Methods of shock wave calculation

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Summary. Certain manipulation with the mass, momentum and energy conservation laws, written in the form of partial differential equations for an ideal non-heat-conducting medium, give a corollary saying about entropy conservation along the particle trajectory.

Conservation laws on the surface of a strong shock are algebraic equations showing that entropy grows across the shock wave. This is the fundamental difference between a shock wave and a continuous solution.

We will discuss only the shock wave methods that treat the strong discontinuity as a layer of a finite width (the shock is smeared within an interval of a finite length called distraction) comparable with the size of the mesh cell. Since states behind and before the shock are related, then there must exist a mechanism that ensures the growth of entropy in the shock distraction region. Only four principally different mechanisms of energy dissipation in the distraction region are known [1]–[4]. Consider four shock wave methods corresponding to these four mechanisms. Many difference schemes can be used to implement them. I suggest that we look only at those that were proposed by the authors of these four methods [1]–[4]. B.L. Rozhdestvensky and N.N. Yanenko [5] were first to try to compare these methods, focusing on approximations and stability.

In this presentation I will focus on energy dissipation, shock distraction and monotonicity.

1 Neumann – Richtmyer method

The basic idea of the method is that energy dissipation and strong shock distraction occupying several mesh cells are provided by adding an artificial viscosity term to the differential equations of motion and energy [1].

Ref. [1] proposes the artificial viscosity term in the form

$$q = -\frac{C^2 \Delta x_0^2}{V} \frac{\partial U}{\partial x_0} \left| \frac{\partial U}{\partial x_0} \right| \tag{1}$$

and offers a difference scheme then slightly modified in [6]. Difference schemes with the artificial viscosity term may differ, as well as expressions for q [7, 8]. The difference schemes may be either explicit or implicit. But given the presence of the artificial viscosity term, all such schemes are implementations of the Neumann-Richtmyer method.

In the difference scheme proposed in [1], thermodynamic quantities are defined at the centers of mesh intervals for m, and velocities and coordinates are defined in mesh nodes. Equations in [6] are written as:

$$\frac{U_i^{n+1}-U_i^n}{\Delta t}+\frac{P_{i+0,5}^n+q_{i+0,5}^n-P_{i-0,5}^n-q_{i-0,5}^n}{h}=0,$$

$$x_i^{n+1}=x_i^n+\tau U_i^{n+1},\quad V_{i+0,5}^{n+1}=\frac{x_{i+1}^n-x_i^{n+1}}{h},\quad h=\frac{x_{i+1}^n-x_i^n}{V_{i+0,5}^n},$$

$$q_{i+0,5}^{n+1}=\begin{cases}\frac{k}{V_{i+0,5}^{n+1}}\left(U_{i+1}^{n+1}-U_i^{n+1}\right)^2, & for \quad U_{i+1}^{n+1}-U_i^{n+1}<0\\ 0, \quad for \quad U_{i+1}^{n+1}-U_i^{n+1}\geqslant 0\end{cases},$$

$$E_{i+0,5}^{n+1}-E_{i+0,5}^n+\left(\frac{P_{i+0,5}^{n+1}+P_{i+0,5}^n}{2}+q_{i+0,5}^{n+1}\right)\left(V_{i+0,5}^{n+1}-V_{i+0,5}^n\right)=0, \tag{2}$$

$$P_{i+0,5}^{n+1}=P\left(V_{i+0,5}^{n+1},E_{i+0,5}^{n+1}\right), \tag{3}$$

Equations (2) and (3) form a system of non-linear equations for P^{n+1} and E^{n+1}.

The method is conditionally stable. The ratio between time and space steps $æ = a\tau/h$ depends on an empirical constant, k, and according to [6], the actual stability condition is

$$æ \leqslant \quad 0,25.$$

Ref. [1] proposes a method of shock distraction analysis. For this purpose they add the artificial viscosity term, q, in form (1) and go to a self-similar variable

$$\xi = m - Wt.$$

This yields

$$WV' + U' = 0, \tag{4}$$

$$WU' - (P+q)' = 0, \tag{5}$$

$$E' + (P+q)V' = 0, \tag{6}$$

where priming means differentiation with respect to ξ.

For the ideal gas

$$PV = (\gamma - 1)E \tag{7}$$

and q taken in the following form:

$$q = \frac{k^2h^2W^2}{V}\left(V'\right)^2, \tag{8}$$

equations (4)-(8) reduce to the single equation for V

$$2k^2h^2\left(\frac{dV}{d\xi}\right)^2+(\gamma+1)\left(V-V_0\right)^2+2V_0\left(V-V_0\right)=0. \tag{9}$$

Its solution is

$$\xi=\pm kh\sqrt{\frac{2}{\gamma+1}}\arcsin\left(\gamma-(\gamma+1)\frac{V}{V_0}\right).$$

For $V=V_0$, $\xi=\xi_0=\dfrac{3kh\pi}{2}\sqrt{\dfrac{2}{\gamma+1}}$ and for $V=V_1$, respectively,

$$\xi=\xi_1=-kh\sqrt{\frac{2}{\gamma+1}}\arcsin\left(\gamma-(\gamma+1)\frac{V_1}{V_0}\right).$$

The maximum compression $V_1=\dfrac{\gamma-1}{\gamma+1}V_0$ is achieved across the infinite shock with $P_0=0$. In this case $\xi_1=-\dfrac{kh\pi}{2}\sqrt{\dfrac{2}{\gamma+1}}$. So, the width of the shock layer, $\Delta\xi$, and the strong shock distraction, D, in the Neumann-Richtmyer method are:

$$\Delta\xi=\xi_0-\xi_1=2kh\pi\sqrt{\frac{2}{\gamma+1}},\quad D_{\mathrm{NR}}=\frac{\Delta\xi}{h}=2k\pi\sqrt{\frac{2}{\gamma+1}}.$$

The effective distraction, $D^{\mathrm{e}}_{\mathrm{NR}}$, is determined by finding points where the straight line $V(\xi)$ with the maximum slope

$$V'_m(\xi)=\frac{V_0}{kh\sqrt{2(\gamma+1)}}$$

intersects with V_0 and V_1

$$\Delta\xi=\frac{V_0-V_1}{V'_M}. \tag{10}$$

Substituting the expression for V'_M and the minimum specific volume

$$V_1=\frac{\gamma-1}{\gamma+1}V_0,$$

and dividing by h yield

$$D^{\mathrm{e}}_{\mathrm{NR}}=2k\sqrt{\frac{2}{\gamma+1}}.$$

2 Lax method

The basic idea of this method [2] is that energy dissipation is provided by the principal terms of approximation errors. Later this method was called the approximation viscosity method.

