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9   Investigation of the Dissipative Properties of Difference Schemes for the Gas-Dynamics Equations

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The gas-dynamics equations describe a wide range of compressible-fluid motions ranging from the very slow movements of the atmosphere to the fast motions of gases in combustion chambers and the very fast motions of gases during an explosion. The mathematical modeling of these motions is of great scientific and technical importance, and this accounts for the endless flow of publications devoted to the development, analysis and application of the corresponding mathematical models. The difference scheme (DS) is an important element in a mathematical model. Its qualities have a direct impact on the quality of the mathematical experiment. The development and use of third and fourth-generation computers have made it possible for us to pass from the investigation of one-dimensional and two-dimensional motions to the mathematical modeling of motions in space, the characteristics of the medium depending on three space coordinates and time. In order to investigate the properties of a DS however it is often sufficient to restrict consideration to the equations for the one-dimensional case.

Modern applied mathematics employs a variety of methods for investigating [1] the properties of difference equations, such as their stability and approximation. The instability of a DS quickly becomes apparent on a finite grid and makes it impossible to continue the calculations. Approximation, on the other hand, is an asymptotic property of a DS and merely indicates the way the approximation errors vanish when the grid is refined. An approximation error is an infinite series of terms which are products of powers of the grid spacings and functions of the solution. These functions are different DS's. It is these functions that determine the quality of the DS on a finite grid. Consider for example, the following two ways the approximation error ω depends on the grid spacing h (a first and a second order DS):

$$\omega_1 = h, \quad \omega_2 = 100 \ h^2.$$

In terms of the rate of convergence $d\omega/dh$ the second DS is preferable to the first. On a finite grid, however, and for $h \geqslant 0.01$ we have $\omega_1 \leqslant \omega_2$, and the first DS turns out to be better than the second in terms of the approximation error.

To investigate the approximation error of a DS on a finite grid the notions of conservatism [1, 2, 3] and complete conservatism [4] of the DS were introduced. It was once believed for difference equations of gas dynamics [4] that the difference equation of energy could not be transformed from its nondivergence form to divergence form and vice versa using the other equations of DS. Naturally therefore several workers wanted to relate the properties of difference equations to their form. Thus [3] identifies the divergence of DS's with their conservatism and [1] identifies the conservatism of DS's with their divergence only if the auxiliary quantities on the faces of a grid cell are invariant under the space index. An analysis of the work so far carried out on the properties of the difference conservation laws indicates that the *a priori* theory of the conservatism of DS's is incomplete and that the estimates are inconsistent, because most writers prefer the divergence form for the equation of energy and the nondivergence form (density equals mass divided by volume) for the equation for the conservation of mass.

We consider a method for investigating the conservatism of a DS and use it to define the dissipative properties of some well-known DS's.

9.1   DIFFERENTIAL AND DIFFERENCE EQUATIONS

In the absence of viscosity, heat conduction, and energy sources, the equations for the conservation of mass, momentum, and energy for a perfect medium in Lagrange coordinates are:

$$\frac{\partial V}{\partial t} - \frac{\partial u}{\partial m} = 0, \tag{9.1.1}$$

$$\frac{\partial u}{\partial t} + \frac{\partial p}{\partial m} = 0, \tag{9.1.2}$$

$$\frac{\partial}{\partial t}(E + 0.5u^2) + \frac{\partial}{\partial m}(pu) = 0. \tag{9.1.3}$$

The system made up of (9.1.1) to (9.1.3) contains four unknown functions (V, the specific volume, p, the pressure, E, the specific internal energy, and u, the mass velocity) which depend on two independent variables (t, the time, and m, the Lagrange coordinate). It is known from thermodynamics that given a number of thermodynamic functions characterizing the state of a material two are independent and the others can be expressed in terms of them. Since (9.1.1)-(9.1.3) contain three thermodynamic functions, to close the system we need only add an equation of state

$$F(p, V, E) = 0.$$

The position of every particle in space is determined by its Euler coordinate $x = x(t, m)$ to find which we may use one of the equations

$$\left(\frac{\partial x}{\partial t}\right)_m - u = 0, \tag{9.1.4}$$

$$\left(\frac{\partial x}{\partial m}\right)_t - V = 0. \tag{9.1.5}$$

Equations (9.1.1), (9.1.4) and (9.1.5) are dependent, one of them following from the other two. We could consider also several equations which are consequences of (9.1.1)-(9.1.3) and other equations of thermodynamics. By multiplying (9.1.2) by u and subtracting from (9.1.3) we get

$$\frac{\partial E}{\partial t} + p\frac{\partial u}{\partial m} = 0. \tag{9.1.6}$$

By multiplying (9.1.1) by p and adding it to (9.1.6) we get

$$\frac{\partial E}{\partial t} + p\frac{\partial V}{\partial t} = 0. \tag{9.1.7}$$

Equations (9.1.6) and (9.1.7) follow from (9.1.1)-(9.1.3). It is possible to write out a great many consequences if we take into consideration the various thermodynamic functions (enthalpy, free energy, temperature, etc.). Of the functions that do not appear in (9.1.1) to (9.1.7) we shall only consider entropy, S, since it is known to remain constant along a streamline of motion in adiabatic flows.

Equations (9.1.1) to (9.1.7) contain three thermodynamic functions, p, V and E. Let V and E be independent. The equation of the rate of change of entropy $S(V, E)$ along a streamline

$$\frac{\partial S}{\partial t} = \left(\frac{\partial S}{\partial V}\right)_E \frac{\partial V}{\partial t} + \left(\frac{\partial S}{\partial E}\right)_V \frac{\partial E}{\partial t}$$

is transformed using familiar thermodynamic equations, i.e.

$$\left(\frac{\partial S}{\partial V}\right)_E + \left(\frac{\partial E}{\partial V}\right)_S\left(\frac{\partial S}{\partial E}\right)_V = 0, \quad \left(\frac{\partial E}{\partial S}\right)_V\left(\frac{\partial S}{\partial E}\right)_V = 1,$$

$$p = -\left(\frac{\partial E}{\partial V}\right)_S, \quad T = \left(\frac{\partial E}{\partial S}\right)_V$$

to the form

$$T\frac{\partial S}{\partial t} = \frac{\partial E}{\partial t} + p\frac{\partial V}{\partial t}. \tag{9.1.8}$$

Equations (9.1.7) and (9.1.8) yield the equation for the conservation of entropy along a streamline

$$T\frac{\partial S}{\partial t} = 0. \tag{9.1.9}$$

Equation (9.1.9) like (9.1.6) and (9.1.7), is a consequence of (9.1.1)-(9.1.3) and the thermodynamic equations.

