_0 = 10$ kPa and an initial temperature of $T_0 = 295$ K, was first considered. For this mixture, the isentropic exponent, the heat release, and the activation energy were set to $\gamma = 1.54$, $Q/RT_0 = 10$, and $E_a/RT_0 = 23.98$, respectively. The reaction order of the two-step chain-branching kinetic was set to 0.5 to have a finite reaction length. A second fictional mixture with a lower isentropic index of $\gamma = 1.17$ was chosen to enhance the jetting and the convection mixing behind the detonation, see [10, 11]. To keep the ratio of induction length to reaction length (Δ_i/Δ_r) and the Mach number the same as in the first mixture, the fictional mixture heat release and activation energy were $Q/RT_0 = 28.23$ and $E_a/RT_0 = 10.61$, respectively. Owing to the weakly unstable nature of the detonation front, the maximum level of mesh refinement was set to 5 yielding a maximum numerical resolution of 16 points per induction length.

Passive massless Lagrangian particles were introduced in the Eulerian mg code. The fluid particles were tracked in time by the numerical integration of the equation of particle motion with the initial particle position (x_0, y_0) at time $t = 0$ as the initial condition. The fluid particle velocity was defined to be the Eulerian velocity field evaluated at the instantaneous particle position, accurate to the first-order.

The detonation was initiated using the steady ZND structure. and allowed to propagate up to a distance of $2000\Delta_i$. The computations were then restarted using the fully developed detonation and 14300 particles were introduced in the two-dimensional channel ahead of the detonation front, as sketched in Fig. 1

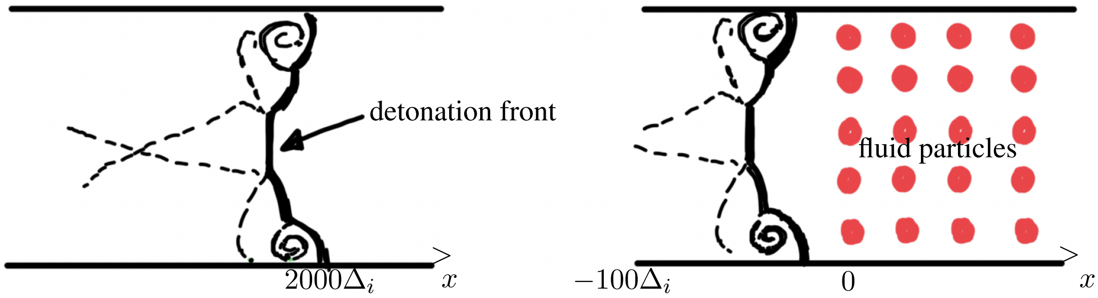

Figure 1: Sketch of the numerical experiment. The detonation were propagating from left to right. Symmetric conditions were imposed in the top and bottom wall. Free boundary conditions were applied at the entrance and the exit of the channel.

3 Eulerian statistics

In this section, we provide a brief overview of the Eulerian statistics, which will be subsequently compared to the Lagrangian statistics. Generally, there are two ways to obtain the Eulerian statistics. In the first approach, the average are conducted in a reference frame attached to the mean detonation speed or to the Chapman-Jouguet (CJ) reference frame. In the second approach, the average are conducted in the instantaneous location of the shock, i.e, in the shock-attached frame. The shock is always located at $x = 0$ in the shock attached-frame while the leading front pulsates around $x = 0$ in the CJ reference frame.

Figure 2 shows the density contour for mixture 2. A Mach bifurcation process occurs upon triple shock reflections. The vortex like structure enhancing the convection mixing behind the detonation are highlighted by the motion of the Lagrangian particles. The two-dimensional quantities obtained from the computations are first averaged in the y-direction to generate 1D quantities depending on the space coordinate x and the time t. The average 1D quantities are then again averaged in time yielding 1D