Difference equations are obtained by integrating the conservation laws over the mesh cell and applying the mean-value theorem:

$$\frac{V_{i+0,5}^{n+1}-V_{i+0,5}^{n}}{\tau}-\frac{U_{i+1}^{*}-U_{i}^{*}}{h}=0, \tag{11}$$

$$\frac{U_{i+0,5}^{n+1}-U_{i+0,5}^{n}}{\tau}+\frac{P_{i+1}^{*}-P_{i}^{*}}{h}=0, \tag{12}$$

$$\frac{\varepsilon_{i+0,5}^{n+1}-\varepsilon_{i+0,5}^{n}}{\tau}+\frac{(PU)_{i+1}^{*}-(PU)_{i}^{*}}{h}=0, \tag{13}$$

$$E_{i+0,5}^{n+1}=\varepsilon_{i+0,5}^{n+1}-0,5\left(U_{i+0,5}^{n+1}\right)^{2}, \tag{14}$$

where the values of sought functions $V_{i+0,5}^{n}$, $P_{i+0,5}^{n}$, $U_{i+0,5}^{n}$, $E_{i+0,5}^{n}$, and $\varepsilon_{i+0,5}^{n}$ are defined at the centers of mesh intervals for m at times t^n, and auxiliary quantities P_i^*, U_i^* and $(PU)_i^*$ are defined at the centers of the time steps, τ, at the faces of the mesh cells with coordinates m_i.

Equations (11)-(14) are general until equations for U_i^*, P_i^* and $(PU)_i^*$ are specified. Ref. [2] proposes a difference scheme that defines auxiliary quantities U^* and P^* across shocks and continuous solutions with the following equations:

$$U_{i}^{*}=\frac{1}{2}\left(U_{i+0,5}^{n}+U_{i-0,5}^{n}\right)+\frac{h}{2\tau}\left(V_{i+0,5}^{n}-V_{i-0,5}^{n}\right), \tag{15}$$

$$P_{i}^{*}=\frac{1}{2}\left(P_{i+0,5}^{n}+P_{i-0,5}^{n}\right)-\frac{h}{2\tau}\left(U_{i+0,5}^{n}-U_{i-0,5}^{n}\right), \tag{16}$$

$$(PU)_{i}^{*}=\frac{1}{2}\left((PU)_{i+0,5}^{n}+(PU)_{i-0,5}^{n}\right)-\frac{h}{2\tau}\left(\varepsilon_{i+0,5}^{n}-\varepsilon_{i-0,5}^{n}\right). \tag{17}$$

Difference equations (11)-(13) and equations (15)-(17) for the auxiliary quantities approximate the differential conservation laws with approximation errors

$$\omega_1=-\frac{1}{2}\frac{\partial^2 V}{\partial t^2}\tau+\frac{1}{2}\frac{\partial^2 V}{\partial m^2}\frac{h^2}{\tau}+O\left(\tau^2,h^2\right), \tag{18}$$

$$\omega_2=-\frac{1}{2}\frac{\partial^2 U}{\partial t^2}\tau+\frac{1}{2}\frac{\partial^2 U}{\partial m^2}\frac{h^2}{\tau}+O\left(\tau^2,h^2\right), \tag{19}$$

$$\omega_3=-\frac{1}{2}\frac{\partial^2 \varepsilon}{\partial t^2}\tau+\frac{1}{2}\frac{\partial^2 \varepsilon}{\partial m^2}\frac{h^2}{\tau}+O\left(\tau^2,h^2\right). \tag{20}$$

When $h \to 0$ and $\tau = \text{const}$, the associated terms in (18)-(20) tend to zero. However, it goes worse with τ. When $\tau \to 0$, the terms proportional to

$\frac{h^2}{\tau}$ in (18)-(20) tend to zero if only $\lim\limits_{\substack{\tau\to 0\\ h\to 0}} \frac{h^2}{\tau} = 0$. If not, equations (11)-(13) do not converge to the initial differential equations because the reduction of τ at constant h increases the error.

According to [9], the equation of entropy production for difference schemes with independent ω_1, ω_2, and ω_3 is

$$T\frac{\partial S}{\partial t} = \omega_3 - U\omega_2 + P\omega_1. \tag{21}$$

Substitute Eqs. (18)-(20) into Eq. (21) and using differential equations replace the second time derivatives in Eq. (20) by m-derivatives. Also assume that $\frac{\partial S}{\partial m} \approx 0$ and then the entropy production equation takes the form:

$$T\left(\frac{\partial S}{\partial t}\right) = \frac{h}{2a}\frac{\left(1-æ^2\right)}{æ}\left(a^2\left(\frac{\partial V}{\partial t}\right)^2 + \left(\frac{\partial U}{\partial t}\right)^2\right) + ...$$

For $æ = \frac{\tau a}{h} \to 0$, the rate of entropy production approaches infinity. So, the difference scheme of Lax is extremely dissipative, according to [8].