An analysis of other familiar thermodynamic functions shows that none of them remain constant along a trajectory.

Finally, let us consider the equation of state $F(p, V, E) = 0$ in greater detail. By differentiating it with respect to t we obtain the rate of change of pressure

$$\frac{\partial p}{\partial t} = \left(\frac{\partial p}{\partial V}\right)_E \frac{\partial V}{\partial t} + \left(\frac{\partial p}{\partial E}\right)_V \frac{\partial E}{\partial t}.$$

Substituting the $\frac{\partial E}{\partial t}$ from (9.1.6) or (9.1.7) into this we get

$$\frac{\partial p}{\partial t} + a^2 \frac{\partial u}{\partial m} = 0, \qquad (9.1.10)$$

$$\frac{\partial p}{\partial t} + a^2 \frac{\partial V}{\partial t} = 0, \qquad (9.1.11)$$

where

$$a^2 = -\left(\frac{\partial p}{\partial V}\right)_S = -\left(\frac{\partial p}{\partial V}\right)_E + p\left(\frac{\partial p}{\partial E}\right)_V.$$

For numerical integration the differential equations are replaced by difference equations. We shall consider below difference equations in differential form. Obtaining difference equations for gas dynamics in differential form and investigating their properties are discussed in more detail in [5].

We shall investigate difference equations approximating (9.1.1) to (9.1.7) and (9.1.9) to (9.1.11) in the form

$$\frac{\partial V}{\partial t} - \frac{\partial u}{\partial m} = \omega_1, \quad \frac{\partial u}{\partial t} + \frac{\partial p}{\partial m} = \omega_2, \qquad (9.1.12),\ (9.1.13)$$

$$\frac{\partial}{\partial t}(E + 0.5u^2) + \frac{\partial}{\partial m}(pu) = \omega_3, \qquad (9.1.14)$$

$$\frac{\partial x}{\partial t} - u = \omega_4, \quad \frac{\partial x}{\partial m} - V = \omega_5, \qquad (9.1.15),\ (9.1.16)$$

$$\frac{\partial E}{\partial t} + p\frac{\partial u}{\partial m} = \omega_6, \quad \frac{\partial E}{\partial t} + p\frac{\partial V}{\partial t} = \omega_7, \qquad (9.1.17),\ (9.1.18)$$

$$T\frac{\partial S}{\partial t} = \omega_8, \qquad (9.1.19)$$

$$\frac{\partial p}{\partial t} + a^2 \frac{\partial u}{\partial m} = \omega_9, \quad \frac{\partial p}{\partial t} + a^2 \frac{\partial V}{\partial t} = \omega_{10}. \qquad (9.1.20),\ (9.1.21)$$

Here ω_i $(i = 1, \ldots, 10)$ are the errors in the approximation of equations (9.1.1) to (9.1.7) and (9.1.9) to (9.1.11) by equations (9.1.12) to (9.1.21) respectively, and have the form

$$\omega_i \sum_{k=0,\ l=0}^{\infty} A_{ikl}\tau^k h^l, \quad (k+l \geqslant 1), \qquad (9.1.22)$$

where the A_{ikl} contain partial derivatives of the functions appearing in the corresponding difference equations and are independent of τ and h.

9.2 TRANSFORMABILITY OF THE FORMS OF DIFFERENCE EQUATIONS

We restrict our consideration here to difference equations (9.1.12) to (9.1.21). In general, this system of equations does not contain all the consequences of the conservation laws since we did not consider every thermodynamic function. However, the only thermodynamic quantity conserved along a streamline, entropy, is in the system of (9.1.12) to (9.1.21). Increasing therefore the number of equations to be considered by including the other thermodynamic functions makes little sense when investigating the conservatism of a DS, although it does play a role when determining the type of a DS. This however is beyond the scope of this paper.

The system of (9.1.12) to (9.1.21), which contains 10 equations and 4 independent functions (x, u and two thermodynamic functions), is overdetermined. To find a numerical solution only some of the equations need be used. Constructing a particular DS consists in choosing the required number of equations from (9.1.12)-(9.1.21), i.e. in choosing particular ω_i. Following well-established terminology [4] we shall refer to the difference equations of (9.1.12) to (9.1.14) as equation in the divergence form and to equations (9.1.15) to (9.1.21) as equations in the nondivergence form or simply as divergent and nondivergent equations.

Theorem 9.1. The divergent difference equations of gas dynamics can be transformed into equations in the nondivergence form and vice versa by using the other equations of the DS.

