A FRONT TRACKING METHOD FOR TRANSITIONAL SHOCK WAVES

Hyun-Cheol Hwang*

Abstract

Non–strictly-hyperbolic and mixed-type conservation laws pose a challenge to computational methods. Specifically, the computation of transitional shock waves, which are dependent on the parabolic regularization of the conservation laws, is sensitive to the numerical viscosity. In this paper, we propose a front tracking algorithm that treats transitional shock waves correctly. The algorithm includes the computation of saddle-to-saddle connections in planar dynamical systems using the multiple shooting method. We compare our results with those of commonly-used shock capturing schemes, including the Lax-Friedrichs, Lax-Wendroff, and higher-order Godunov schemes.

1. Introduction

Discontinuities, such as shock waves and material interfaces, are a common and significant feature of solutions of systems of conservation laws. A discontinuous wave is, at each point, characterized by the limiting states on its two sides and by its normal propagation speed, which are related by jump conditions derived from the conservation laws. The discontinuity, however, is a mathematical idealization: physically there are regularization mechanisms that provide a discontinuous wave with a continuous internal structure on a small length scale [6]. Usually the internal structure can be ignored, but certain types of discontinuities are sensitively dependent on the regularization procedure, not only

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in their internal structure, but also in their propagation speeds and limiting states. These waves occur in applications such as combustion [4], three-phase flow through a porous medium [2, 20], and magneto-hydrodynamics [22]. It is important to be able to correctly simulate them using numerical methods.

One type of regularization-sensitive wave, the transitional (or undercompressive) shock wave, has been the subject of recent studies of Riemann solutions in non–strictly-hyperbolic systems of conservation laws [18, 12]. A transitional shock wave differs from a classical shock wave in that fewer characteristic families impinge on the wave. Therefore the dynamical information carried into the wave along characteristics is insufficient to determine the evolution of the wave. The missing information comes from the internal structure of the shock wave, which means that the internal structure strongly influences wave propagation.

Most numerical methods for shock waves rely on numerical diffusion for stability, and thus provide discontinuous waves with an artificial internal structure. Such methods are successful only if they are applied to waves that are insensitive to this numerical regularization. Difficulties can arise when they are used for regularization-sensitive waves: for example, excess diffusion can cause significant errors in detonation wave speeds [3], and the limiting states of a deflagration wave are sensitive to heat conduction and viscosity [4]. In order to circumvent these difficulties, numerical methods must account for the true internal structure of discontinuities.

In this paper, we propose a numerical method that accomplishes this for transitional shock waves, and we compare it with some commonly-used shock capturing methods. Our method uses front tracking to locate the position of the transition wave and solves Riemann problems to account for the internal wave structure. This strategy is similar to that of Hilditch and Colella [9], who track a deflagration front, solving Riemann problems using a phenomenological flame speed law. The difference is that, in our solution of the Riemann problem, we construct the exact internal structure of the wave corresponding to viscous regularization. Our method has been implemented for pairs of conservation laws with quadratic fluxes and for a single space dimension; its extension to other systems and multiple dimensions is under development.

2. Transitional Shock Waves

We consider a system of conservation laws,

$$U_t + F(U)_x = 0, \tag{2.1}$$

where $U = (u, v)$ is a two-component state vector, F is the flux function, t is time, and x represents the one space coordinate. The characteristic speeds, which are the eigenvalues of the Jacobian $F'(U)$ of the flux function, are denoted $\lambda_i(U)$, $i = 1, 2$. The system of conservation laws is not necessarily strictly hyperbolic, *i.e.,* characteristic speeds may be indistinct or complex in the subregion of state space called the elliptic region. In the hyperbolic region, where the characteristic speeds are real, we order them so that

$$\lambda_1(U) \leq \lambda_2(U). \tag{2.2}$$

The need to admit weak solutions of Eq. (2.1), which contain discontinuous waves (shock waves), is well-known. A shock wave propagating at speed s and having limiting states U_- and U_+ on its left and right sides, respectively, must satisfy the Rankine-Hugoniot jump condition

$$-s(U_+ - U_-) + F(U_+) - F(U_-) = 0. \tag{2.3}$$

However, weak solutions of Eq. (2.1) are not unique. Therefore we require shock waves to satisfy an admissibility condition that selects physically correct solutions. In the present paper, we choose the viscous profile criterion as an admissibility condition, since it is the most realistic for many physical models.