Consider the distraction of a stationary discontinuity in the Lax method. For this end write difference equations (11)-(13) in the differential form with approximation errors (18)-(20) and go to the variable $\xi = m - Wt$. We obtain

$$WV' + U' + \frac{h^2}{2\tau}\left(1-æ^2\right)V'' + O\left(\tau^2, h^2\right) = 0,$$

$$WU' - P' + \frac{h^2}{2\tau}\left(1-æ^2\right)U'' + O\left(\tau^2, h^2\right) = 0,$$

$$W\varepsilon' - (PU)' + \frac{h^2}{2\tau}\left(1-æ^2\right)\varepsilon'' + O\left(\tau^2, h^2\right) = 0.$$

Integrate these equations with respect to ξ. Find constants of integration for $\xi = +\infty$, where $U = U_0$, $V = V_0$, $P = P_0$, $E = E_0$, $\varepsilon = \frac{1}{2}U_0^2 + E_0$, $V' = 0$, $U' = 0$, $P' = 0$, $\varepsilon' = 0$. This yields

$$WV + U + AV' - WV_0 - U_0 + O\left(\tau^2, h^2\right) = 0,$$

$$WU - WU_0 - P + P_0 + AU' + O\left(\tau^2, h^2\right) = 0,$$

$$W\varepsilon - W\varepsilon_0 - PU + A\varepsilon' + P_0U_0 + O\left(\tau^2, h^2\right) = 0, \tag{22}$$

where $A = \frac{h^2}{2\tau}\left(1-æ^2\right)$. Substitute the Clapeyron equation into (22). Then express all quantities in terms of V and derivatives in terms of V'. We obtain an ordinary differential equation for the profile $V(\xi)$

$$\frac{4AV}{W(\gamma+1)}\frac{dV}{d\xi} - \frac{(V_0 - V)(V - V_1)}{V} = O\left(\tau^2, h^2\right), \tag{23}$$

where $V_1 = V_0 \left(\frac{\gamma - 1}{\gamma + 1} + \frac{2}{\gamma + 1} \left(\frac{a_0}{W} \right)^2 \right)$. Omitting the second order infinitesimals gives the following solution:

$$\xi = \frac{2h^2 \left(1 - æ^2\right)}{\tau W \left(\gamma + 1\right) \left(V_0 - V_1\right)} \left(V_1 \ln \left(V - V_1\right) - V_0 \ln \left(V_0 - V\right)\right). \tag{24}$$

It follows from (24) that $\xi = \xi_0 = +\infty$ for $V = V_0$ and $\xi = \xi_1 = -\infty$ for $V = V_1$. So, the strong shock distraction in the Lax method is infinite:

$$D_{\mathrm{L}} = \infty.$$

To determine the effective distraction, differentiate (23), and find V_M and the maximum value V'_M for $V'' = 0$

$$V_M = \sqrt{V_0 V}, \quad V'_M = \frac{(\gamma + 1)\, æ}{2h \left(1 - æ^2\right)} \left(\sqrt{V_0} - \sqrt{V_1}\right)^2. \tag{25}$$

Using (23) and (10) yields

$$D^{\mathrm{e}}_{\mathrm{L}} = \frac{2\left(1 - æ^2\right)}{(\gamma + 1)\, æ} \left(\frac{\sqrt{V_0} + \sqrt{V_1}}{\sqrt{V_0} - \sqrt{V_1}} \right). \tag{26}$$

It is seen from (25) that $D^{\mathrm{e}}_{\mathrm{L}} \to 0$ for $æ \to 1$ and $D^{\mathrm{e}}_{\mathrm{L}} \to \infty$ for $æ \to 0$ or $V_1 \to V_0$.

Finally, check monotonicity of the Lax scheme. Go from P and U to invariants:

$$\alpha = P + aU, \quad \beta = P - aU.$$

Express P and U in terms of α and β:

$$P = 0,5(\alpha + \beta), \quad U = 0,5\left(\alpha - \beta\right)/a. \tag{27}$$

For a matter with EOS

$$P = a^2 \left(V_0 - V\right), \tag{28}$$

replace V by P in Eq. (11). We obtain

$$P^{n+1}_{i+0.5} = \frac{1}{2}\left(P^n_{i+1.5} + P^n_{i-0.5}\right) - \frac{1}{2}\frac{\tau a^2}{h}\left(U^n_{i+1.5} - U^n_{i-0.5}\right). \tag{29}$$

Substituting (27) in (29) and (12) yields

$$\begin{gathered} \alpha^{n+1}_{i+0.5} + \beta^{n+1}_{i+0.5} = 0,5 \cdot \alpha^n_{i-0.5}\left(1 + æ\right) + \\ +0,5 \cdot \alpha^n_{i+1.5}\left(1 - æ\right) + 0,5 \cdot \beta^n_{i-0.5}\left(1 - æ\right) + 0,5 \cdot \beta^n_{i+1.5}\left(1 + æ\right), \end{gathered} \tag{30}$$

$$\begin{gathered} \alpha^{n+1}_{i+0.5} - \beta^{n+1}_{i+0.5} = 0,5 \cdot \alpha^n_{i-0.5}\left(1 + æ\right) + \\ +0,5 \cdot \alpha^n_{i+1.5}\left(1 - æ\right) - 0,5 \cdot \beta^n_{i-0.5}\left(1 - æ\right) - 0,5 \cdot \beta^n_{i+1.5}\left(1 + æ\right). \end{gathered} \tag{31}$$

Sum (2) and (2), and then subtract (2) from (2)

$$\left.\begin{aligned}\alpha_{i+0.5}^{n+1} &= 0,5\,(1-æ)\,\alpha_{i+1.5}^{n} + 0,5\,(1+æ)\,\alpha_{i-0.5}^{n},\\ \beta_{i+0.5}^{n+1} &= 0,5\,(1+æ)\,\beta_{i+1.5}^{n} + 0,5\,(1-æ)\,\beta_{i-0.5}^{n}.\end{aligned}\right\} \tag{32}$$

It follows from (32) that for $0\leqslant æ \leqslant 1$, all coefficients of the invariants in the right-hand sides are nonnegative and hence the difference scheme by Lax is monotonic by the Godunov theorem.