Proof. We transform the left-hand sides of (9.1.12) to (9.1.21) and obtain a system of equations that contain ω_i from the difference equations of (9.1.12) to (9.1.21). We multiply (9.1.12) by p, add it to (9.1.17) and subtract (9.1.18) from the resulting expression

$$p\omega_1 + \omega_6 - \omega_7 = 0 \qquad (9.2.1)$$

We differentiate (9.1.15) with respect to m and (9.1.16) with respect to t

$$\frac{\partial^2 x}{\partial m\, \partial t} - \frac{\partial u}{\partial m} = \bar{\omega}_4, \quad \frac{\partial^2 x}{\partial t\, \partial m} - \frac{\partial V}{\partial t} = \bar{\omega}_5,$$

where $\bar{\omega}_4 = \frac{\partial \omega_4}{\partial m}$ and $\bar{\omega}_5 = \frac{\partial \omega_5}{\partial t}$. We then express $\frac{\partial u}{\partial m}$ and $\frac{\partial V}{\partial t}$, omitting the bar above $\bar{\omega}_4$ and $\bar{\omega}_5$, for convenience and substitute them into (9.1.12):

$$\omega_1 - \omega_4 + \omega_5 = 0. \qquad (9.2.2)$$

We multiply (9.1.13) by u, subtract (9.1.14) from the resulting expression and add (9.1.17) to get

$$u\omega_2 - \omega_3 + \omega_6 = 0. \tag{9.2.3}$$

We next substitute (9.1.18) and (9.1.19) into (9.1.8), hence

$$\omega_7 - \omega_8 = 0. \tag{9.2.4}$$

By multiplying (9.1.12) by a^2, adding it to (9.1.20) and subtracting (9.1.21) we get

$$a^2\omega_1 + \omega_9 - \omega_{10} = 0. \tag{9.2.5}$$

Finally, (9.1.18), (9.1.21), and the equation for the rate of increase of pressure yield

$$\left(\frac{\partial p}{\partial E}\right)_V \omega_7 - \omega_{10} = 0. \tag{9.2.6}$$

Equations (9.2.1) to (9.2.6) form a system of six equations linear in ω_i with two unknowns. The rank of the matrix of coefficients of the system is six. Hence the system formed by (9.2.1) to (9.2.6) has fundamental solutions, each consisting of six linearly independent solutions. The number of fundamental solutions $K \leqslant C_{10}^6 = 210$. Let us consider them. We begin with the most common type of DS in the literature, i.e. in which ω_2, ω_3, ω_4, and ω_5 are independent. We transfer the terms of the equations that correspond to elements 2 to 5 of the columns to the right-hand sides of the equations. As a result we obtain a system of nonhomogeneous equations linear in ω_i. The matrix of this system

$$A_1 = \begin{Vmatrix} p & 1 & -1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 \\ a^2 & 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & \frac{\partial p}{\partial E} & 0 & 0 & -1 \end{Vmatrix}$$

and the augmented matrix

$$B_1 = \begin{Vmatrix} p & 1 & -1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & \omega_4 - \omega_5 \\ 0 & 1 & 0 & 0 & 0 & 0 & \omega_3 - u\omega_2 \\ 0 & 0 & 1 & -1 & 0 & 0 & 0 \\ a^2 & 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & \frac{\partial p}{\partial E} & 0 & 0 & -1 & 0 \end{Vmatrix}$$

both have rank $r = 6$. Consequently the system is compatible, the fundamental solution exists and is of the form

$$\omega_1 = \omega_4 - \omega_5,$$

$$\omega_6 = -u\omega_2 + \omega_3,$$

$$\omega_7 = p(\omega_4 - \omega_5) - u\omega_2 + \omega_3,$$

$$\omega_8 = p(\omega_4 - \omega_5) - u\omega_2 + \omega_3,$$

$$\omega_9 = \left(p\frac{\partial p}{\partial E} - a^2\right)(\omega_4 - \omega_5) + \frac{\partial p}{\partial E}(\omega_3 - u\omega_2),$$

$$\omega_{10} = \frac{\partial p}{\partial E}(p(\omega_4 - \omega_5) - u\omega_2 + \omega_3).$$

By considering all of the 210 systems in a similar way we find that only some of them are compatible, and hence that there are less than 210 fundamental solutions. We shall restrict ourselves to constructing fundamental solutions for those types of DS's which are found in the literature. The DS type numbering and their corresponding sets of independent and dependent ω_i are given in Table 9.1.

Table 9.1

DS type	Independent				Dependent					
1	ω_2	ω_3	ω_4	ω_5	ω_1	ω_6	ω_7	ω_8	ω_9	ω_{10}
2	ω_2	ω_4	ω_5	ω_6	ω_1	ω_3	ω_7	ω_8	ω_9	ω_{10}
3	ω_2	ω_4	ω_5	ω_7	ω_1	ω_3	ω_6	ω_8	ω_9	ω_{10}
4	ω_1	ω_2	ω_3	ω_4	ω_5	ω_6	ω_7	ω_8	ω_9	ω_{10}
5	ω_1	ω_2	ω_4	ω_6	ω_3	ω_5	ω_7	ω_8	ω_9	ω_{10}
6	ω_1	ω_2	ω_4	ω_7	ω_3	ω_5	ω_6	ω_8	ω_9	ω_{10}

The existence of these fundamental solutions implies that:

1. If a DS uses the energy equation of (9.1.14) in divergence form, then it can be transformed by using the corresponding fundamental solution to any of equations (9.1.17) to (9.1.18) in nondivergence form (DS of type 1).

2. If a DS uses the energy equation of (9.1.17) or (9.1.18) in nondivergence form, then it can be transformed by using the corresponding fundamental solution to equation (9.1.14) in divergence form (DS of types 2 and 3).

3. If a DS uses the mass conservation equation of (9.1.12) in divergence form, then it can be transformed to the mass conservation equation of (9.1.16) in nondivergence form (DS of types 4, 5, and 6).

4. If a DS uses the mass conservation equation of (9.1.16) in non-divergence form, then it can be transformed to the equation of (9.1.12) in divergence form (DS of types 1, 2, and 3).

The theorem is proved.

9.3   THE CONSERVATISM AND DISSIPATIVE PROPERTIES OF A DIFFERENCE SCHEME

Definition. If a difference scheme preserves unchanged one, or a combination, of the functions that appear in equations (9.1.12) to (9.1.21), or preserves unchanged integrals of combinations of functions over any domain or contour then it is called conservative.

Of the functions in (9.1.1)-(9.1.7), or (9.1.9), only S and m are constant along a streamline. When considering a DS we must restrict our attention as to whether they preserve S and m exactly or approximately along a streamline. Since these properties become apparent on every streamline, they are local properties of conservatism.