2.1. Viscous Profile Criterion

The viscous profile criterion requires that a shock wave arise as the limit, as $\epsilon \to 0$, of a traveling wave solution to a parabolic equation associated with Eq. (2.1), *viz.*,

$$U_t + F(U)_x = \epsilon[D(U)U_x]_x, \tag{2.4}$$

where $D(U)$ is the viscosity matrix, which models certain physical effect that have been neglected in Eq. (2.1). The viscosity matrix $D(U)$ is required to be positive definite. A traveling wave solution takes the form

$$U(x,t) = \hat{U}(\xi), \quad := \frac{x - st}{\epsilon}, \tag{2.5}$$

where $\hat{U}(\xi) \to U_{\pm}$ as $\xi \to \pm\infty$ and s is the propagation speed. In order for U to satisfy Eq. (2.4), $\hat{U}$ must be a solution of the dynamical system

$$-s[\hat{U}(\xi) - U_-] + F(\hat{U}(\xi)) - F(U_-) = D(\hat{U}(\xi))\hat{U}'(\xi). \tag{2.6}$$

The limiting states U_- and U_+ are equilibria of this dynamical system, according to the Rankine-Hugoniot condition (2.3). If a solution of system (2.6) leads from U_- to U_+, then we say that the shock wave has a viscous profile. Only those shock waves having viscous profiles are accepted as admissible solutions; this is the viscosity profile criterion.

2.2. Saddle-to-Saddle Connections

A transitional shock wave is a non-classical wave satisfying the viscosity profile criterion, as we now explain. For a system of two conservation laws, the question of shock wave admissibility reduces to the study of planar dynamical systems and their equilibria. The behavior of solutions of the dynamical system (2.6) in the vicinity of an equilibrium U_c is determined by the matrix

$$D(U_c)^{-1}\left[-sI + F'(U_c)\right], \tag{2.7}$$

provided that the eigenvalues $\mu_i(U_c)$, $i = 1, 2$ of this matrix are nonzero. For example, if the viscosity matrix $D(U)$ is the identity matrix, then the eigenvalues at U_c are

$$\mu_i(U_c) = \lambda_i(U_c) - s, \quad i = 1, 2. \tag{2.8}$$

Therefore a shock wave satisfying the Lax admissibility condition [14] corresponds either to a connection from a repelling node to a saddle point, in the case of a 1-family wave, or to a connection from a saddle point to an attracting node, in the case of a 2-family wave. When $D(U)$ is not necessarily a multiple of the identity matrix, the node can be a spiral point, but the phase portrait is still generically stable, in that the sum of the dimensions of the unstable manifold of U_- and the stable manifold of U_+ is three.

In contrast, a transitional shock wave is a so-called crossing discontinuity: the inequalities

$$\lambda_1(U_-) < s < \lambda_2(U_-), \tag{2.9}$$

$$\lambda_1(U_+) < s < \lambda_2(U_+) \tag{2.10}$$

hold, so that both characteristic families cross through the wave. Since $D(U)$ has a positive determinant, it follows that the eigenvalues of system (2.6) at U_- and U_+ satisfy $\mu_1(U_-)\,\mu_2(U_-) < 0$ and $\mu_1(U_+)\,\mu_2(U_+) < 0$, respectively. Therefore a viscous profile for a transitional wave connects two saddle points, and the phase portrait is generically unstable. (See Fig. 2.1.) The structural instability of a saddle-saddle connection usually entails that that only special crossing discontinuities, those in a codimension-1 set, have viscous profiles [1, 19]. Moreover, the set of transitional shock wave generally varies with the viscosity matrix $D(U)$. In other words, not only is the internal structure sensitive to the precise form of the viscosity matrix, but so too are the limiting states U_+ and U_- and the speed s.

2.3. Numerical Difficulties

Transitional waves pose difficulties for computational methods. In the numerical simulation of systems of conservation laws, almost every scheme utilizes some form of artificial viscosity to make it stable. Transitional shock waves computed using such schemes are generally different from those corresponding to the physical viscosity matrix. Since the limiting states and the propagation speed are sensitive to the viscosity matrix, the difference between the computed and physical solutions cannot be ignored.