3 Godunov method

In this method all quantities that characterize the response of media to loads are defined at the centers of mesh intervals for m. Coordinates x_i are defined in mesh nodes. The difference equations are written in forms (11)-(13). Auxiliary quantities P_i^*, U_i^* are defined as follows. All tabular functions at time t^n are assumed piecewise constant. Therefore, arbitrary discontinuities appear in nodes. They split at $t > t^n$. Pressures and velocities across the contact discontinuity are taken to be auxiliary quantities. If an arbitrary discontinuity is such as a shock wave propagates to the right of x_i and a rarefaction wave does to the left, then equations for the quantities across the contact discontinuity are

$$P_i^* + a_{i-0.5}^n U_i^* = P_{i-0.5}^n + a_{i-0.5}^n U_{i-0.5}^n,$$

$$P_i^* - W_{i+0.5} U_i^* = P_{i+0.5}^n - W_{i+0.5} U_{i+0.5}^n.$$

Generally $W_{i+0.5}$ depends on P_i^* and U_i^* because the problem of discontinuity splitting is non-linear. However, for a weak shock with $W_{i+0.5} = a + O(h)$, $a_{i-0.5} = a + O(h)$, equations for P_i^*, U_i^* take the form

$$P_i^* = 0,5\left(P_{i+0.5}^n + P_{i-0.5}^n\right) - 0,5a\left(U_{i+0.5}^n - U_{i-0.5}^n\right), \tag{33}$$

$$U_i^* = 0,5\left(U_{i+0.5}^n + U_{i-0.5}^n\right) - 0,5\left(P_{i+0.5}^n - P_{i-0.5}^n\right)/a. \tag{34}$$

Write difference equations (11)-(13), (33) and (34) in the differential form. The approximation errors ω_1, ω_2, and ω_3 are:

$$\omega_1 = -\frac{\tau}{2}\frac{\partial^2 V}{\partial t^2} - \frac{h}{2a}\frac{\partial^2 P}{\partial m^2} + O\left(\tau^2, h^2\right),$$

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

$$\omega_3 = -\frac{\tau}{2}\frac{\partial^2 \varepsilon}{\partial t^2} - \frac{ah}{2}U\frac{\partial^2 U}{\partial m^2} + \frac{ah}{2}\left(\frac{\partial U}{\partial m}\right)^2 + \frac{h}{2a}\left(\frac{\partial P}{\partial m}\right)^2 + \frac{h}{2a}P\frac{\partial^2 P}{\partial m^2} + O\left(\tau^2, h^2\right).$$

Since ω_1, ω_2, and ω_3 are independent, then, by [9], the right-hand side of the entropy equation is in form (21). Substitute ω_1, ω_2, and ω_3 in (21). Then using differential conservation laws and their derivatives, replace time derivatives by m-derivatives. This gives the following equation of entropy production:

$$T\frac{\partial S}{\partial t} = \frac{h}{2W}\left(1 - æ\right)\left(\left(\frac{\partial P}{\partial m}\right)^2 + W^2\left(\frac{\partial U}{\partial m}\right)^2\right) + O\left(\tau^2, h^2\right). \tag{35}$$

It follows from (35) that for $æ = \dfrac{\tau a}{h} < 1$, this difference scheme, being an acoustic approximation to the Godunov scheme, is extremely dissipative. Since the principal term in the right-hand side of Eq. (35) is nonnegative, entropy grows across both shock and rarefaction waves. The rate of entropy production is limited and achieves maximum at $æ = 0$:

$$T\frac{\partial S}{\partial t} < \frac{h}{2W}\left(\left(\frac{\partial P}{\partial m}\right)^2 + W^2\left(\frac{\partial U}{\partial m}\right)^2\right).$$

Analyze shock distraction. For this end go to the self-similar variable $\xi = m - Wt$ and write the difference equations in the differential form:

$$WV' + U' - \frac{\tau W^2}{2}V'' - \frac{h}{2W}P'' + O\left(\tau^2, h^2\right) = 0,$$

$$WU' - P' - \frac{\tau W^2}{2}U'' + \frac{hW}{2}U'' + O\left(\tau^2, h^2\right) = 0,$$

$$W\varepsilon' - (PU)' - \frac{\tau W^2}{2}\varepsilon'' + \frac{hW}{2}\left(UU'\right)' + \frac{h}{2W}\left(PP'\right)' + O\left(\tau^2, h^2\right) = 0.$$

Integrating with respect to ξ and eliminating P, U, ε, P', U', ε' gives the following equation for $V(\xi)$ for the ideal gas:

$$\frac{2h\left(1 - æ\right)}{(\gamma + 1)} \cdot \frac{dV}{d\xi} + \frac{\left(V - V_0\right)\left(V - V_1\right)}{V} + O\left(\tau^2, h^2\right) = 0.$$

Its solution is

$$\xi = \frac{2h\left(1 - æ\right)}{(\gamma + 1)\left(V_0 - V_1\right)}\left(V_1 \ln\left(V - V_1\right) - V_0 \ln\left(V_0 - V\right)\right).$$

From this equation:

$$\xi = \xi_0 = +\infty \text{ for } V = V_0,$$

$$\xi = \xi_1 = -\infty \text{ for } V = V_1,$$

So, in the Godunov method, the shock distraction for $æ < 1$ is infinite:

$$D_{\mathrm{G}} = \infty,$$

and for $æ = 1$, D_{G}=0.