Theorem 9.2. The necessary and sufficient condition for a difference scheme to be M-conservative is that

$$\bar{\omega}_5 = \omega_M, \tag{9.3.1}$$

where

$$\omega_M = -\sum_{k=1}^{\infty} \frac{\Delta m^{2k}}{2^{2k}(2k+1)!} \frac{\partial^{2(k+1)}x}{\partial t\,\partial m^{2k+1}}$$

Proof. Consider the difference mass-conservation equation in non divergence form

$$\frac{\Delta x}{\Delta m} = V, \tag{9.3.2}$$

where $\Delta x = x_1 - x_{-1}$. We expand x_1 and x_{-1} into Taylor series about the point $x_0 = 0.5\,(x_1 + x_{-1})$ and substitute them into (9.3.2):

$$\frac{\Delta x}{\Delta m} - V = \frac{\partial x}{\partial m} - V + \sum_{k=1}^{\infty} \frac{\Delta m^{2k}}{2^{2k}(2k+1)!} \frac{\partial^{2k+1}x}{\partial m^{2k+1}} = 0.$$

Equation (9.1.16) is subtracted from this to get

$$\omega_5 + \sum_{k=1}^{\infty} \frac{\Delta m^{2k}}{2^{2k}(2k+1)!} \frac{\partial^{2k+1}x}{\partial m^{2k+1}} = 0. \tag{9.3.3}$$

Differentiating (9.3.3) with respect to t and then obtaining the expression for $\frac{\partial \Delta m}{\partial t}$, we get

$$\frac{\partial \Delta m}{\partial t} = \frac{\omega_M - \bar{\omega}_5}{\sum_{k=1}^{\infty} \frac{2k\Delta m^{2k-1}}{2^{2k}(2k+1)!} \frac{\partial^{2k+1}x}{\partial m^{2k+1}}}. \tag{9.3.4}$$

Necessity. Suppose that (9.3.1) does not hold, i.e. that $\bar{\omega}_5 \neq \omega_M$. Then it follows from (9.3.4) that

$$\frac{\partial \Delta m}{\partial t} \neq 0$$

along the streamline and that the mass is not conserved.

Sufficiency. Let $\frac{\partial \Delta m}{\partial t} = 0$. Then (9.3.4) implies (9.3.1).

The theorem is proved.

Corollary 9.1. A DS containing the mass-conservation equation of (9.1.16) in nondivergence form is always M-conservative.

Corollary 9.2. A DS containing the mass-conservation equation of (9.1.12) in divergence form is M-conservative provided

$$\bar{\omega}_4 - \omega_1 = \omega_M. \tag{9.3.5}$$

Indeed ω_1 and $\bar{\omega}_4$ are known in DS's of types 4, 5, and 6. According to Theorem 9.2.1 and using the appropriate fundamental solution we get

$$\bar{\omega}_5 = \bar{\omega}_4 - \omega_1. \tag{9.3.6}$$

If this $\bar{\omega}_5$ satisfies (9.3.1), then the DS's of types 4, 5, and 6 are all M-conservative. But if $\bar{\omega}_5 \neq \omega_M$, then the DS's are M-conservative.

Since ω_M and $\bar{\omega}_5$ are approximation errors of the form in (9.1.22), the mass-production equation (9.3.4) has the following form in M-nonconservative DS's

$$\frac{\partial \Delta m}{\partial t} = \sum_{k=0,\,l=0}^{\infty} B_{mkl}\tau^k h^l, \quad (k+l \geqslant 1). \tag{9.3.7}$$

Definition. The nth differential approximation of a DS is M-conservative if $B_{Mkl} = 0$ for all $k + l \leqslant n$ in the mass-production equation of (9.3.7).

Theorem 9.3. The necessary and sufficient condition for a difference scheme to be S-conservative is that

$$\omega_8 = 0. \tag{9.3.8}$$

Necessity. Suppose that $\omega_8 \neq 0$. When it is substituted into (9.1.19) we get $\frac{\partial S}{\partial t} \neq 0$. The entropy changes.

Sufficiency. Let $\frac{\partial S}{\partial t} = 0$. When $\frac{\partial S}{\partial t}$ is substituted into (9.1.19), we get (9.3.8).

The theorem is proved.

None of the DS types given in Table 9.1 has an independent ω_8. For each DS type ω_8 must be expressed in terms of independent ω_i thus:

Type 1. $\omega_8 = p\,(\overline{\omega}_4 - \overline{\omega}_5) + \omega_3 - u\omega_2$,

Type 2. $\omega_8 = p\,(\overline{\omega}_4 - \overline{\omega}_5) + \omega_6$,

Type 3. $\omega_8 = \omega_7$,

Type 4. $\omega_8 = p\omega_1 + \omega_3 - u\omega_2$,   (9.3.9)

Type 5. $\omega_8 = p\omega_1 + \omega_6$,

Type 6. $\omega_8 = \omega_7$.

Evaluating the changes in entropy along a streamline over time is an effective way of controlling locally the accuracy of a thermodynamic calculation. Since all ω_i are of the form of (9.1.22), we can obtain a general entropy-production equation from (9.3.9) and (9.1.19), viz.

$$T\frac{\partial S}{\partial t} = \sum_{k=0,\,l=0}^{\infty} B_{Skl}\tau^k h^l, \quad (k+l \geqslant 1). \qquad (9.3.10)$$

Definition. The nth differential approximation of a DS is S-conservative if $B_{Skl} = 0$ for all $k + l \leqslant n$ in entropy-production equation (9.3.10).

Consider DS's of types 1 and 4 with the divergent equation of energy of (9.1.14). It follows from (9.3.9) that the right-hand side of entropy-production equation (9.3.10) may contain values of the mass velocity u and the derivatives $\frac{\partial^\nu u}{\partial t^\nu}$. This means that the class of DS's with the divergent equation of energy contains schemes in which the entropy changes when an undeformable material is translated or accelerated, and this contradicts the laws of thermodynamics.

Definition. A DS is said to be thermodynamically normal if the rate of entropy production in it is independent of the mass velocity and acceleration of the material. But if $\frac{\partial S}{\partial t}$ does depend on u or on $\frac{\partial^\nu u}{\partial t^\nu}$, then the DS is thermodynamically abnormal.

