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Title: THE EFFECT OF A NON-ZERO SHOCK WIDTH ON WAVE PROPAGATION IN MULTI-DIMENSIONS

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THE EFFECT OF A NON-ZERO SHOCK WIDTH ON WAVE PROPAGATION IN MULTI-DIMENSIONS

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ABSTRACT. It is known that a numerical shock width in one dimension can lead to a localized entropy error when waves interact. In multi-dimensions the wave width, either numerical or physical, can also affect the propagation of the wave, and thus have a global effect on fluid flow. A well known physical example is the diameter effect for detonation waves. This effect is due to reaction zone dynamics; the competition between a source term for the release of chemical energy and a geometric source term due to front curvature. When the reaction zone is underresolved, the effective reaction zone dynamics leads to mesh dependent numerical results. The mesh dependence is due to an artificial numerical curvature effect. An explanation of this effect is given based on the conservation laws. Because of the non-zero wave width, the standard Hugoniot jump conditions must be modified. Correction terms are proportional to the wave width. It follows when the width is proportional to the cell size, as occurs in shock capturing schemes, that the curvature effect is mesh dependent. A similar modification of the jump conditions can be expected whenever there are multiple length scales determining the dissipation which gives rise to the wave width. As a consequence, the wave curve depends on the local front curvature and the divergence of the velocity field in the tangent plane in addition to the usual state variables. In computations, the length scales affecting the wave curve may either be physical or artificial in nature. Artificial length scales lead to numerical errors which may not vanish under mesh refinement.

1. INTRODUCTION

Shock capturing algorithms are widely used to obtain numerical solutions of hyperbolic partial differential equations (PDEs). In these algorithms a shock wave is not truly discontinuous but rather a very rapid change in state over a small number of cells. There are two reasons for the numerical shock width: (i) to control the truncation errors for numerical stability, and (ii) to add the necessary dissipation in order to select out the physical shock waves. The heuristic motivation for shock capturing algorithms is that the state behind a shock wave is determined by the Hugoniot jump conditions and giving a shock a narrow profile causes only a local error that doesn't affect the global solution.

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Though shock capturing algorithms are generally effective, the artificial shock width can lead to non-trivial errors which manifest themselves as incorrect values for the entropy. Only for a steady-state shock wave is the entropy increase determined solely by the Hugoniot jump conditions and independent of the form of the numerical dissipation. A transient, when a shock wave is formed or when a shock profile changes abruptly, gives rise to a localized entropy error. This has been analyzed in one-dimension for shock wave interactions [3]. The same analysis explains many commonly occurring and widely ignored numerical errors such as excess wall heating, shock start-up error, the error when a shock impinges on a material interface, and the error when a shock passes through an abrupt change in cell size

Here we show that for a curved shock the wave width gives rise to correction terms in the Hugoniot jump conditions. As a consequence, there is a curvature effect on propagating shock waves. This is a generalization of the well known diameter effect for detonation waves. The diameter effect has been observed experimentally and in numerical simulations. We will briefly describe the diameter effect in Section 2. Latter sections will use detonation waves as an illustrative example. A qualitatively similar curvature effect occurs for partially and fully dispersed shock waves resulting from relaxation effects described by source terms in hyperbolic PDEs.

Our analysis of a curved shock with non-zero wave width is based on a quasi-steady 1-D approximation. The approximation is developed in Section 3. Assuming the dimensionless product of wave width and front curvature is small, we show that there is a distinguished frame of reference in which the dominant multi-dimensional effects are well approximated by steady nozzle flow, i.e., a flow in a duct with variable cross sectional area. The geometric source term for the nozzle is determined by the front curvature and the divergence of the velocity in the plane tangent to the front.

The quasi-steady 1-D approximation is used to derive modified jump conditions. In Section 4 we show that the leading order correction is proportional to the dimensionless product of wave width and front curvature. As discussed in Section 5, the same analysis applies equally well to conservative difference schemes. Consequently, the numerical shock width can give rise to an artificially large and mesh dependent curvature effect. This is a generic problem with shock capturing algorithms.

2. Diameter Effect for Detonation Waves

An explosive may be modeled by the reactive fluid flow equations [2]. In 1-D, this leads to the Zel'dovich-von Neumann-Doering (ZND) model for a detonation wave. In the ZND model a detonation wave consists of a lead shock followed by a thin reaction zone. It can be viewed as a partially dispersed wave in which chemical equilibrium is established in the reaction zone.