The effective distraction is obtained in the same manner as in the Lax method:

$$D^{\mathrm{e}}_{\mathrm{G}} = \frac{2}{(\gamma+1)}\,(1-æ)\left(\frac{\sqrt{V_0}+\sqrt{V_1}}{\sqrt{V_0}-\sqrt{V_1}}\right).$$

To check the Godunov scheme for monotonicity, go to the invariants. Express P and U in terms of α and β, and for equation of state (28), replace V by P in Eq. (11). For $a = W$, we obtain

$$\alpha^{n+1}_{i+0.5}+\beta^{n+1}_{i+0.5} = \alpha^{n}_{i+0.5}+\beta^{n}_{i+0.5}+æ\left(\beta^{n}_{i+1.5}-\alpha^{n}_{i+0.5}-\beta^{n}_{i+0.5}+\alpha^{n}_{i-0.5}\right), \quad (36)$$

$$\alpha^{n+1}_{i+0.5}-\beta^{n+1}_{i+0.5} = \alpha^{n}_{i+0.5}-\beta^{n}_{i+0.5}+æ\left(-\beta^{n}_{i+1.5}-\alpha^{n}_{i+0.5}+\beta^{n}_{i+0.5}+\alpha^{n}_{i-0.5}\right). \quad (37)$$

Summing (36) and (37), and subtracting (37) from (36) give equations for α and β:

$$\alpha^{n+1}_{i+0.5} = \alpha^{n}_{i+0.5}(1-æ)+\alpha^{n}_{i-0.5}æ,$$

$$\beta^{n+1}_{i+0.5} = \beta^{n}_{i+0.5}(1-æ)+\beta^{n}_{i-0.5}æ.$$

For $0 \leqslant æ \leqslant 1$, all coefficients of α and β are nonnegative and by the Godunov theorem, the difference scheme, being an acoustic approximation of the Godunov scheme, is monotonic.

4 Kuropatenko method [4]

The basic idea of this method is as follows. All mesh intervals (basic and auxiliary) are referred to one of two types depending on solution: compression or rarefaction. The former is treated as shock compression defined by the local (only within the current interval) shock wave. States before and behind the shock wave relate as conservation laws:

$$P_1 - P_0 - W(U_1 - U_0) = 0, \quad (38)$$

$$U_1 - U_0 + W(V_1 - V_0) = 0, \quad (39)$$

$$P_1U_1 - P_0U_0 - W(E_1 - E_0) - \frac{W}{2}(U_1^2 - U_0^2) = 0. \quad (40)$$

The state before the shock $(P_0,\ V_0,\ E_0,\ U_0)$ is the solution in the mesh interval. One of the quantities, either on the boundary or in the neighbor interval, is taken as the quantity behind the shock. Other quantities behind the shock are determined from Eqs. (38)-(40) and the equation of state. They are taken as auxiliary quantities. For example, if define U_1 [4], then P_1, V_1, E_1, and W are sought from Eqs. (38)-(40), or if define P_1 [10,11,12], then V_1, E_1, U_1, and W are sought.

The method can be implemented on different meshes [4], [9]–[14]. Discuss two of them.

4.1 Non-divergent scheme

Meshes proposed in [4] for velocity and thermodynamic quantities differ. Quantities P, V, and E are defined at the centers of mass intervals, and velocities are defined in nodes t^n, m_i.

For a compression wave, the difference equations take the form:

$$\frac{U_i^{n+1} - U_i^n}{\tau} + \frac{\overline{P}_{i+0.5}^n - \overline{P}_{i-0.5}^n}{h} = 0, \tag{41}$$

$$x_i^{n+1} = x_i^n + \tau U_i^{n+1}, \tag{42}$$

$$V_{i+0,5}^{n+1} = \frac{x_{i+1}^{n+1} - x_i^{n+1}}{h}, \quad h = \frac{x_{i+1}^n - x_i^n}{V_{i+0,5}^n} \tag{43}$$

$$E_{i+0.5}^{n+1} - E_{i+0.5}^n + 0,5\left(\overline{P}_{i+0.5}^{n+1} + \overline{P}_{i+0.5}^n\right)\left(V_{i+0.5}^{n+1} - V_{i+0.5}^n\right) = 0. \tag{44}$$

The dynamic pressure $\overline{P}$ is a solution of these equations across the strong shock. Before the shock, we take quantities in the mesh interval at time t^n

$$V_0 = V_{i+0,5}^n,\ \mathrm{P}_0 = P_{i+0,5}^n,\ \mathrm{E}_0 = E_{i+0,5}^n,$$

and as the velocity jump we take the difference of U in nodes at time t^{n+1}

$$\Delta U = |U_1 - U_0| = \left|U_{i+1}^{n+1} - U_i^{n+1}\right|.$$

Substituting these quantities in the equations for the strong shock yields

$$\overline{P}_{i+0.5}^{n+1} = P_{i+0.5}^n - W\left(U_{i+1}^{n+1} - U_i^{n+1}\right), \tag{45}$$

where W depends on P_0, V_0, E_0 and ΔU.

For a simple equation of state for condensed matter

$$P = (\gamma - 1)\rho E + C_{0k}^2(\rho - \rho_{0k}),$$

Eq. (45) takes the form

$$\overline{P}_{i+0,5}^{n+1} = P_{i+0,5}^n + b\Delta U^2 + \sqrt{\left(b\Delta U^2\right)^2 + \left(a_{i+0,5}^n\right)^2 \Delta U^2}, \tag{46}$$

where $b = \frac{\gamma+1}{4}\rho_{i+0,5}^n$.

Eq. (46) has two asymptotes:

1. Weak shock, $b\Delta U \ll a_{i+0,5}^n$. In this case the dynamic pressure is a linear function of ΔU:
$$\overline{P}_{i+0,5}^{n+1} \approx P_{i+0,5}^n + a_{i+0,5}^n \Delta U. \tag{47}$$

2. Strong shock, $b\Delta U \gg a^n_{i+0,5}$. In this case the function is quadratic:

$$\overline{P}^{n+1}_{i+0,5} \approx P^n_{i+0,5} + \frac{\gamma+1}{2}\rho^n_{i+0,5}\Delta U^2. \tag{48}$$

Using these asymptotes, M. Wilkins [8] introduced a linear-quadratic artificial viscosity.