To overcome this difficulty, we adopt the front tracking method [16, 7]. In this method, a standard finite-difference scheme is coupled to a lower-dimensional dynamic grid (the front) that follows the most important waves. Associated with each point of the front is a pair of states [8] representing the limiting states of the wave, which are updated as the front moves. The main advantage of this method is that, by avoiding finite differencing across the front, there is no diffusion at the tracked waves. Therefore it offers a suitable framework for the computation of regularization-sensitive waves, such as transitional shock waves.

In the front tracking method for shock waves, the shock position and limiting states, which constitute five unknown quantities, are updated at each time step. In the case of a Lax shock wave, these quantities are determined by the two Rankine-Hugoniot equations and the state information carried along the three impinging charactersitic curves. In the case of transitional shock wave, however, there are only two impinging characteristic curves. To resolve the resulting indeterminacy, one more equation is needed, *viz.*, the constraint that the shock wave should lie on the codimension-1 surface of crossing shock waves having viscous profiles.

3. Riemann Solutions near a Transitional Shock Wave

To update a tracked shock wave, we solve the Riemann problem defined by the states on either side. In general, solving a Riemann problem is extremely complicated (see, for example, Ref. [18]). However, the Riemann problems that occur in tracking usually have a simplifying feature: except for the tracked wave, all waves in the solution are weak. Indeed, the Riemann problem at a particular time level arises from the interaction, during the previous time step, of the tracked wave and the (usually) weak waves that have impinged on it. We say that a Riemann problem is near a certain wave type if its solution consists of a wave of this type together with small amplitude waves of other types.

The algorithm we now describe works for a Riemann problem near a transitional shock wave. As illustrated in Fig. 3.1, the solution of such a Riemann problem comprises a 1-wave from U_L to U_M, a transitional shock wave from U_M to U_N, and a 2-wave from U_N to U_R. Given U_L and U_R, we shall calculate U_M, U_N , and the speed s of the transitional wave.

Since U_M and U_N lie on the wave curves from U_L and U_R, they can be expressed as

$$U_M = \mathcal{W}_1^+(U_L, \varepsilon_L) \approx U_L + \varepsilon_L\, r_1(U_L), \tag{3.1}$$

$$U_N = \mathcal{W}_2^-(U_R, \varepsilon_R) \approx U_R + \varepsilon_R\, r_2(U_R), \tag{3.2}$$

where $\mathcal{W}_1^+$ (respectively, $\mathcal{W}_2^-$) parameterizes the forward 1-family (resp., backward 2-family) wave curve in terms of the parameter ε_L (resp., ε_R). As indicated, we approximate the wave curves by straight lines, since U_M and U_N are close to U_L and U_R, but this approximation can easily be avoided. The states U_M and U_N are also saddle points of dynamical system

$$U' = D(U)^{-1}\left[-s(U - U_M) + F(U) - F(U_M)\right] =: G(U, s, \varepsilon_L). \tag{3.3}$$

To calculate the saddle-to-saddle connection from U_M to U_N, we employ the multiple shooting method [21], as follows. (Refer to Fig. 3.2 .)

First, the ξ-axis is divided into the intervals $(-\infty, -T_1]$, $[-T_1, T_2]$, and $[T_2, \infty)$, where T_1 and T_2 are suitably large (see below); then the interval $[-T_1, T_2]$ is divided into n subintervals defined by the endpoints $\xi_0 := -T_1 < \xi_1 < \cdots < \xi_{n-1} < \xi_n := T_2$. State variables $U_0, \ldots, U_n$ corresponding to points $\xi_0, \ldots, \xi_n$ are introduced; U_M corresponds to $\xi = -\infty$, and U_N to $\xi = \infty$. The object is to have successive states joined by integral curves of the dynamical system (3.3). The state U_0 at $\xi = -T_1$ can be approximated as

$$U_0 \approx U_M + \varepsilon_M\, \tilde{r}_2(U_M), \tag{3.4}$$

for some value of ε_M. Here $\tilde{r}_2(U_M)$ denotes an eigenvector of $G_U(U_M, s, \varepsilon_L)$ corresponding to the eigenvalue $\mu_2(U_M)$; this eigenvector is tangent to the unstable manifold at U_M. Similarly,

$$U_n \approx U_N + \varepsilon_N\, \tilde{r}_1(U_N). \tag{3.5}$$

This linearized approximation also motivates choosing the values $T_1 = a/\mu_2(U_M)$ and $T_2 = a/|\mu_1(U_N)|$, where a is a dimensionless constant (taken to be 4 or 5 in the numerical experiments of Sec.). For $i = 0, \ldots, n-1$, we let $H(U_i, s, \varepsilon_L)$ denote the state obtained by numerically integrating the dynamical system (3.3) from $\xi = \xi_i$ to $\xi = \xi_{i+1}$ starting from the state U_i.