An important property of a detonation is that there exists a self-sustaining detonation wave known as a Chapman-Jouguet (CJ) detonation; the shock heating initiates the chemical reaction and the energy release drives the shock wave. The state behind a CJ detonation wave is sonic relative to the front, and hence the wave is acoustically decoupled from the flow behind. Moreover, a CJ detonation has the minimum wave speed of any steady detonation wave. The CJ detonation speed

can be determined from the equation of state of the detonation products and the Hugoniot jump conditions. It is independent of the reaction rate law.

Rate stick experiments are used to determine the CJ detonation speed. In a rate stick experiment, a cylinder of explosive is detonated at one end. After a distance of run of a few diameters a steady-state is approached and the wave speed is measured. It is found that the detonation speed decreases as the diameter of the explosive cylinder is decreased. This is known as the diameter effect. The diameter effect is related to rarefactions from the side which lead to a curved detonation front. An infinite diameter would correspond to a 1-D planar CJ detonation wave. This gives rise to the question; Why is the detonation speed of a curved wave less than the minimum allowed value for the planar case?

Furthermore, in numerical experiments the magnitude of the diameter effect is mesh dependent. A systematic numerical study varying the cell size was carried out by Donguy & Legrand [1]. The normalized velocity deficit, showing the diameter effect as a function of cell size is plotted in Fig. 1. We note that the numerical effect is qualitatively the same as the physical effect.

With the typical cell size used for a calculation, the curvature effect is quantitatively inaccurate and leads to a significant error when the cylinder diameter is small. As the cell size is decreased and the reaction zone is resolved, rather than captured, the artificial numerical effect decreases compared to the real physical effect. Moreover, as the number of cells in the reaction zone increases, the width of the reaction zone decreases until the value intrinsic to the reaction rate model is reached. The subsequent analysis shows that the artificially large numerical width is the dominant cause of the numerical curvature effect.

Our analysis shows that the curvature effect is not limited to detonation waves. However, the effect stands out in detonation waves. Because of the minimum wave speed, it can be demonstrated with the measurement of a single variable. In addition, the effect is insensitive to boundary conditions because acoustic waves can not catch up with and influence a self-sustaining detonation. Most importantly, the effect has been measured experimentally and can not be accurately computed with shock capturing algorithms.

3. Quasi-Steady 1-D Approximation

Our analysis is based on a long wavelength, low frequency approximation. We assume that (i) the reaction zone width w is much smaller than the principal radii of curvature of the front, and that (ii) the wave speed normal to the front is slowly varying in both position and time. A consequence of these assumptions is that the derivatives of the flow variables tangent to the front are much smaller than those normal to the front. Locally, the tangential flow can be neglected relative to the normal flow. However, the normal directions are not parallel to each other when the front is curved. This effect can not be neglected, but to leading order it can be accounted for with geometric source terms in a quasi one-dimensional model.

For a small areal patch on the detonation front, the streak lines form a flow tube. Let A be the cross sectional area of the flow tube, and x the coordinate along a

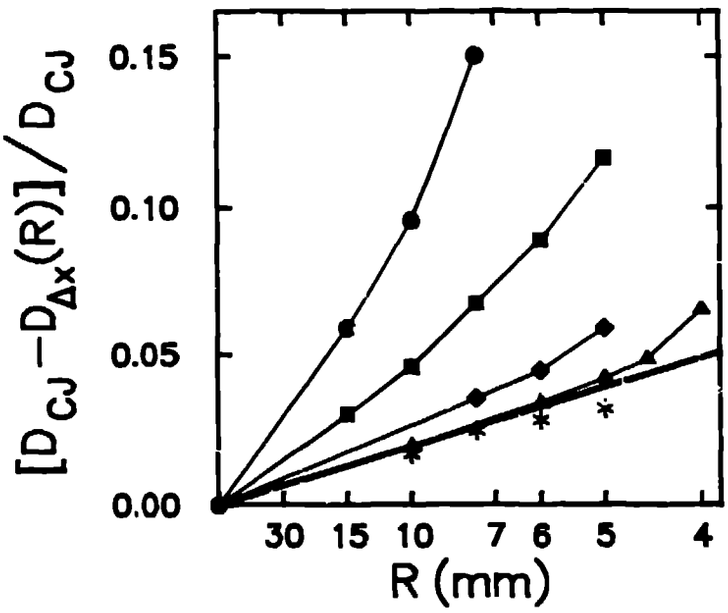

FIGURE 1. Mesh dependence of curvature effect; numerical data from Table I of Ref. [1]. Thick solid line is fit to experimental data. Circle, square, diamond and triangle are calculations with cell size of $\Delta x = 0.5, 0.25, 0.125$ and 0.075 mm respectively. The symbol * corresponds to the extrapolation of the last two points to $\Delta x = 0$ assuming second order convergence.

