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Errors when Shock Waves Interact due to Numerical Shock Width*

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ABSTRACT

A simple test problem proposed by Noh, a strong shock reflecting from a rigid wall, demonstrates a generic problem with numerical shock capturing algorithms at boundaries that Noh called "excess wall heating." We show that the same type of numerical error occurs in general when shock waves interact. The underlying cause is the non-uniform convergence to the hyperbolic solution of the inviscid limit of the solution to the PDEs with viscosity. The error can be understood from an analysis of the asymptotic solution. For a propagating shock, there is a difference in the total energy of the parabolic wave relative to the hyperbolic shock. Moreover, the relative energy depends on the strength of the shock. The error when shock waves interact is due to the difference in the relative energies between the incoming and outgoing shock waves. It is analogous to a phase shift in a scattering matrix. A conservative differencing scheme correctly describes the Hugoniot jump conditions for a steady propagating shock. Therefore, the error from the asymptotics occurs in the transient when the waves interact. The entropy error that occurs in the interaction region remains localized but does not dissipate. A scaling argument shows that as the viscosity coefficient goes to zero, the error shrinks in spatial extend but is constant in magnitude. Noh's problem of the reflection of a shock from a rigid wall is equivalent to the symmetric impact of two shock waves of the opposite family. The asymptotic argument shows that the same type of numerical error would occur when the shocks are of unequal strength. Thus, Noh's problem is indicative of a numerical error that occurs when shocks interact due to the numerical shock width.

Key words: hyperbolic conservation laws, shock interactions, viscous profiles

AMS (MOS) subject classification: 35L65, 35L67, 65M12, 76M20

1. Introduction

The equations for ideal fluid flow form a hyperbolic system of conservation laws

$$\partial_t \begin{pmatrix} \rho \\ \rho u \\ \rho(\frac{1}{2}u^2 + E) \end{pmatrix} + \partial_x \begin{pmatrix} \rho u \\ \rho u^2 + P \\ \rho(\frac{1}{2}u^2 + E)u + Pu \end{pmatrix} = \vec{0} \qquad (1.1)$$

where ρ is the density, u is the particle velocity, E is the specific energy, $P(V, E)$ is the pressure and $V = 1/\rho$ is the specific volume. Dissipation only occurs across a shock wave and physically is accounted for by imposing the Rankine-Hugoniot jump relations across the shock discontinuity. Finite difference shock capturing algorithms are frequently used to obtain a numerical solution to the fluid flow equations. These schemes have a numerical dissipation that gives a shock wave a small width measured in grid cells, but an artificially large spatial width compared to the typical shock width that physically occurs. The effect of the artificial shock width is largest when shock waves interact. To determine the effect of the numerical shock width, we analyze the asymptotic solution for a simple shock interaction when a viscous dissipative term is added to the ideal fluid equations.

The problem we consider in detail is a strong shock in an ideal gas reflecting from a rigid wall. This is equivalent to the interaction between equal strength shocks of the opposite family. It is similar to a test problem Noh [3] introduced that exemplify errors in numerical calculations due to artificial viscosity. In Noh's problem the initial data consists of a uniform state of cold gas with a constant velocity directed towards a rigid wall. Its solution has a strong outgoing shock. Because of the zero initial sound speed, an analytic solution exists in planar, cylindrical and spherical geometry. Typically, numerical solutions have an entropy error at the boundary. The shock interaction problem considered here is less singular then the Noh problem. The initial state is assumed to have a smooth viscous profile rather than a discontinuity in the velocity. Furthermore, the Mach number of the reflected shock is finite. Nevertheless, the same type of entropy error occurs in the numerical solution of the shock interaction problem.

The hyperbolic solution of the shock interaction problem consists of an outgoing shock wave. Because the flux at the boundaries is constant, the total mass, momentum and

energy in the viscous solution have the same value as those in the hyperbolic solution. We define the shock position of the viscous wave to have the same total mass and momentum as the hyperbolic shock wave. An important quantity in the asymptotic analysis is the energy of the viscous shock relative to the energy of hyperbolic shock.

We show that there is a shift in the relative energy between the incoming and outgoing waves. This implies that an entropy error must occur during the transient shock inter-action. For a shock reflection, the transient takes place when the shock profile overlaps with the boundary. After the transient, the entropy is frozen in place, i.e., convects along particle trajectories, and the error does not dissipate.