We have $2n+3$ unknown quantities, namely ε_L, ε_R, ε_M, ε_N, s, $U_1, \ldots, U_{n-1}$ (treating U_M, U_N, U_0, and U_n as given by the approximations described above), for which we require $2n+3$ equations. The $2n$ matching conditions and the Rankine-Hugoniot condition constitute $2n+2$ equations:

$$\begin{aligned} H(U_0, s, \varepsilon_L) - U_1 &= 0, \\ H(U_1, s, \varepsilon_L) - U_2 &= 0, \\ &\vdots \\ H(U_{n-2}, s, \varepsilon_L) - U_{n-1} &= 0, \\ H(U_{n-1}, s, \varepsilon_L) - U_n &= 0, \\ G(U_N, s, \varepsilon_L) &= 0. \end{aligned} \tag{3.6}$$

There is one remaining degree of freedom, which reflects nonuniqueness of solutions: since the dynamical system is autonomous, replacing t by $t + \text{const.}$ in one solution yields another. To fix the solution uniquely, we impose the phase condition of Ref. [5], which requires that

$$\int_{-T_1}^{T_2} \Big\langle G(U) - G(U_{\text{ref}}), G_U(U) \cdot G(U) \Big\rangle \, d\xi = 0 \tag{3.7}$$

for some reference solution U_{ref}. (Here the arguments s and ε_L of G are suppressed, and the angle brackets denote the inner product.) We choose U_{ref} to be the solution calculated at the previous time level in the front tracking method, and we discretize the integral using the trapezoid rule. Now we have a complete set of equations, which we solve using a damped Newton method [21], with Broyden update of the Jacobian, to obtain U_M, U_N, and s.

4. Tracking Algorithm

The algorithm to track the shock waves comprises four steps. Given the states U_L and U_R at time t, we:

1. solve the Riemann problem and find U_M, U_N, and s;

2. find the states U_{LL} and U_{RR} at the feet of characteristics drawn from the new shock position, as shown in Fig. 4.1;

3. calculate a characteristic correction, for improved accuracy, by solving the equations

$$l_2(U_M^{\text{char}})(U_M^{\text{char}} - U_M) = l_2(U_{LL})(U_{LL} - U_L), \tag{4.1}$$

$$l_1(U_M^{\text{char}})(U_M^{\text{char}} - U_M) = 0, \tag{4.2}$$

$$l_1(U_N^{\text{char}})(U_N^{\text{char}} - U_N) = l_1(U_{RR})(U_{RR} - U_R), \tag{4.3}$$

$$l_2(U_N^{\text{char}})(U_N^{\text{char}} - U_N) = 0 \tag{4.4}$$

for the states U_M^{char} and U_N^{char} at time $t + dt - 0$;

4. solve the Riemann problem with data U_M^{char} and U_N^{char} to obtain U_M^{new}, U_N^{new}, and s^{new} at time $t + dt + 0$, and revise the shock position using the average shock speed $\frac{1}{2}(s + s^{\text{new}})$.

5. Application to Quadratic Models

We have implemented our front tracking method for pairs of conservation laws with quadratic flux functions:

$$u_t + \left[\frac{1}{2}\left(a_1u^2 + 2b_1uv + c_1v^2\right) + d_1u + e_1v\right]_x = 0, \tag{5.1}$$

$$v_t + \left[\frac{1}{2}\left(a_2u^2 + 2b_2uv + c_2v^2\right) + d_2u + e_2v\right]_x = 0. \tag{5.2}$$

Generally, such a model fails to be strictly hyperbolic; for example, when linear terms are absent, the characteristics speeds coincide at $U = 0$. Furthermore, an elliptic region, where characteristic speeds are not real, can occur. Schaeffer and Shearer [17] classified homogeneous quadratic models into four cases, I–IV. In the following we describe some of the results of testing our tracking algorithm and some commonly-used shock capturing methods, as applied to a homogeneous model in Case II and on an inhomogeneous model for which the homogeneous quadratic part belongs to Case I.