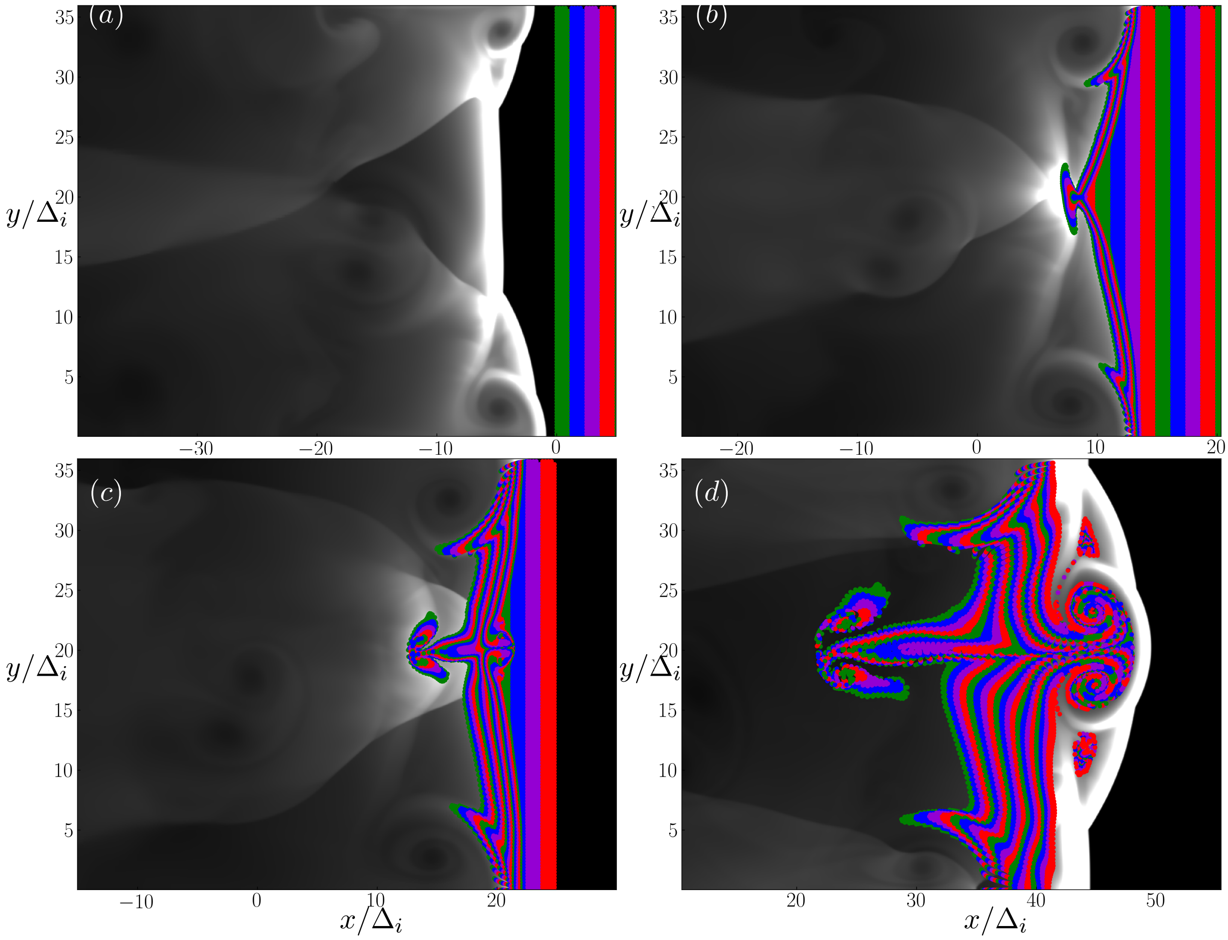

Figure 2: Contour of density for mixture 2 and Lagrangian particle locations. The time sequence evolves from a) to d).

quantities depending only on space coordinate x. Some particles are kept near the shock front while the rest fall behind.

The profiles of pressure, density, reaction progress variable, and Mach number as well as the ZND profiles are shown in Fig. 3. The von Neumann state is, unsurprisingly, largely under predicted by averaging in the CJ frame. The difference is related to the spatial and temporal averaging over the pulsating leading front in the CJ frame. Taking the statistics in the shock-attached frame, the difference with ideal ZND structure is a lot less noticeable. Similar observations were reported by Sow et al. [] in there statistical analysis of pulsating 1D detonations. Furthermore, the hydrodynamic surfaces obtained in the two averaging strategy we conducted in this study are located at approximately $20\Delta_i$. This result is in good accordance with the previous studies [4] which show that the effective sonic surface is located at $20\Delta_i$ for weakly unstable detonations.