Taking Taylor series expansion of all quantities in Eqs. (41)-(44) gives independent approximation errors:

$$\omega_2 = -\frac{\tau}{2}\frac{\partial^2 U}{\partial t^2} + hW\frac{\partial^2 U}{\partial m^2} + \tau\frac{\partial^2 P}{\partial t \partial m} + O\left(\tau^2, h^2\right), \tag{49}$$

$$\omega_4 = \frac{\tau}{2}\frac{\partial U}{\partial t} - \frac{\tau^2}{6}\frac{\partial^2 U}{\partial t^2} + O\left(\tau^3\right), \tag{50}$$

$$\omega_5 = -\frac{h^2}{24}\frac{\partial^3 x}{\partial m^3} + O\left(h^3\right), \tag{51}$$

$$\omega_7 = -\frac{\tau}{2}\left(\frac{\partial^2 E}{\partial t^2} - \frac{\partial P}{\partial t}\frac{\partial V}{\partial t} + P\frac{\partial^2 V}{\partial t^2}\right) + hW\frac{\partial V}{\partial t}\frac{\partial U}{\partial m} + O\left(\tau^2, h^2, \tau h\right). \tag{52}$$

Differentiate (42) and (43) with respect to t and m, and using the equation

$$\frac{\partial P}{\partial t} + a^2\frac{\partial U}{\partial m} = \omega_{10}$$

write ω_7 as

$$\omega_7 = hW\left(1 - æ\frac{\mathrm{a}}{\mathrm{W}}\right)\left(\frac{\partial V}{\partial t}\right)^2 + O\left(\tau^2, h^2\right).$$

Since ω_7 is independent, then the entropy production equation for $W = a + O(\tau, h)$ takes the form:

$$T\left(\frac{\partial S}{\partial t}\right)_m = hW(1 - æ)\left(\frac{\partial V}{\partial t}\right)^2 + O(\tau^2, h^2).$$

What about distraction in this non-divergent scheme? As earlier, go to the self-similar variable $\xi = m - Wt$. The differential conservation laws with approximation errors (50), (51), (49) and (52) are

$$WU' - P' - \frac{\tau W^2}{2}U'' + hWU'' - \tau WP'' + O\left(\tau^2, h^2\right) = 0, \tag{53}$$

$$Wx' + U - \frac{\tau W}{2}U' + O\left(\tau^2\right) = 0, \tag{54}$$

$$x' - V + O\left(\tau^2\right) = 0, \tag{55}$$

$$E' + PV' - \frac{\tau W}{2}\left(E'' - P'V' + PV''\right) - hWV'U' + O\left(\tau^2, h^2\right) = 0. \tag{56}$$

By differentiating (53)-(56), eliminating x', E'', U', P' and integrating with respect to ξ we obtain a differential equation for $V(\xi)$ that is identical with the equation in the Godunov scheme. Thus, the first differential approximation of the Kuropatenko non-divergent scheme has the same distraction that the approximation of the Godunov scheme.

Is the scheme monotonic? For equation of state (28) across the compression wave, we write the consequence of Eqs. (41)-(44) as

$$P_{i+0,5}^{n+1} - P_{i+0,5}^{n} + \frac{\tau a^2}{h}(U_{i+1}^{n+1} - U_i^{n+1}) = 0. \tag{57}$$

Substituting (45) in (41) yields

$$U_i^{n+1} - U_i^n + \frac{\tau}{h}(P_{i+0,5}^{n-1} - P_{i-0,5}^{n-1}) - æ(U_{i+1}^n - 2U_i^n + U_{i-1}^n) = 0. \tag{58}$$

Substitute (27) in (57) and (58)

$$\alpha_{i+0,5}^{n+1} + \beta_{i+0,5}^{n+1} + æ(\alpha_{i+1}^{n+1} - \beta_{i+1}^{n+1}) - æ(\alpha_i^{n+1} - \beta_i^{n+1}) = \alpha_{i+0,5}^n + \beta_{i+0,5}^n, \tag{59}$$

$$\begin{aligned}\alpha_i^{n+1} - \beta_i^{n+1} = \alpha_i^n - \beta_i^n - æ(\alpha_{i+0,5}^{n-1} + \beta_{i+0,5}^{n-1}) + æ(\alpha_{i-0,5}^{n-1} + \beta_{i-0,5}^{n-1}) + \\ + æ(\alpha_{i+1}^n - \beta_{i+1}^n) - 2æ(\alpha_i^n - \beta_i^n) + æ(\alpha_{i-1}^n - \beta_{i-1}^n).\end{aligned} \tag{60}$$

Write Eq. (60) for $i+1$ and multiply by $-æ$, then multiply Eq. (60) by $æ$, and add all to Eq. (59). For β=const, we obtain

$$\begin{aligned}\alpha_{i+0,5}^{n+1} = \alpha_{i+0,5}^n + (3æ^2 - æ)(\alpha_{i+1}^n - \alpha_i^n) - æ^2(\alpha_{i+2}^n - \alpha_{i-1}^n) + \\ + æ^2\alpha_{i+1,5}^{n-1} - 2æ^2\alpha_{i+0,5}^{n-1} + æ^2\alpha_{i-0,5}^{n-1}.\end{aligned}$$

Take the Taylor series expansions of all α in the right-hand side. We obtain the following equation:

$$\alpha_{i+0,5}^{n+1} = \alpha_{i+0,5}^n - æh\left(\frac{\partial\alpha}{\partial m}\right)_{i+0,5} + æ^2h^2\left(\frac{\partial^2\alpha}{\partial m^2}\right)_{i+0,5} + O(h^3). \tag{61}$$

Decrease the index by 1 and subtract from (61). Then take the Taylor series expansions at t^n and m_i of all quantities in the right-hand side of the obtained equation. This gives

$$\Delta_i^{n+1} = \alpha_{i+0,5}^{n+1} - \alpha_{i-0,5}^{n+1} = h\left(\left(\frac{\partial\alpha}{\partial m}\right)_i - æh\left(\frac{\partial^2\alpha}{\partial m^2}\right)_i\right) + O(h^3). \tag{62}$$

For β=const, the compression wave propagates in the positive direction. Since on the backside of the compression wave $\alpha' \leqslant 0$, $\alpha'' \leqslant 0$, then for $\tau \approx 0$ ($æ \approx 0$), it follows from (62) that $\Delta_i^n \leqslant 0$. In order that Δ_i^n remain nonpositive, it is required that the following condition be satisfied

$$\left|\frac{\partial\alpha}{\partial m}\right| - \tau a\left|\frac{\partial^2\alpha}{\partial m^2}\right| \geqslant 0.$$

So, the scheme is conditionally monotonic.