For the homogeneous Case II model, the coefficients are $a_1 = 0.5$, $b_1 = 0.2$, $c_1 = 1$, $d_1 = e_1 = 0$, $a_2 = 0.2$, $b_2 = 1$, $c_2 = d_2 = e_2 = 0$; the viscosity matrix is taken to be constant and diagonal, with diagonal entries 1 and 0.3. We solve the initial-value problem with Riemann data $U_L = (1.632, 1.278)$ and $U_R = (-1.658, -1.269)$. The exact solution comprises a 1-shock wave, a transitional wave, and a 2-shock wave [10]; the connecting orbit for the transitional wave lies along a line through the origin (a viscosity line) that can be determined analytically [12]. This solution is to be contrasted with the solution when $D(U)$ is a multiple of the identity matrix, or, more generally, a function of $F'(U)$: then the transitional wave lies along a different line through the origin (a secondary bifurcation line).

Figures 5.1 and 5.2 show results of using the Lax-Friedrich (LF) [13] and Bell-Colella-Trangenstein (BCT) [1] methods with front tracking. Graphs of u and v plotted vs. x for several time steps are shown superimposed. For both methods, the calculated solution shows the 1- and 2-family shock waves moving away from the tracked transitional wave; of course the untracked waves are sharper for the BCT method. For comparison, Figs. 5.3 and 5.4 show the results of using the LF and BCT schemes without front tracking. Naturally, for these schemes, the transitional wave is less sharply defined, but more significantly, the limiting states of this wave are very different, leading to 1- and 2-family waves that are very different as well.

To compare these results with the exact solution, we have plotted the computed solutions in state space; see Figures 5.5 and 5.6. In each figure there are two sets of dashed lines: short-dashed lines are secondary bifurcation lines, whereas long-dashed lines are viscosity lines corresponding to the chosen viscosity matrix. These lines have been computed using the formulae in Ref. [12]. For the front tracking solutions, the orbit for the transitional wave lies along a viscosity line, and thus approximates the exact solution well. For the untracked solutions, however, the orbit lies along a bifurcation line; this is consistent with the fact that the numerical viscosity matrices for these schemes (*i.e.*, the viscosity matrices for the corresponding modified equations) are functions of $F'(U)$.

The next set of figures shows the test results for the Case I model. The coefficients for this model are $a_1 = -1$, $b_1 = 0$, $c_1 = 1$, $d_1 = 0$, $e_1 = 0.23$, $a_2 = 0$, $b_2 = 1$, $c_2 = 0$, $d_2 = -0.23$, $e_2 = 0$; the viscosity matrix is taken to be the identity matrix. This model has a elliptic region, the boundary of which is a circle shown in the state-space figures. The Riemann initial values are $U_L = (0.273, 0.182)$ and $U_R = (-0.246, 0.310)$. The exact solution, as computed using the Riemann Problem Package of Isaacson *et al* [11], comprises a 1-rarefaction wave, a transitional wave with a curved connecting orbit, and a 2-shock wave.

The results of using the front tracking method are shown in Figs. 5.7, 5.8, and 5.11. The underlying finite-difference schemes are the Lax-Friedrich and the Lax-Wendroff (LW) [15] schemes; the LW scheme is modified by adding artificial viscosity [16]. The comparable results without front tracking are shown in Figs. 5.9, 5.10, and 5.12. In the state space figures are drawn not only the solutions for several time steps but also the orbits of the dynamical system corresponding to the transitional shock wave (particularly the connecting orbit), the Hugoniot locus based at the point U_L, and the circle bounding the elliptic region. As seen in the state-space figures, the front tracking solution approximates the exact solution well, whereas the untracked solutions are significantly different.

6. Conclusion

The front tracking method we have described is effective for computing transitional shock waves in quadratic models, and we expect that it can be applied to other regularization-sensitive waves, such as deflagration waves in reactive gas dynamics, and extended to multi-dimensional calculations.

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Department of Applied Mathematics and Statistics
State University of New York at Stony Brook
Stony Brook, NY 11794-3600
Email: hchwang@ams.sunysb.edu

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