stream line. Locally, the reaction zone is described by the reactive flow equations in a duct of variable cross sectional area

$$(\rho A)_t + (\rho A u)_x = 0 , \tag{3.1}$$

$$(\rho A u)_t + (\rho A [u^2 + PV])_x = PA_x . \tag{3.2}$$

$$(\rho A \mathcal{E})_t + (\rho A u [\mathcal{E} + PV])_x = -PA_t , \tag{3.3}$$

$$(\rho A \lambda)_t + (\rho A u \lambda)_x = \rho A \mathcal{R} , \tag{3.4}$$

where ρ, u, E and λ are the fluid density, particle velocity along a stream line, specific internal energy (thermal + chemical), and mass fraction of the reaction products ($\lambda = 0$ unburnt, $\lambda = 1$ completely burnt), $V = 1/\rho$ is the specific volume, $\mathcal{E} = \frac{1}{2}u^2 + E$ is the total specific energy, $P(V, E, \lambda)$ is the pressure, and $\mathcal{R}(V, E, \lambda)$ is the specific reaction rate.

It is important to note that the flow tube is not Galilean invariant. There are two special frames in which the equation simplify because to leading order $\partial_t A = 0$: (i) the co-moving frame, and (ii) the normal frame. In these frames the only geometric term that enters the equations is the local divergence of the streak lines,

$\kappa = \lim_{A\to 0}(\partial_x A/A)$. The co-moving frame is not a good choice because $\kappa(x)$ is not *a priori* known.

The angle between a streamline and the local normal to the front depends on the ratio of the tangential and normal velocity components. In our approximation, the tangential component is constant but the normal component varies dramatically through the reaction zone. In 2-D, the shape of the stream tube depends on the reaction zone dynamics unless one chooses the normal frame in which the tangential velocity vanishes in first order. In 3-D there is no frame in which the tangential velocity vanishes over a local region. However, we have shown in Ref. [4] that there is a unique frame in which the residual tangential velocity affects only the shape but not the cross sectional area $A(x)$. Since only the area enters into the quasi 1-D model, this is sufficient for our analysis to apply in 3-D as well.

In the normal frame the velocity ahead of the front is on average normal to the front and has the magnitude u_{ahead} determined by the relation

$$\kappa_f u_{ahead} = \nabla_T \cdot \vec{u} \ , \tag{3.5}$$

where κ_f is the local front curvature and $\nabla_T \cdot \vec{u}$ is the velocity divergence in the tangent plane. Moreover, $\kappa = \kappa_f$ is constant to $O(\kappa_f w)$. In the typical case with solid high explosives, the material ahead of the front is standing still. This happens to correspond to the normal frame.

The time and length scales in the reaction zone are much smaller than the bulk flow. Consequently, we can assume the reaction zone profile varies adiabatically, i.e., rapidly equilibrates to slow changes of the front curvature. To leading order the PDEs reduce to ODEs for the quasi-steady reaction zone profile

$$[\rho(D-u)]_x = \rho u \kappa_f \ , \tag{3.6}$$

$$[\rho(D-u)^2 + P]_x = \rho \cdot (D-u)\, u \kappa_f \ , \tag{3.7}$$

$$[E + PV + \tfrac{1}{2}(D-u)^2]_x = 0 \ , \tag{3.8}$$

$$(u-D)\lambda_x = \mathcal{R} \ , \tag{3.9}$$

where D is the detonation wave speed and x is the distance relative to the front. For these ODEs, κ_f and D are to be treated as parameters determined by the bulk flow.

4. Modified Jump Conditions

The Hugoniot jump conditions are an expression of the conservation laws across a shock wave. When the wave has a width, the jump conditions are obtained by integrating the quasi-steady 1-D equations. To leading order this gives the modified jump conditions

$$\Delta[\rho(D-u)] = \kappa_f w \langle \rho u \rangle \ , \tag{4.1}$$

$$\Delta\left[(\rho(D-u))^2 V + P\right] = \kappa_f w \langle \rho(D-u)u \rangle \ , \tag{4.2}$$

$$\Delta\left[E + PV + \tfrac{1}{2}(D-u)^2\right] = 0 \ , \tag{4.3}$$

where $\Delta[f] = f(x_0) - f(x_1)$ is the change of variable f across the detonation wave, $w = x_0 - x_1$ is the reaction zone width, and

$$\langle f \rangle = \frac{1}{w} \int_{x_1}^{x_0} dx\, f \tag{1.1}$$

is the average value of f in the reaction zone. The averages result from the fact that the source terms are not perfect derivatives.