A scaling argument due to Noh shows that as the viscous coefficient goes to zero the entropy error decreases in spatial extent but not in magnitude. It implies that the convergence of the inviscid limit to the hyperbolic solution is non-uniform in regions where shocks have interacted.

2. Asymptotics

Let us consider a steady state viscous shock wave. Suppose the wave is right facing and propagating with velocity σ. Furthermore, let the reference points r_a and r_b be in the ahead and behind state respectively, with $r_b < r_a$. The position of the wave can be defined by comparing the viscous profile with a discontinuous shock and adjusting the discontinuity such that the two waves have the same total mass.

The condition that the waves have the same mass is given by

$$0 = \int_{r_b}^{r_c} dx\,(\rho - \rho_b) + \int_{r_c}^{r_a} dx\,(\rho - \rho_a)$$ (2.1)

Relative to r_b the shock position based on the mass is given by

$$r_s = r_b + (\rho_b - \rho_a)^{-1} \int_{r_b}^{r_a} dx\,(\rho(x) - \rho_a)$$ (2.2)

Similarly, the position of the wave could be defined by matching the total momentum. The shock position based on momentum is obtained from Eq. (2.2) by replacing the mass density ρ with the momentum density ρu.

In steady state the mass flux is everywhere constant

$$\rho(u - \sigma) = m$$

Hence, there is a linear relation between mass density and momentum density $\rho u = \rho\sigma + m$. Consequently the shock positions, based on either the mass or momentum of the waves, are the same.

One could also base the shock position on the total energy. However the energy density $\mathcal{E} = (\frac{1}{2}u^2 + E)\rho$ is not Galilean invariant. This would lead to a non-uniqueness in the shock position. Instead, we define the relative energy between the viscous profile and the discontinuous shock with the shock position based on mass

$$\delta\mathcal{E}^\Gamma = \int_{r_b}^{r_s} dr\,(\mathcal{E} - \mathcal{E}_b) + \int_{r_c}^{r_s} dr\,(\mathcal{E} - \mathcal{E}_a)$$
$$= \int_{r_b}^{r_s} dr\,(\mathcal{E} - \mathcal{E}_a) - (r_s - r_b)(\mathcal{E}_b - \mathcal{E}_a) \qquad (2.3)$$

We note that $\delta\mathcal{E}^\Gamma > 0$ corresponds to an excess energy in the viscous profile over the discontinuous shock.

We next show that the relative energy is Galilean invariant and hence well defined. In a reference frame moving with relative velocity u' the energy density is transformed to $\mathcal{E}' = \mathcal{E} + \rho u u' + \frac{1}{2}\rho(u')^2$. Substituting $\mathcal{E}'$ into Eq. (2.3) one finds that the additional terms are proportional to the mass and momentum density and have the same form as in Eq. (2.1). Hence, the additional terms vanish when r_s is chosen to be the shock position based on mass or equivalently momentum.

3. Von Neumann-Richtmyer Viscosity

Viscosity can be incorporated into the fluid equations by adding a viscous pressure onto the fluid pressure, $P \to P + Q$ in Eq. (1.1). We analyze the viscous fluid equations using a von Neumann-Richtmyer viscosity [2] and an ideal gas equation of state. The von Neumann-Richtmyer viscosity is defined by the viscous pressure

$$Q = \begin{cases} C_\nu \, \rho \, \ell^2 (\partial_x u)^2, & \text{if } \partial_x u < 0; \\ 0, & \text{otherwise.} \end{cases} \tag{3.1}$$

where C_ν is a dimensionless viscosity and ℓ is a length scale proportional to the shock width. Without loss of generality we can set $C_\nu = 1$. For an ideal gas

$$PV = (\gamma - 1)E \tag{3.2}$$

with $\gamma > 1$.