Definition. The nth differential approximation of a DS is said to be thermodynamically normal if the B_{Skl} functions of (9.3.10), for which $k + l \leqslant n$, do not contain the mass velocity of the mate-

rial or its acceleration $\frac{\partial^\nu u}{\partial t^\nu}$; if they do, it is thermodynamically abnormal.

To determine whether a divergent DS is thermodynamically normal the right-hand side of (9.3.10) must be investigated and it has to be shown that it is independent of u and $\frac{\partial^\nu u}{\partial t^\nu}$.

It is obvious that changes in entropy due to approximation errors must not exceed its changes in characteristic physical processes. As an illustration consider a weak shock wave at whose front we have the equation

$$E - E_0 = -0.5\,(p + p_0)\,(V - V_0) \qquad (9.3.11)$$

relating the values of p_0, V_0, and E_0 before the discontinuity to the values of the p, V and E after it. We represent E and p as Taylor series at the point p_0, V_0, E_0:

$$E = E_0 + \left(\frac{\partial E}{\partial V}\right)_S \Delta V + \frac{1}{2}\left(\frac{\partial^2 E}{\partial V^2}\right)_S \Delta V^2$$
$$+ \frac{1}{6}\left(\frac{\partial^3 E}{\partial V^3}\right)_S \Delta V^3 + \left(\frac{\partial E}{\partial S}\right)_V \Delta S + \frac{1}{2}\left(\frac{\partial^2 E}{\partial S^2}\right)_V \Delta S^2 + \ldots,$$

$$p = p_0 + \left(\frac{\partial p}{\partial V}\right)_S \Delta V + \frac{1}{2}\left(\frac{\partial^2 p}{\partial V^2}\right)_S \Delta V^2 + \left(\frac{\partial p}{\partial S}\right)_V \Delta S + \ldots,$$

where $\Delta V = V - V_0$ and $\Delta S = S - S_0$. By substituting E and p in (9.3.11) and using $T = \left(\frac{\partial E}{\partial S}\right)_V$ and $p = -\left(\frac{\partial E}{\partial V}\right)_S$ we get

$$T_0 \Delta S = -\frac{1}{12}\left(\frac{\partial^2 p}{\partial V^2}\right)_S \Delta V^3 + O\,(\Delta V^4, \Delta S^2). \qquad (9.3.12)$$

Thus the change in the entropy on a weak shock wave is proportional to the cube of the change in the specific volume. This well-known [6] equation, (9.3.12), will be used as the accuracy criterion for the calculation of entropy. Assuming that S and V depend on time t and that ΔS and ΔV are changes in S and V for a single time step τ, we represent them as Taylor series. By substituting these series into (9.3.12) we get

$$T\frac{\partial S}{\partial t} = \omega_S,$$

where

$$\omega_S = -\frac{\tau^2}{12}\left(\frac{\partial^2 p}{\partial V^2}\right)_S \left(\frac{\partial V}{\partial t}\right)^3 + \ldots. \qquad (9.3.13)$$

Equation (9.3.13) makes it possible to divide DS's as strongly dissipative and weakly dissipative schemes.

Definition. A DS is said to be strongly dissipative if the FDA (first differential approximation) of its entropy-production equation is S-nonconservative.

Definition. A DS is said to be weakly dissipative if the FDA of its entropy-production equation is S-conservative.

9.4 AN ANALYSIS OF THE S-CONSERVATISM OF SOME DIFFERENCE SCHEMES FOR THE GAS-DYNAMICS EQUATIONS

We discuss to what degree of accuracy the law of the conservation of entropy is satisfied in DS's with the divergent and the nondivergent equation of energy. A detailed analysis of the changes in entropy in some DS's is given in [7]. Here we partly repeat this analysis but in a different form and for a wider class of equations.

We first examine the S-conservatism of DS's of type 4. Let the unknown quantities p, V, E, u, S and T be defined at grid points with half-integer indices (referred to the midpoints of grid intervals). Following [7] we write the difference equations in their general form, viz.

$$\frac{V_{i+0.5}^{n+1} - V_{i+0.5}^{n}}{\tau} - \frac{u_{i+1}^{*} - u_i^{*}}{h} = 0,$$

$$\frac{u_{i+0.5}^{n+1} - u_{i+0.5}^{n}}{\tau} + \frac{p_{i+1}^{*} - p_i^{*}}{h} = 0, \qquad (9.4.1)$$

$$\frac{E_{i+0.5}^{n+1} - E_{i+0.5}^{n}}{\tau} + \frac{(u_{i+0.5}^{n+1})^2 - (u_{i+0.5}^{n})^2}{2\tau} + \frac{p_{i+1}^{*} u_{i+1}^{*} - p_i^{*} u_i^{*}}{h} = 0.$$

The quantities with an asterisk are auxiliary quantities.

We examine the character of the changes in the entropy in some difference schemes of the two-parameter family of the IIIA schemes of [7] where the auxiliary quantities are defined by the formulas

$$u_i^{*} = 0.5\left((1 - l_1)(u_{i+0.5}^{n} + u_{i-0.5}^{n}) + l_1(u_{i+0.5}^{n+1} + u_{i-0.5}^{n+1})\right),$$

$$\qquad (9.4.2)$$

$$p_i^{*} = 0.5\left((1 - l_2)(p_{i+0.5}^{n} + p_{i-0.5}^{n}) + l_2(p_{i+0.5}^{n+1} + p_{i-0.5}^{n+1})\right).$$