In contrast to the standard jump conditions, additional information about the reaction zone dynamics is needed for the modified jump conditions. In particular, $\lim_{w \to 0} \langle f \rangle$ does not vanish, nor can it be expressed in terms of the values of f at the end points. Thus, the conservation relations applied to a wave with non-zero width are no longer algebraic conditions.

The modified jump conditions reduce to the standard Hugoniot jump conditions when either the front is planar $\kappa_f = 0$ or the width of the wave is zero $w = 0$. In effect the correction terms express the dynamics of the reaction zone; the competition between the source term for energy release due to the chemical reaction and the geometric source term due to front curvature. We note that the correction terms are not Galilean invariant. The modified jump conditions are valid *only* in the normal frame described in the previous section.

Even though the short length scale of the reaction zone may not be of interest, the reaction zone dynamics does affect the propagation of a detonation wave and hence the flow on the hydrodynamic length scale of interest. Instead of computing a quasi-steady reaction zone, its dynamics can be accounted for in the wave curve; *i.e.*, locus of final states connected to a given initial state. In contrast to a discontinuous shock, the detonation wave curve depends on front curvature and the tangential velocity divergence ahead of the wave as well as the initial state. The curvature effect is a material property described by the wave curve. The diameter effect is merely a special application of the curvature effect to a rate stick experiment

5. Conclusion

To capture shock waves correctly, it is important that numerical algorithms are written in conservation form. Moreover, when the wave profile is not resolved, the assumptions of the quasi-steady 1-D approximation are applicable. Since the modified jump conditions are derived from the conservation laws, they also apply to finite difference algorithms. Hence, there is an artificial curvature effect from the numerical shock width.

The averages in the modified jump conditions are slowly varying functions of three parameters; D, κ_f and $\nabla_T \cdot \vec{u}$. The factor $w\kappa_f$ has a large effect on the magnitude of the correction terms. In shock capturing algorithms, the wave width is several cells and hence proportional to the cell size. Consequently, the numerical curvature effect is mesh dependent.

The mesh dependence of the numerical curvature effect can be reduced with adaptive mesh algorithms. This has the effect of partially resolving the reaction zone and is computationally expensive. Since an adaptive algorithm must place a fine mesh around the detonation wave, in effect, it is a crude tracking algorithm. Front tracking is a more natural algorithm for dealing with the curvature effect. It provides a clean separation between the long length scales of the non-reactive flow

and the short length scales required for the reaction zone dynamics. The analytic information needed to propagate a detonation wave is contained in the wave curve. By empirically calibrating the average quantities in the modified jump conditions, the wave curve can be determined without a detailed knowledge of the complicated chemical reactions which are impractical to obtain experimentally.

Our analysis is based on the conservation equations and the quasi-steady approximation. It is not limited to detonation waves. The curvature effect occurs in general whenever a wave has a width. Therefore, partially dispersed and fully dispersed shock waves due to relaxation phenomena are also subject to a curvature effect.

A narrow wave front may have a local region of high curvature. This can occur when waves interact to form multi-dimensional wave patterns. In this case the 1-D assumption in the quasi-steady model breaks down. Consequently, the region where wave profiles overlap may be fully multi-dimensional. This undoubtably will affect the threshold for the bifurcation of wave patterns, such as the transition between regular and Mach reflection. Thus, we hypothesize that the physical dissipative mechanism that determine shock profiles can in certain instances affect the global behavior of fluid flow.

REFERENCES

1. P. Donguy and N. Legrand, *Numerical simulations of non-ideal detonations of a heterogeneous explosive with the two dimensional Eulerian code C.E.E.*, Proceedings of the Seventh International Symposium on Detonation, 1981, pp. 695-702.
2. W. Fickett and W. C. Davis, *Detonation*, Univ. of California Press, Berkeley, 1979.
3. R. Menikoff, *Errors when shock waves interact due to numerical shock width*, SIAM J. Sci. Comput. 15 (1994), xx–xx.
4. R. Menikoff, K. S. Lackner, and B. G. Bukiet, *Modeling flows with curved detonation waves*, preprint LA-UR-94-481, Los Alamos National Lab., 1994, (submitted to Combustion Flame).

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