In this case, there is an exact analytic formula for the viscous profile of a shock wave [4]. Let σ be the shock velocity and the variable

$$w = \left(\frac{\gamma + 1}{2} \right)^{\frac{1}{2}} \cdot \left(\frac{x - \sigma t}{\ell} \right) \tag{3.3}$$

be a scaled length relative to the shock front. Then the viscous profile is given by

$$V(w) = \tfrac{1}{2}(V_a + V_b) + \tfrac{1}{2}(V_a - V_b)\sin(w) \tag{3.4}$$

$$P(w) = \tfrac{1}{2}(P_a + P_b) - \tfrac{1}{2}(P_b - P_a)\left[\sin(w) + \frac{\tfrac{1}{2}(\gamma + 1)(V_a - V_b)\cos^2(w)}{(V_a + V_b) + (V_a - V_b)\sin(w)}\right] \tag{3.5}$$

$$Q(w) = \tfrac{1}{4}(\gamma + 1)(P_b - P_a)\left[\frac{(V_a - V_b)\cos^2(w)}{(V_a + V_b) + (V_a - V_b)\sin(w)}\right] \tag{3.6}$$

$$u(w) = \sigma - m\,V(w) \tag{3.7}$$

where $m = \rho_a(\sigma - u_a)$ is the mass flux through the shock front. From the Hugoniot jump conditions $m^2 = (P_b - P_a)/(V_a - V_b)$. We note the shock profile is of finite width extending from the ahead state at $w_a = -\tfrac{1}{2}\pi$ to the behind state at $w_b = \tfrac{1}{2}\pi$.

The shock position based on mass is given by

$$w_* = w_b + (\rho_b - \rho_a)^{-1}\left[\int_{-\pi/2}^{\pi/2} dw \frac{2}{(V_a + V_b) + (V_a - V_b)\sin(w)} - \pi\rho_a\right] \tag{3.8}$$

The integral is of the form evaluated in the appendix. It can be simplified to give

$$w_s = w_b + \pi \left(\frac{\eta^{\frac{1}{2}} - 1}{\eta(\eta - 1)} \right) \qquad (3.9)$$

where $\eta = V_a/V_b$ is the compression ratio of the shock. We note the limiting cases: for a weak shock $\eta \to 1$ and $w_s \to 0$ while for a strong shock $\eta \to (\gamma + 1)/(\gamma - 1)$ and $-\frac{1}{2}\pi < w_s < 0$.

It is convenient to calculate the relative energy of the shock profile in the rest frame of the shock front, i.e., $\sigma = 0$. In this case the kinetic energy is $\frac{1}{2}\rho u^2 = \frac{1}{2}m^2 V$ and the energy density can be expressed as

$$\mathcal{E} = \tfrac{1}{2} m^2 V + (\gamma - 1)^{-1} P \qquad (3.10)$$

Substituting this expression into Eq. (2.3) for the relative energy we obtain

$$\delta\mathcal{E}^T = \left(\frac{2}{\gamma + 1} \right)^{\frac{1}{2}} \ell \left[\tfrac{1}{2}m^2 \int_{-\pi/2}^{\pi/2} dw\, V(w) + \frac{1}{\gamma - 1} \int_{-\pi/2}^{\pi/2} dw\, P(w) - \pi\mathcal{E}_a - (w_s - w_b)(\mathcal{E}_b - \mathcal{E}_a) \right] \qquad (3.11)$$

The integrals can be evaluated with the formulae in the appendix.

$$\int_{-\pi/2}^{\pi/2} dw\, V(w) = \tfrac{1}{2}\pi(V_a + V_b)$$

$$\int_{-\pi/2}^{\pi/2} dw\, P(w) = \tfrac{1}{2}\pi \left[(P_a + P_b) - \tfrac{1}{2}(\gamma + 1)(\eta^{\frac{1}{2}} - 1)^2(\eta - 1)^{-1}(P_b - P_a) \right]$$

After straightforward algebraic manipulation, we obtain for the relative energy

$$\delta\mathcal{E}^T = \tfrac{1}{2}\pi \frac{1}{\gamma - 1} \left(\frac{2}{\gamma + 1} \right)^{\frac{1}{2}} \ell(P_b - P_a) \left\{ (\gamma - 3)\left[\frac{\eta^{\frac{1}{2}} - 1}{\eta(\eta - 1)} - \tfrac{1}{2} \right] - \tfrac{1}{2}(\gamma + 1)\frac{(\eta^{\frac{1}{2}} - 1)^2}{\eta(\eta - 1)} \right\} \qquad (3.12)$$

We note three general properties of the relative energy.

(1) $\delta\mathcal{E}^T$ is a function of the shock width.

In particular, $\delta\mathcal{E}^T \to 0$ as the shock width goes to zero.

(2) $\delta\mathcal{E}^T$ is a function of the shock strength.