In the general case, the independent ω_i for the family of DS's under consideration have the form

$$\omega_1 = \tau\,(l_1 - 0.5)\frac{\partial^2 V}{\partial t^2} - \tau^2\left(l_1^2 - l_1 + \frac{1}{6}\right)\frac{\partial^3 V}{\partial t^3} + O(\tau^3,\ h^2),$$

$$\omega_2 = \tau\,(l_2 - 0.5)\frac{\partial^2 u}{\partial t^2} - \tau^2\left(l_2^2 - l_2 + \frac{1}{6}\right)\frac{\partial^3 u}{\partial t^3} + O(\tau^3,\ h^2),$$

$$\omega_3 = -\tau\left[(l_1 - 0.5)\frac{\partial}{\partial m}\left(p\,\frac{\partial u}{\partial t}\right) + (l_2 - 0.5)\frac{\partial}{\partial m}\left(u\,\frac{\partial p}{\partial t}\right)\right]$$

$$-\frac{\tau^2}{12}\left[p\,\frac{\partial^3 V}{\partial t^3} + \frac{\partial^2 p}{\partial t^2}\frac{\partial V}{\partial t} - \frac{\partial p}{\partial t}\frac{\partial^2 V}{\partial t^2} - u\,\frac{\partial^3 u}{\partial t^3}\right.$$

$$\qquad (9.4.3)$$

$$\left. + 12\,(l_1 - 0.5)(l_2 - 0.5)\frac{\partial}{\partial m}\left(\frac{\partial p}{\partial t}\frac{\partial u}{\partial t}\right)\right] + O(\tau^3,\ h^2).$$

When (9.4.3) is substituted into type 1 of (9.3.9) and the ω_8 is substituted into (9.1.19) we obtain an entropy-production equation from which it follows that those type IIIA DS's, for which $l_1 \neq l_2$ and $l_1 = l_2 \neq 0.5$, are thermodynamically abnormal and strongly dissipative. The only DS of this family, for which $l_1 = l_2 = 0.5$, has the entropy-production equation of the form

$$T\,\frac{\partial S}{\partial t} = -\frac{\tau^2}{12}\left(\frac{\partial^2 p}{\partial t^2}\frac{\partial V}{\partial t} - \frac{\partial p}{\partial t}\frac{\partial^2 V}{\partial t^2}\right) + O(\tau^3,\ h^2). \qquad (9.4\ 4)$$

In other words, the FDA of that difference scheme is S-conservative and its second differential approximation is thermodynamically normal.

We use the equations

$$\frac{\partial p}{\partial t} = \left(\frac{\partial p}{\partial V}\right)_S\frac{\partial V}{\partial t}, \quad \frac{\partial^2 p}{\partial t^2} = \left(\frac{\partial^2 p}{\partial V^2}\right)_S\left(\frac{\partial V}{\partial t}\right)^2 + \left(\frac{\partial p}{\partial V}\right)_S\frac{\partial^2 V}{\partial t^2}$$

and simplify (9.4.4) to get

$$T\,\frac{\partial S}{\partial t} = -\frac{\tau^2}{12}\left(\frac{\partial^2 p}{\partial V^2}\right)_S\left(\frac{\partial V}{\partial t}\right)^3 + O(\tau^3,\ h^2) \qquad (9.4.5)$$

Thus the principal term in (9.4.5) coincides with (9.3.13) and hence the errors arising in determining the entropy in that scheme do not exceed its changes on weak shock waves. In other words, none of the IIIA DS's of [7] are weakly dissipative except for the one with $l_1 = l_2 = 0.5$. The other DS's are thermodynamically abnormal and cannot be recommended for calculations. We show that the dissipative properties of IIIA DS's remain unchanged if the mass-conservation equation of (9.1.12) is replaced by the nondivergent equation of (9.1.16) in the form

$$\frac{x_{i+1}^{n+1} - x_i^{n+1}}{h} - V_{i+0.5}^{n+1} = 0$$

and the equation of the streamline is taken in the form

$$\frac{x_i^{n+1} - x_i^{n}}{\tau} - u_i^{*} = 0$$

The DS containing these equations belongs to type 1. If we take u_i^{*} and p_i^{*} in the form of (9.4.2), then the independent approximation errors ω_2 and ω_3 have the same form they do in (9.4.3) and the $\bar{\omega}_4$

and $\overline{\omega}_5$ are as follows:

$$\overline{\omega}_4 = (l_1 - 0.5)\,\tau\,\frac{\partial^2 u}{\partial t\,\partial m} + \frac{\tau^2}{12}\,\frac{\partial^3 u}{\partial m\,\partial t^2} + \frac{h^2}{8}\,\frac{\partial^3 u}{\partial m^3} + \cdots .$$

$$\overline{\omega}_5 = -\frac{h^2}{24}\,\frac{\partial^3 u}{\partial m^3} + \cdots .$$

By substituting ω_2, ω_3, $\overline{\omega}_4$, and $\overline{\omega}_5$ into (9.1.19) we obtain an entropy-production equation from which it follows that when $l_1 \neq l_2$, $l_1 \neq 0.5$ or $l_2 \neq 0.5$ the DS's are thermodynamically abnormal and strongly dissipative. When $l_1 = l_2 = 0.5$ the entropy-production equation is of the form (9.4.4). This scheme is weakly dissipative and thermodynamically normal.

Now we consider the second two-parameter family of schemes IIIB of [7], where the auxiliary quantities are defined as follows:

$$u_i^* = 0.5\,(u_{i+0.5}^n + u_{i-0.5}^n) - \frac{\tau l_3}{h}\,(p_{i+0.5}^n - p_{i-0.5}^n),$$

$$p_i^* = 0.5\,(p_{i+0.5}^n + p_{i-0.5}^n) - \frac{\tau l_4}{h}\,(u_{i+0.5}^n - u_{i-0.5}^n). \qquad (9.4.6)$$

In differential form, together with (9.4.1) the equations of (9.4.6) assume the forms in (9.1.12) to (9.1.14), where

$$\omega_1 = (l_3 - 0.5)\,\tau\,\frac{\partial^2 V}{\partial t^2} + O\,(\tau^2,\ h^2),$$

$$\omega_2 = \tau\left(l_4\,\frac{\partial^2 u}{\partial m^2} - 0.5\,\frac{\partial^2 u}{\partial t^2}\right) + O\,(\tau^2,\ h^2),$$

$$\omega_3 = \tau\left(0.5\,\frac{\partial p}{\partial t}\,\frac{\partial V}{\partial t} + l_4\left(\frac{\partial V}{\partial t}\right)^2 - 0.5u\,\frac{\partial^2 u}{\partial t^2} + l_4 u\,\frac{\partial^2 u}{\partial m^2}\right)$$
$$- \tau\,(l_3 - 0.5)\left(p\,\frac{\partial^2 V}{\partial t^2} - \left(\frac{\partial u}{\partial t}\right)^2\right) + O\,(\tau^2,\ h^2).$$