4 Lagrangian statistics

For a better comparison between the Lagrangian and the Eulerian statistics, the Lagrangian average is conducted in the shock-attached frame. A visualization (not shown here) of the trajectories of few

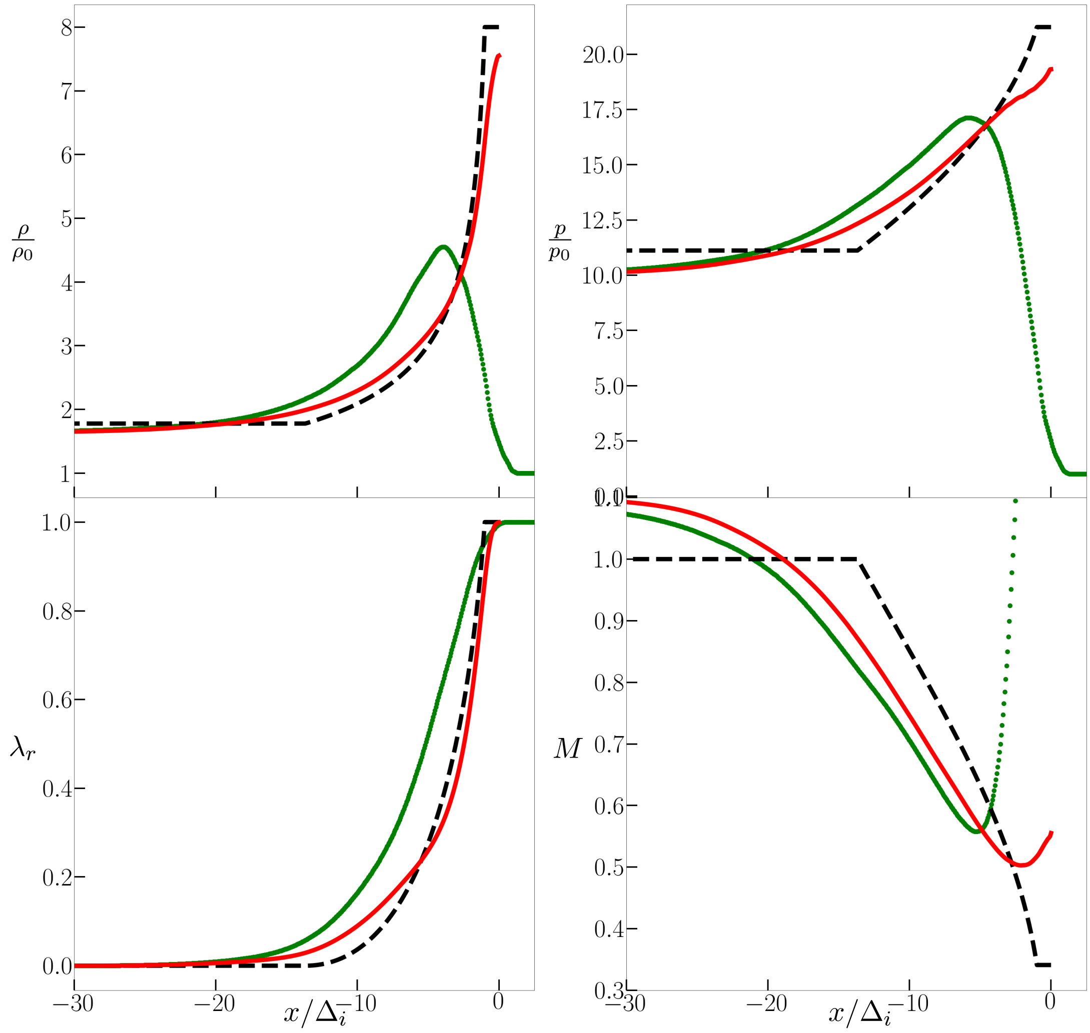

Figure 3: Eulerian averaged profiles of density, pressure, reactant progress variable, and Mach number; The dotted lines are the ZND profiles, the red lines are for the averaged quantities in the shock-attached frame and the green symbols are for the averaged quantities in the CJ frame.

particles selected based on their initial position x_0 and y_0 shows noticeable differences in the path of particles even for particles sitting initially close to each other highlighting the anisotropic nature of the detonation flow.

To conduct the statistical analysis for the Lagrangian particles in the shock-attached frame, the time at which each particle is shocked (t_s) is recorded. The time that elapses since a particle has been shocked ($t - t_s$) is used to place all Lagrangian properties in the shock-attached frame. The lead shock front is always located at $t - t_s = 0$. The 1D average profiles are obtained by averaging a property over the number of particles. The profiles of density, pressure, and reaction progress variable as well as the ZND profiles are shown in Fig.4. A substantial difference can be seen between is Lagrangian an its Eulerian counterpart. For instance, the Lagrangian reaction zone is ends after an elapsed time of 3 while in the Euler structure the reaction ends after an elapsed time of 26.