For weak shocks $\delta\mathcal{E}^T/\ell \sim (P_b - P_a)^2$ and for strong shocks $\delta\mathcal{E}^T/\ell \sim (P_b - P_a)$.

(3) $\delta\mathcal{E}^T$ varies with γ, and hence the equation of state.

This is a consequence of the fact that the viscous pressure depends only on the density and velocity, hence the shock profile depends on the equation of state.

These important properties are expected to be true for any reasonable viscosity and equation of state.

4. Example of Reflected Strong Shock

The effect of the shock width on a shock interaction can be seen in the simple case of a strong shock reflecting from a rigid wall. To compare the viscous solution with the hyperbolic solution, we compute the difference in the relative energy between the incoming shock and the outgoing shock, $\Delta\mathcal{E}^T = \delta\mathcal{E}^T_{rs} - \delta\mathcal{E}^T_s$. We note that $\Delta\mathcal{E}^T > 0$ corresponds to a net excess energy in the viscous shock profiles compared to the hyperbolic shocks.

Let the pressure behind the incoming shock be P_s. The compression ratio of a strong shock is $\eta_s = (\gamma + 1)/(\gamma - 1)$. The reflected shock is characterized by its pressure ratio, $P_{rs}/P_s = 1 + 2\gamma/(\gamma - 1)$, and its compression ratio, $\rho_{rs}/\rho_s = \gamma/(\gamma - 1)$.

The scale for the relative energies is $\epsilon = \frac{1}{2}\pi\frac{1}{\gamma-1}\left(\frac{2}{\gamma+1}\right)^{\frac{1}{2}}\ell P_s$. Substituting the values for the pressure and compression ratio into Eq. (3.11) we obtain for the relative energies

$$\delta\mathcal{E}^T_s/\epsilon = \tfrac{1}{2}(\gamma-3)\left\{\frac{(\gamma-1)^2}{\gamma+1}\left[\left(\frac{\gamma+1}{\gamma-1}\right)^{\frac{1}{2}}-1\right]-1\right\} - \tfrac{1}{4}(\gamma-1)^2\left[\left(\frac{\gamma+1}{\gamma-1}\right)^{\frac{1}{2}}-1\right]^2$$

$$\delta\mathcal{E}^T_{rs}/\epsilon = (\gamma-3)\left\{2(\gamma-1)\left[\left(\frac{\gamma}{\gamma-1}\right)^{\frac{1}{2}}-1\right]-\frac{\gamma}{\gamma-1}\right\} - (\gamma+1)(\gamma-1)\left[\left(\frac{\gamma}{\gamma-1}\right)^{\frac{1}{2}}-1\right]^2$$

From the above formulae, the difference in the relative energies can easily be evaluated numerically as a function of γ. A plot shows the following general properties for the difference of the relative energy:

(1) $\Delta \mathcal{E}^T \to \infty$ as $\gamma \to 1$

This singularity is due to the singularity in the compression ratio at $\gamma = 1$.

(2) $\Delta \mathcal{E}^T = 0$ at $\gamma \approx 2.4$

(3) The minimum value of $\Delta \mathcal{E}^T \approx -0.34$ occurs at $\gamma \approx 4.65$

(4) $\Delta \mathcal{E}^T \to 0$ as $\gamma \to \infty$.

We note that in general $\Delta \mathcal{E}^T$ is not zero.

The constant flux ahead of the outgoing wave can be accounted for by comparing the position of the shock in the viscous solution to that of the hyperbolic solution. The shift in the energy of the viscous shock profiles implies that a steady state outgoing wave can not simultaneously satisfy the flux relations for mass, momentum and energy. Instead, the shock interaction must result in a transient. The transient occurs on both a fast and slow time scale and results in an entropy error when comparing the viscous solution to the hyperbolic solution.

Over the fast time scale, (shock width)/(shock velocity), the viscous pressure smoothes out any discontinuity in the non-degenerate or acoustic modes. This is important when the positions of the incoming and outgoing shock waves are within a few shock widths of the wall. The pressure and particle velocity rapidly equilibrate towards the values of the hyperbolic solution as the incoming shock profile changes to the outgoing profile. On the slow time scale, the viscous solution is close to the solution to the Riemann problem and the outgoing shock profile approaches its steady state solution.