4.2 Divergent scheme [10]

All thermodynamic quantities and velocities are defined at the centers of mesh intervals and mesh nodes have coordinates t^n and m_i. The difference equations are in form (11)-(14). To define auxiliary quantities P_i^*, U_i^*, the solution in the auxiliary interval $m_{i-0.5} \leqslant m \leqslant m_{i+0.5}$ is divided in two: rarefaction and compression.

Compression wave. Auxiliary quantities are found from equations (38)-(40) for the strong shock surface. Quantities across the discontinuity are defined as follows.

If $U^n_{i+0.5} - U^n_{i-0.5} < 0$, then

1. $U_1 = U^n_{i-0.5}, \quad (P, V, E, U)_0 = (P, V, E, U)^n_{i+0.5} \quad$ for $P^n_{i-0.5} > P^n_{i+0.5}$,
2. $U_1 = U^n_{i+0.5}, \quad (P, V, E, U)_0 = (P, V, E, U)^n_{i-0.5} \quad$ for $P^n_{i-0.5} < P^n_{i+0.5}$.

All other quantities subscripted 1 are found from (38)-(40). If consider only W¿0, then P_i^*, U_i^* are defined by equations

$$U_i^* = U^n_{i-0.5}, \quad P_i^* = P^n_{i+0.5} - W\left(U^n_{i+0.5} - U^n_{i-0.5}\right). \tag{63}$$

Check monotonicity of this scheme across the compression wave. Constitutive equations with auxiliary quantities (63) take the form:

$$P^{n+1}_{i+0.5} = P^n_{i+0.5} - \frac{\tau a^2}{h}\left(U^n_{i+0.5} - U^n_{i-0.5}\right),$$

$$U^{n+1}_{i+0.5} = U^n_{i+0.5} - \frac{\tau}{h}\left(P^n_{i+1.5} - P^n_{i+0.5} - a\left(U^n_{i+1.5} - 2U^n_{i+0.5} + U^n_{i-0.5}\right)\right).$$

Replace P and U by their expressions for the invariants α and β

$$\alpha^{n+1}_{i+0.5} + \beta^{n+1}_{i+0.5} = \alpha^n_{i+0.5} + \beta^n_{i+0.5} - æ\left(\alpha^n_{i+0.5} - \beta^n_{i+0.5} - \alpha^n_{i-0.5} + \beta^n_{i-0.5}\right),$$

$$\alpha^{n+1}_{i+0.5} - \beta^{n+1}_{i+0.5} = \alpha^n_{i+0.5} - \beta^n_{i+0.5} - æ\left(\alpha^n_{i+1.5} + \beta^n_{i+1.5} - \alpha^n_{i+0.5} - \beta^n_{i+0.5}\right) +$$
$$+ æ\left(\alpha^n_{i+1.5} - \beta^n_{i+1.5} - 2\alpha^n_{i+0.5} + 2\beta^n_{i+0.5} + \alpha^n_{i-0.5} - \beta^n_{i-0.5}\right).$$

Sum these equations

$$\alpha^{n+1}_{i+0.5} = \alpha^n_{i+0.5}(1 - æ) + æ\alpha^n_{i-0.5} - æ\beta^n_{i+1.5} + 4æ\beta^n_{i+0.5} - æ\beta^n_{i-0.5}. \tag{64}$$

If β=const, Eq. (64) takes the form

$$\alpha^{n+1}_{i+0.5} = \alpha^n_{i+0.5}(1 - æ) + \alpha^n_{i-0.5}æ.$$

Both coefficients are positive for $0 \leqslant æ \leqslant 1$ and hence the divergent scheme [10], [12] is monotonic across the compression wave.

Now consider shock distraction. For this end write difference conservation laws (11)-(14) and auxiliary quantities (63) in the differential form with approximation errors:

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

$$\omega_2 = -\frac{\tau}{2}\frac{\partial^2 U}{\partial t^2} - hW\frac{\partial^2 U}{\partial m^2} - \frac{h}{2}\frac{\partial^2 P}{\partial m^2} + O\left(\tau^2, h^2\right),$$

$$\omega_3 = -\frac{\tau}{2}\frac{\partial^2 \varepsilon}{\partial t^2} - \frac{h}{2}\frac{\partial}{\partial m}\left(U\frac{\partial P}{\partial m}\right) + \frac{h}{2}\frac{\partial}{\partial m}\left(P\frac{\partial U}{\partial m}\right) + hW\frac{\partial}{\partial m}\left(U\frac{\partial U}{\partial m}\right) +$$

$$+O\left(\tau^2, h^2\right).$$

Go to the self-similar variable $\xi = m - Wt$. Then the equations take the form

$$WV' + U' - \frac{\tau W^2}{2}V'' - \frac{h}{2}U'' + O\left(\tau^2, h^2\right) = 0, \tag{65}$$

$$WU' - P' - \frac{\tau W^2}{2}U'' - \frac{h}{2}P'' + hWU'' + O\left(\tau^2, h^2\right) = 0, \tag{66}$$

$$W\varepsilon' - (PU)' - \frac{\tau W}{2}PU'' - \frac{h}{2}\left(UP'\right)' + \frac{h}{2}\left(PU'\right)' - hW\left(UU'\right)' + O\left(\tau^2, h^2\right) = 0. \tag{67}$$