5 Discussion and future works

We have shown in this paper through quantitative statistical analysis that the hydrodynamic structure can be substantially different if a Lagrangian perspective is used in opposition to the traditional Eulerian perspective. Unlike previous studies pointing out to an average lengthening of the reaction length compared to the ZND structure, the Lagrangian perspective shows a significant shortening of the reaction length. This rise an important questions: where this difference comes from? Is the effective hydrodynamic thickness much sorter than previously expected ? We are planning to further investigate the Lagrangian statistics. We are investigating the influence of the observation time of the particles which can affect the statistics. We will increase considerably the number of Lagrangian particles to evaluate the impact of the population of Lagrangian particles in the statistics. In this study we presented only the results of a weakly unstable mixture. As a perspective, we will study highly unstable mixtures to determine if the observed trend can be generalized to all detonations.

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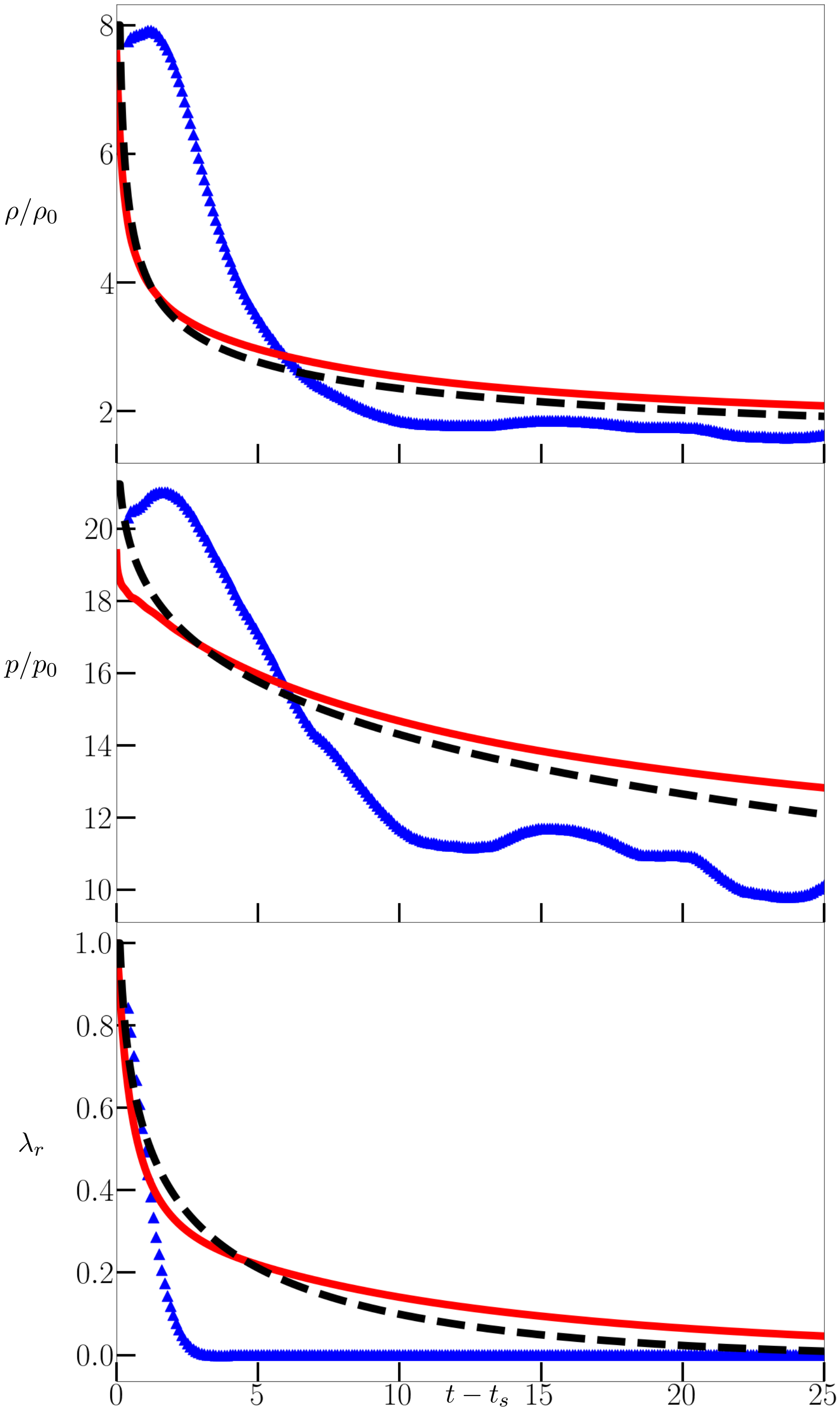

Figure 4: Profiles of density, pressure, and reactant progress variable; The dotted lines are the ZND profiles, the red lines are for the Eulerian averaged quantities in the shock-attached frame and the blue symbols are for the Lagrangian averaged quantities in the shock-attached frame.