On the slow time scale, the shift in energy is small compared to the total energy behind the shock. The energy mismatch in the shock profiles can be distributed over the region between the wall and the shock front by acoustic waves. The entropy error at the shock front is small and further decrease as $1/t$ for large t. This is a consequence of the fact that the Hugoniot jump conditions give the correct entropy jump across a steady state shock profile independent of the form of dissipation.

On the fast time scale, the energy shift is significant compared to the total energy in the shock profile. This results in a significant entropy error in the interaction region

during the transient in which the shock profiles change. After the pressure and particle velocity have equilibrated, the viscous pressure in the interaction region approaches zero and the subsequent change in entropy is negligible. Without heat conduction which would give rise to diffusion of entropy, the entropy error is frozen into the particle trajectories. Thus, the bulk of the entropy error from the interaction is confined to within a few shock widths of the wall.

Let us consider in more detail the interaction region for the case when $\Delta \mathcal{E}^T > 0$. Near the wall the outgoing viscous wave must have a deficit in energy equal to $\Delta \mathcal{E}^T$ in order to compensate for the energy difference in the shock profiles. Because the wall causes the particle velocity to go to zero, the energy density reduces to $\mathcal{E} = \rho E = P/(\gamma - 1)$ and is proportional to P. When the reflected wave has propagated a couple of shock widths, the pressure has approximately equilibrated to the value behind the outgoing hyperbolic shock. In order to conserve total energy, the viscous shock front must be slightly behind the hyperbolic shock front. Then to conserve mass, on average ρ must be above the value for the hyperbolic shock. Since P is approximately constant, a high value for ρ implies on average the entropy $S \propto \log(P/\rho^\gamma)$ is low.

At the wall, the pressure rise is more characteristic of a single strong shock then a double shock. Since the entropy is greater for a single strong shock then for two sequential shocks to the same final pressure, right at the wall we expect the entropy to be high and the density to be low. This implies there is an oscillation in the density and entropy in the vicinity of the wall. The pressure and density determine the specific energy through the equation of state. At the wall, a low value of ρ results in a high value of E. This agrees with the results of numerical calculations and is what Noh [3] called excessive wall heating, even though there is a damped oscillation in the energy about the value behind the hyperbolic shock.

Finally, to conserve total momentum the velocity profile overshoots and becomes slightly negative immediately behind the viscous shock front. As the wave moves further away from the wall, the viscous profile more closely approaches that of a steady state shock wave. Consequently, the entropy jump across the viscous wave rapidly approaches

the value for the hyperbolic shock. As time progresses, further errors in entropy outside the interaction region are negligible.

We note that the initial data for Noh's test problem corresponds in effect to taking the relative energy of the incoming wave to be zero. In this case, the energy difference for the interaction is $\Delta \mathcal{E}^T = \delta \mathcal{E}_s^T$. Again, in general $\Delta \mathcal{E}^T$ is not zero and an entropy error occurs from the transient interaction that forms the outgoing shock.

Finally, to understand the small distance it take for the shock to form and the pressure and velocity to equilibrate we estimate the magnitude of $\delta \mathcal{E}_s^T$ relative to the energy in the shock profile. For illustrative purposes we assume $\gamma = 5/3$. From Eq. (3.3) the shock width is $\Delta x = 2.72\ell$. The compression ratio of a strong shock is $\eta = (\gamma + 1)/(\gamma - 1) = 4$. From Eq. (3.12), the energy ratio is $\delta \mathcal{E}_s^T / \Delta x \mathcal{E}_s = 1/9$. Thus the energy in the shock profile will have a small effect on the shock interaction after the outgoing shock has propagated a couple of shock widths.

5. Non-uniform convergence of Inviscid Limit

One important consequence of shock interactions is that the convergence of the inviscid limit to the hyperbolic solution is non-uniform. This may be deduced through a scaling argument introduced by Noh [3].

The inviscid fluid equations are scale invariant. Scaling space and time amounts to a choice of units. Viscosity introduces a length scale which breaks the invariance. However, under scaling, the viscous pressure is multiplied by a constant. Therefore, by scaling the coefficient of viscosity along with the length and time scales, the equations are again invariant A solution to the fluid equations with the von Neumann-Richtmyer viscosity is invariant under the transformation $x' = \alpha x$, $t' = \alpha t$ and $C_\nu' = \alpha^2 C_\nu$. Furthermore, this transformation preserves velocity and hence the initial value data. As $\alpha \to 0$, the entropy error at the wall is constant in magnitude but decreases in spatial extent. Hence the inviscid limit for this case converges in L^1 or L^2 but not in L^∞.