Integrating with respect to ξ gives

$$WV + U - \frac{\tau W^2}{2}V' - \frac{h}{2}U' = WV_0 + U_0 + O\left(\tau^2, h^2\right), \tag{68}$$

$$WU - P - \frac{\tau W^2}{2}U' - \frac{h}{2}P' + hWU' = W_0U_0 - P_0 + O\left(\tau^2, h^2\right), \tag{69}$$

$$W\varepsilon - PU - \frac{\tau W}{2}(PU)' - \frac{h}{2}UP' + \frac{h}{2}PU' - hWUU' =$$
$$= W\varepsilon_0 - P_0U_0 + O\left(\tau^2, h^2\right). \tag{70}$$

Using (65)-(67), replace U' and P' in (68)-(4.2) by V'. Then using (68)-(4.2), replace U and P by V. We obtain an equation describing the profile $V(\xi)$ for the ideal gas. The equation is identical to that in the Godunov scheme. Therefore, the distraction and the effective distraction in this scheme are identical with D_G and D_G^e.

5 Other difference schemes

5.1 Lax-Wendroff scheme

The scheme of Lax and Wendroff [15], [16] is worthy of considering because of its rather wide use. Lax and Wendroff proposed that auxiliary quantities P_i^*, U_i^* in (11)-(13) should be defined as

$$P_i^* = P_i^n - \frac{\tau}{2h}\left(a_i^n\right)^2\left(U_{i+0,5}^n - U_{i-0,5}^n\right) - \frac{B}{4}\left|a_{i+0,5}^n - a_{i-0,5}^n\right|(U_{i+0,5}^n - U_{i-0,5}^n),$$

$$U_i^* = U_i^n - \frac{\tau}{2h}\left(P_{i+0,5}^n - P_{i-0,5}^n\right) - \frac{B}{4\left(a_i^n\right)^2}\left|a_{i+0.5}^n - a_{i-0.5}^n\right|\left(P_{i+0,5}^n - P_{i-0,5}^n\right),$$

$$(PU)_i^* = (PU)_i^n - \left(P_i^n\left(P_{i+0.5}^n - P_{i-0.5}^n\right) + \left(a_i^n\right)^2 U_i^n\left(U_{i+0,5}^n - U_{i-0,5}^n\right)\right) \times$$

$$\times\left(\frac{\tau}{2h} + \frac{B}{4\left(a_i^n\right)^2}\left|a_{i+0,5}^n - a_{i-0,5}^n\right|\right),$$

where

$$P_i^n = \frac{1}{2}\left(P_{i+0,5}^n + P_{i-0,5}^n\right), \quad a_i^n = \frac{1}{2}\left(a_{i+0,5}^n + a_{i-0,5}^n\right),$$

$$U_i^n = \frac{1}{2}\left(U_{i+0,5}^n + U_{i-0,5}^n\right), \quad (PU)_i^n = \frac{1}{2}\left((PU)_{i+0,5}^n + (PU)_{i-0,5}^n\right).$$

Using these equations for shock wave computing is the same as adding three artificial viscosity terms:

$$q_p = -\frac{B}{4}h^2\left|\frac{\partial a}{\partial m}\right|\frac{\partial U}{\partial m}, \quad q_u = -\frac{B}{4}\frac{h^2}{a^2}\left|\frac{\partial a}{\partial m}\right|\frac{\partial P}{\partial m},$$

$$q_{pu} = -\frac{B}{4}\frac{h^2}{a^2}\left|\frac{\partial a}{\partial m}\right|\left(P\frac{\partial P}{\partial m} + a^2 U\frac{\partial U}{\partial m}\right).$$

They are not approximation viscosities and therefore, the Lax-Wendroff scheme is an implementation of the Neumann-Richtmyer method. This scheme has an empirical constant, $B \approx 1-2$, defining the boundary of the stability region. The stability condition is

$$æ(æ + \frac{1}{2}\mathrm{B}) \leqslant 1.$$

The scheme is non-monotonic.

5.2 Eulerian difference schemes

These difference schemes are widely used in aerodynamic calculations. In rather detail their merits and shortcomings are considered in [17], [18]. The only thing I would like to attract your attention to is that all these schemes can be considered as consisting of two steps. At the first step the mesh is Lagrangian and one of the shock wave methods in the Lagrangian formulation is used. During the second step the quantities are recalculated to transfer from the Lagrangian mesh to the Eulerian one. The solution obtained at the first step permits the approximation of mass, momentum and energy fluxes acting across Eulerian cell faces without disturbing the conservation laws.

5.3 Non-monotony reduction

Obtained solutions can be made monotonic by using special methods that allow their smoothing without disturbing the conservation laws. These methods can be used along with any of the above shock wave methods. As a rule, these methods are developed without considering the problems of energy dissipation and entropy conservation across continuous solutions.

6 Conclusion

In conclusion I would like you to look at this table and compare the basic parameters of the methods we have just discussed.

Parameter	Difference Schemes				
	Neumann-Richtmyer	Lax	Godunov	Kuropatenko	
				Non-divergent	Divergent
1 Distraction, D	$2k\pi\sqrt{\dfrac{2}{\gamma+1}}$	∞	∞	∞	∞
2 Effective distraction, D^{e}	$2k\sqrt{\dfrac{2}{\gamma+1}}$	$\dfrac{2(1-æ^2)}{æ\,(\gamma+1)}$ $\dfrac{\sqrt{V_0}+\sqrt{V_1}}{\sqrt{V_0}-\sqrt{V_1}}$	$\dfrac{2(1-æ)}{(\gamma+1)}$ $\dfrac{\sqrt{V_0}+\sqrt{V_1}}{\sqrt{V_0}-\sqrt{V_1}}$		
3 Monotonicity	No	Yes	Yes	Conditional	Yes
4 Empirical constants	k	No	No	No	No
5 Stability	$æ \leqslant \dfrac{\sqrt{\gamma}}{2k}$	$æ \leqslant 1$	$æ \leqslant 1$	$æ \leqslant 1$	$æ \leqslant 1$

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