By substituting ω_1, ω_2, and ω_3 into (9.3.9) and (9.1.18) we get

$$T\,\frac{\partial s}{\partial t} = \tau\left((l_3 - 0.5)\left(\frac{\partial u}{\partial t}\right)^2\right.$$
$$+ \left.\left(0.5\left(\frac{\partial p}{\partial V}\right)_s + l_4\right)\left(\frac{\partial V}{\partial t}\right)^2\right) + O\,(\tau^2,\ h^2).$$

It follows from this that the FDA's of all the DS's in this family, for which $l_3 \neq 0.5$, are thermodynamically abnormal, but the DS, for which $l_3 = 0.5$ and $l = 0.5\,a^2$, is thermodynamically normal and strongly dissipative.

Godunov's scheme [8] is obtained for IIIB DS with $l_3 = \dfrac{h}{2\tau a}$ and $l_4 = \dfrac{ha}{2\tau}$, where $a = \sqrt{-\left(\dfrac{\partial p}{\partial V}\right)_s}$ is the velocity of sound. In this scheme $l_3 = 0.5$ and $l_4 = 0.5$ only when the grid spacing ratio

$\dfrac{\tau a}{h} = 1$. For other spacing ratios, i.e. $\dfrac{\tau a}{h} < 1$, the FDA of the scheme is thermodynamically abnormal.

In Lax's scheme [9], which is obtained for a IIIB DS with $l_3 = \dfrac{1}{2}\left(\dfrac{h}{\tau a}\right)^2$ and $l_4 = \dfrac{1}{2}\left(\dfrac{h}{\tau}\right)^2$, the FDA is also abnormal for $\dfrac{\tau a}{h} < 1$.

We now consider the dissipative properties of a type 4 DS [10] in which the auxiliary quantities are defined in terms of functions that have discontinuities at the contact boundaries. In the mass-conservation and momentum (9.4.1) equations the auxiliary values of velocity and pressure are taken as:

$$u_i^* = 0.25\left[u_{i+0.5}^n + u_{i-0.5}^n + u_{i+0.5}^{n+1} + u_{i-0.5}^{n+1}\right.$$
$$- \left.\frac{h}{\tau}\,(V_{i+0.5}^{n+1} - V_{i+0.5}^n - V_{i-0.5}^{n+1} + V_{i-0.5}^n)\right],$$

$$p_i^* = 0.25\left[p_{i+0.5}^n + p_{i-0.5}^n + p_{i+0.5}^{n+1} + p_{i-0.5}^{n+1}\right.$$
$$+ \left.\frac{h}{\tau}\,(u_{i+0.5}^{n+1} - u_{i+0.5}^n - u_{i-0.5}^{n+1} + u_{i-0.5}^n)\right].$$

In the energy equation (9.4.1) the auxiliary values $(pu)_i^*$ are chosen according to the formula

$$(pu)_i^* = 0.5\,[(pu)_{i+0.5}^{n+1} + (pu)_{i-0.5}^{n+1}]$$
$$+ \frac{h}{4\tau}\,(\varepsilon_{i+0.5}^{n+1} - \varepsilon_{i+0.5}^n - \varepsilon_{i-0.5}^{n+1} + \varepsilon_{i-0.5}^n),$$

where $\varepsilon = E + 0.5u^2$. The approximation errors in this DS are of the form

$$\omega_1 = \frac{\tau^2}{12}\,\frac{\partial^3 V}{\partial t^3} - \frac{h^2}{12}\,\frac{\partial^3 u}{\partial m^3} + O\,(\tau^3,\ h^3),$$

$$\omega_2 = \frac{\tau^2}{12}\,\frac{\partial^3 u}{\partial t^3} + \frac{h^2}{12}\,\frac{\partial^3 p}{\partial m^3} + O\,(\tau^3,\ h^3),$$

$$\omega_3 = \frac{\tau}{2}\left(\frac{\partial^2 E}{\partial t^2} + u\,\frac{\partial^2 u}{\partial t^2} + \left(\frac{\partial u}{\partial t}\right)^2\right)$$
$$- \frac{\tau^2}{6}\,\frac{\partial^3 \varepsilon}{\partial t^3} + \frac{h^2}{12}\,\frac{\partial^3 (pu)}{\partial m^3} + O\,(\tau^3,\ h^3).$$

By substituting these ω_1, ω_2, and ω_3 into (9.3.9) and (9.1.19) we get

$$T\,\frac{\partial S}{\partial t} = \frac{\tau}{2}\left[\frac{\partial^2 E}{\partial t^2} + u\,\frac{\partial^2 u}{\partial t^2} + \left(\frac{\partial u}{\partial t}\right)^2\right] + O\,(\tau^2,\ h^2).$$

Hence the DS of [10] is thermodynamically abnormal and strongly dissipative on adiabatic solutions.