A shock reflecting from a rigid wall is equivalent to the symmetric collision of two shocks, i.e., equal strength shocks of the opposite family. The argument that the cause of the error is due to the asymptotic shift in the relative energy between the incoming waves and the outgoing waves implies t. at the fact that the incoming waves are of equal strength is not important. Hence, shock interactions in general will result in non-uniform convergence of the inviscid limit.

6. Effect of Source terms

Noh also has a version of the shock reflection test problem in cylindrical and spherical geometry. This introduces an additional effect on shock propagation due to geometrical source terms.

The geometrical source terms are singular at the origin. Consequently, as the shock approaches the origin the source terms become comparable in magnitude to the viscous dissipation within the shock profile. When this occurs, the conservation form of the equations no longer implies the Hugoniot jump condition across a shock.

A real effect in which the Hugoniot jump conditions are modified occurs for detonation waves [1]. In this case the competition between chemical reactions and geometrical source terms gives rise to the curvature effect in which the detonation velocity depends on the curvature of the shock front. An artificially large numerical shock width and geometric source terms can have a similar effect near the origin.

An ideal converging shock, from the Gurdeley similarity solution, is singular at the origin. The shock width provides a length scale which regularizes the singularity when the shock reflects from the origin. After reflection there are large gradients behind the shock front. The shock has to propagate a sufficient distance from the origin in order for the gradients behind the shock to be small compared to those in the shock profile. This is a necessary condition for the Hugoniot jump conditions to apply across the shock independent of the form of dissipation.

Thus, when source terms or gradients behind the shock front are large compared to the dissipation within the shock profile, the viscous solution can differ significantly from the hyperbolic solution. Again the error is in the entropy and is expected to be localized. Finite difference shock capturing algorithms have an artificially large shock width. Numerical solutions with schemes that have the smallest shock width will minimize errors of this type and be closest to the hyperbolic solution

7. Conclusion

We have analyzed the problem of a strong viscous shock reflecting from a rigid wall. For the von Neumann-Richtmyer viscosity, we have shown that the same type of entropy error occurs as in Noh's test problem. The error is due to the difference in energy relative to the hyperbolic solution of the viscous profiles for the incoming and outgoing shock waves. A scaling arguments shows that as the viscous coefficient goes to zero the entropy error decreases in spatial extent but not in magnitude. Furthermore, the entropy error is convected with the fluid and does not dissipate.

From the asymptotic energy argument, we expect the same behavior to occur for an arbitrary shock interaction with any dissipative mechanism that results in a non-zero shock width, provided there is no heat conduction to diffuse entropy. The dissipation may correspond to a term added to the hyperbolic PDEs, *e.g.*, an artificial viscosity, or can be numerical in nature, *e.g.*, resulting from truncation errors in the differencing scheme or a Riemann solver used in the Godunov method. The fact that hyperbolic finite difference schemes **deliberately** underresolve the shock profile is not critical. The truncation errors merely introduce an oscillation in the shock profile as the position of the shock front propagates between grid points.

The entropy error when viscous shock profiles interact implies a non uniform convergence of the inviscid limit to the hyperbolic solution. Non-uniform convergence can be expected at the shock front. An additional non-uniformity can occur in a region in which

the solution is smooth resulting from a shock interaction that occurred in the region's past history.

A more **severe** form of this entropy error occurs when a shock wave is incident on a material interface or contact. For materials with different equations of state or when the contact is a discontinuous change in zoning, there can be a large transient resulting from the change in profiles for the incident, transmitted and reflected shock waves. In Lagrangian algorithms the effect is partially ameliorated by choosing the grid such that the wave speed in units of zones per time step is the same for the outgoing shocks on each side of the interface. However, the minimal error is similar to that which occurs for the shock interaction discussed here.

In more complicated fluid flows, additional errors can result from the inhomogeneities caused by the entropy error from shock interactions. For example, subsequent shock waves will scatter off the inhomogeneities and spread the spatial extent of the error. This effect is partially ameliorated by the fact that shock heating raises the sound speed. Hence subsequent reflected shocks have a lower Mach number and the additional entropy errors they cause decrease as the shocks weaken. Another example occurs in an unstable two dimensional flow. The inhomogeneities from shock interactions can be the seed for a perturbation which leads to instability growth.

For some applications, the non-uniform convergence is important. One example is when comparing the calculated temperature at a wall to experimental data. The numerical entropy error from a reflected shock results in a high wall temperature which does not dissipate in time. Moreover, the calculated wall temperature does not improve under mesh refinement. Having understood the cause, one can compensate for this error, e.g., with sufficient resolution by averaging over a small region in the vicinity of the wall. Another example is when the material is chemically reactive. In particular, for an explosive a numerical hot spot caused by a shock interaction can initiate a detonation and greatly effect the fluid flow.

The spatial extend of the entropy error when shocks interact is proportional to the shock width. Thus, this error is smallest for those numerical scheme that minimize the artificial shock width. In particular, this type of error can be eliminated by using a front tracking algorithm.

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Appendix: Evaluation of Integral

The needed integrals can be evaluated by contour integration as follows. Suppose $a > b > 0$ and n is a non-negative integer. Let $z = e^{ix}$. Then the basic integral of interest can be expressed as

$$\int_0^\pi dx \, \frac{\cos(nx)}{a + b\cos(x)} = Re \int_{C_0} \frac{-i\,dz}{z} \cdot \frac{z^n}{a + \frac{1}{2}b(z + 1/z)}$$
$$= Im \int_{C_0} dz \, \frac{z^n}{\frac{1}{2}bz^2 + az + \frac{1}{2}b}$$

where C_0 is the arc of a unit circle in the upper half of the complex plane.

The denominator of the integrand on the RHS has two zeros located at

$$z_\pm = \left[-a \pm (a^2 - b^2)^{\frac{1}{2}} \right] /b \, .$$

These lie along the real axis with $z_- < -1$ and $-1 < z_+ < 0$. Let C be the path formed by closing the path C_0 along the x axis but going around the pole at z_+ in the upper half plane. By applying Cauchy's residue formulae we obtain

$$\int_0^\pi dx \, \frac{\cos(nx)}{a + b\cos(x)} = Im \left(\int_C dz \, \frac{z^n}{\frac{1}{2}bz^2 + az + \frac{1}{2}b} - PV \int_{-1}^1 dx \, \frac{x^n}{\frac{1}{2}bx^2 + ax + \frac{1}{2}b} \right.$$
$$\left. + i\pi \, \text{Residue}(z_+) \right)$$
$$= \pi \, \text{Residue}(z_+)$$
$$= \frac{\pi}{(a^2 - b^2)^{\frac{1}{2}}} \left(\frac{(a^2 - b^2)^{\frac{1}{2}} - a}{b} \right)^n$$

Using the symmetry of the sin and cos functions over a half cycle we note two special cases of the above formula

$$\int_{-\frac{1}{2}\pi}^{\frac{1}{2}\pi} dx \, \frac{1}{a + b\sin(x)} = \int_0^\pi dx \, \frac{1}{a + b\cos(x)}$$
$$= \frac{\pi}{(a^2 - b^2)^{\frac{1}{2}}}$$

$$\int_{-\frac{1}{2}\pi}^{\frac{1}{2}\pi} dx \, \frac{\cos^2(x)}{a + b\sin(x)} = \int_0^\pi dx \, \frac{\sin^2(x)}{a + b\cos(x)}$$
$$= \frac{1}{2}\int_0^\pi \frac{1 - \cos(2x)}{a + b\cos(x)}$$
$$= \frac{\pi}{b^2} \left[a - (a^2 - b^2)^{\frac{1}{2}} \right]$$

References

[1] B. BUKIET AND R. MENIKOFF, *Detonation waves and the Front Tracking Method*, Phys. Fluids A, 4 (1992), pp. 2070-2081.

[2] J. von NEUMANN AND R. D. RICHTMYER, *A Method for the Numerical Calculation of Hydrodynamic Shocks*, J. Appl. Phys., 21 (1950), pp. 232-237.

[3] W. F. NOH, *Errors for Calculations of Strong Shocks Using an Artificial Viscosity and an Artificial Heat Flux*, J. Comp. Phys., 72 (1987), pp. 78-120..

[4] R. D. RICHTMYER AND K. W. MORTON, *Difference Methods for Initial-Value Problems*, Interscience, New York, 1967.

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