We now consider types 5 and 6 DS's with the energy equation in nondivergence form. A "completely conservative" DS with $\sigma_1 = 1$, $\sigma_2 = 0$ and $\sigma_4 = 0.5$ is recommended in [4]. The difference equations in this scheme are of the form:

$$\frac{V_{i+0.5}^{n+1} - V_{i+0.5}^n}{\tau} - \frac{u_{i+1}^n - u_i^n}{h} = 0,$$

$$\frac{u_i^{n+1} - u_i^n}{\tau} + \frac{p_{i+0.5}^{n+1} - p_{i-0.5}^{n+1}}{h} = 0, \qquad (9.4.7)$$

$$\frac{E_{i+0.5}^{n+1} - E_{i+0.5}^n}{\tau} + p_{i+0.5}^n \frac{u_{i+1}^n + u_{i+1}^{n+1} - u_i^n - u_i^{n+1}}{2h} = 0.$$

We write the first two equations in the differential form of (9.1.12)–(9.1.13) with the approximation errors

$$\omega_1 = -0.5\tau \frac{\partial^2 V}{\partial t^2} + O(\tau^2, h^2),$$

$$\omega_2 = -0.5\tau \frac{\partial^2 u}{\partial t^2} + O(\tau^2, h^2).$$

The third equation of (9.4.7) is written in form (9.1.17), where

$$\omega_6 = -0.5\tau \frac{\partial p}{\partial t} \frac{\partial V}{\partial t} = O(\tau^2, h^2).$$

By substituting these ω_1 and ω_6 into (9.3.9) and (9.1.19) we get

$$T \frac{\partial S}{\partial t} = -0.5\tau \frac{\partial}{\partial t}\left(p \frac{\partial V}{\partial t}\right) + O(\tau^2, h^2). \qquad (9.4.8)$$

In this DS the FDA is S-nonconservative.

Equation (9.4.8) implies that the approximation errors in the "completely conservative" DS in question are more powerful sources of entropy than physical sources (weak shock waves). "Complete conservatism" does not remove these sources.

The class of "completely conservative" DS's has weakly dissipative schemes in which the computational sources of entropy do not exceed physical sources by an order of magnitude. An example is the DS of [4] with $\sigma_1 = \sigma_2 = \sigma_4 = 0.5$ which coincides with the DS of [11]. In these DS's the approximation errors are of order τ^2 and their FDA's are S-conservative.

We now consider DS's with the nondivergent energy equation of (9.1.18). Following [7] we approximate (9.1.7) by a one-parameter family of difference schemes

$$\frac{E^{n+1} - E^n}{\tau} + ((1-\beta)p^{n+1} + \beta p^n) \frac{V^{n+1} - V^n}{\tau} = 0. \qquad (9.4.9)$$

Transforming (9.4.9) to the differential form of (9.1.18) we get

$$\omega_7 = \tau \left(\frac{\partial p}{\partial V}\right)_S \left(\frac{\partial V}{\partial t}\right)^2 (\beta - 0.5) - \tau^2 \left(\frac{\partial^2 P}{\partial V^2}\right)_S \left(\frac{\partial V}{\partial t}\right)^3$$

$$\times \left(\beta^2 - \beta + \frac{1}{3}\right) - \tau^2 \left(\frac{\partial p}{\partial V}\right)_S \frac{\partial V}{\partial t} \frac{\partial^2 V}{\partial t^2} 2(\beta - 0.5)^2 + O(\tau^3). \qquad (9.4.10)$$

It follows from (9.4.10) that regardless of the value of β, all the DS's of that family are thermodynamically normal. In one DS obtained from (9.4.9) for $\beta = 0.5$ we find that $\omega_7 = \omega_s$ of (9.3.13) and that DS is weakly dissipative. All the other DS's obtained from (9.4.9), (9.1.18) and (9.4.10) for $\beta \neq 0.5$ are strongly dissipative.

The difference energy equation of (9.4.9) was first used by Neumann and Richtmyer [12]. This class also contains the difference schemes of [13] and [14].

9.5   CONCLUSIONS

The above discussion as well as a number of other examples [15] suggest the following:

1. The properties of M and S-conservatism are not related to the form of difference equations, i.e. whether they are in divergent or nondivergent form.
2. The construction of the entropy-production equation for every DS allows the dissipative properties of that DS to be determined.
3. Some of the DS's with the divergent energy equation of (9.1.14) are thermodynamically abnormal.
4. Most DS's with the nondivergent energy equation of (9.1.17) or (9.1.18) are thermodynamically normal. Some are weakly dissipative.
5. Some completely conservative (according to [4]) DS's are strongly dissipative.
6. Strongly dissipative DS's produce "computational noise" which renders a whole class of physical processes indistinguishable (weak shock waves, for example).

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10   On Complete Conservatism of Difference Schemes

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Numerical calculations of gas flows show that one of the important properties of the difference schemes in use is their complete conservatism [1, 2]. This paper gives an analysis of completely conservative difference schemes by the differential approximation method [3]. The terminology and definitions follow [2] and [3].

10.1   THE LAGRANGIAN COORDINATE CASE

10.1.1 Before describing the relation of the complete conservatism of difference schemes to their first differential approximations (FDA's) we define the notion of the equivalence of difference schemes [3].

Given some domain G of variables x and t, consider two systems of differential equations,

$$F_1\left(x, t, w, \frac{\partial w}{\partial t}, \frac{\partial w}{\partial x}\right) = 0 \qquad (10.1.1)$$

and

$$F_2\left(x, t, w, \frac{\partial w}{\partial t}, \frac{\partial w}{\partial x}\right) = 0, \qquad (10.1.2)$$

where $w = w(x, t)$ and F_1 and F_2 are m-dimensional vector functions, there being an inverse matrix $R = R(x, t, w)$ in $C(G)$ relating (10.1.1) and (10.1.2) as follows:

$$RF_1\left(x, t, w, \frac{\partial w}{\partial t}, \frac{\partial w}{\partial x}\right) = F_2\left(x, t, w, \frac{\partial w}{\partial t}, \frac{\partial w}{\partial x}\right).$$

Let the difference schemes

$$\Lambda_1(w, \tau, S_\tau) = 0 \qquad (10.1.3)$$

and

$$\Lambda_2(w, \tau, S_\tau) = 0 \qquad (10.1.4)$$

approximate respectively (10.1.1) and (10.1.2) to an order of approximation γ. Here $t = n\tau$, $x = ih$, $\tau/h = \varkappa = $ const, and S_τ is the star.

Definition. Difference schemes (10.1.3) and (10.1.4) are said to be equivalent if there is an inverse difference operator R_τ in $C(G)$