COMPLETELY CONSERVATIVE DIFFERENCE SCHEMES*

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1. THE system of equations of gas dynamics expresses three laws of conservation - of mass, momentum and energy.

In the numerical calculation of gas dynamical problems by the method of finite differences the system of differential equations is approximated by a difference scheme, which is equivalent to the replacement of the continuous medium by some discrete model of it. This model must reflect the fundamental properties of the medium. Therefore, it is natural in the first place to require that the corresponding difference analogs of the conservation laws be satisfied, that is, that the difference scheme be conservative. A. N. Tikhonov and A. A. Samarskii directed attention to this important fact at the beginning of the fifties. An example was constructed [1], where a non-conservative difference scheme, having a second order of approximation to the smooth solutions, diverges in the case of a discontinuous solution of the differential equation.

It is usually considered that to obtain a conservative difference scheme it is sufficient to approximate the three fundamental laws of conservation (balance) (see [2, 3], chapter III of the book [4], where a review is given of references on the numerical methods of gas dynamics).

However, there is a theoretical aspect here.

In the system of equations of gas dynamics the energy equation can be written in one of two forms - divergent and non-divergent. In differential form these forms are completely equivalent and may be transformed into one another by means of the remaining equations of the differential system. Therefore, for the system of equations of gas dynamics in differential form both the law of conservation of the total energy, and the balance of the internal energy are simultaneously valid and imply one another.

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For the system of difference equations the position is otherwise. In general, the non-divergent difference equation of the energy cannot be reduced to the divergent difference form by the use of the remaining difference equations. In the course of the transformations, on account of "mismatch" of the other equations of the scheme, remainder terms appear leading to violation of the law of conservation of the total energy.

The use of a difference scheme with a divergent energy equation leads to a similar defect: when the law of conservation of the total energy is satisfied, there are violations of the balance for the individual forms of energy, internal and kinetic.

The magnitude of the energy imbalance depends on the nature of the solution itself. On smooth solutions it is small and decreases as the time step of the net decreases. On strongly varying solutions the value of the imbalance may become comparable with the total energy and considerably distort the nature of the phenomenon calculated.

We will call the difference scheme completely conservative if both the laws of conservation of mass, momentum, and total energy, and also the detailed balance of energy, that is, the balance for the individual forms of energy - internal and kinetic, are valid for it.

In this paper completely conservative difference schemes for the system of equations of gas dynamics are constructed. These difference schemes may be obtained, for example, by means of the well-known [1] integro-interpolational method with the observation of some formal selection rule. This rule is as follows: completely conservative difference schemes must possess the same property as the system of differential equations, that is, a non-divergent energy equation must, by the use of the remaining difference equations, be reduced to a divergent difference equation, and conversely.

A strong imbalance effect was noticed in calculating a system of magneto-hydrodynamic equations where an extra form of energy, magnetic energy, appears, and where an extra energy balance relation must be satisfied.

However, so as not to complicate the treatment, in this paper the theoretical aspect of the question is considered by the simplest example, the "cross" scheme for one-dimensional gas dynamics. For the same reason the reasoning is confined to the case of uniform nets. (Similar questions were considered by V. Ya. Gol'din and N. N. Kalitkin).

2. The system of equations of gas dynamics (for the plane one-dimensional non-stationary case) in Lagrangian mass coordinates has the form

$$\frac{\partial v}{\partial t} = -\frac{\partial p}{\partial x}, \quad \frac{\partial r}{\partial t} = v, \quad \frac{\partial \eta}{\partial t} = \frac{\partial v}{\partial x}, \quad \frac{\partial \varepsilon}{\partial t} = -p\frac{\partial v}{\partial x}. \tag{I}$$

Notation: t is the time, r is the Eulerian coordinate, η is the specific volume, x $(dx = \eta^{-1}dr)$ is the Lagrangian mass coordinate, p is the pressure, ϵ is the internal energy of the gas, and v is the velocity.

The "cross" difference scheme for the system (1) is written as follows [5, 6] (scheme II):

$$\frac{v_i^{j+1} - v_i^j}{\tau} = -\frac{p_{i+1/2}^{j+1/2} - p_{i-1/2}^{j+1/2}}{m}, \tag{2.1}$$

$$\frac{r_i^{j+1} - r_i^j}{\tau} = v_i^{j+1}, \tag{2.2}$$

$$\frac{\eta_{i+1/2}^{j+3/2} - \eta_{i+1/2}^{j+1/2}}{\tau} = \frac{v_{i+1}^{j+1} - v_i^{j+1}}{m}, \tag{2.3}$$

$$\frac{\varepsilon_{i+1/2}^{j+3/2} - \varepsilon_{i+1/2}^{j+1/2}}{\tau} = -p_{i+1/2}^{j+3/2}\frac{v_{i+1}^{j+1} - v_i^{j+1}}{m}. \tag{2.4}$$

The scheme (II) is recorded on the uniform net $\{x_i, t^j\}$, $x_{i+1} = x_i + m$, $i = 0, 1, \ldots N$, $t^{j+1} = t^j + \tau$, $j = 0, 1, \ldots$, which is introduced into the domain of the space x, t considered. The values of the net functions r_i^j, v_i^j related to the nodes of the net (x_i, t^j), the values of the net functions $p_{i+1/2}^{j+1/2}$, $\varepsilon_{i+1/2}^{j+1/2}$, $\eta_{i+1/2}^{j+1/2}$ related to the half-integral points

From the physical point of view the difference equations (2.2), (2.3) are obviously equivalent to the relation

$$\eta_{i+1/2}^{j+3/2} = \frac{r_{i+1}^{j+1} - r_i^j}{m}, \tag{2.5}$$

which guarantees for the scheme (II) the satisfaction of the difference analog of the law of conservation of mass. In calculations, (2.5) is often used instead of the continuity equation for determining the specific volume.

The law of conservation of momentum is also valid for the difference scheme (II), as follows from the divergent form of writing the equations of motion (2.1).

The energy equation (2.4) is non-divergent. We consider for the scheme (II) the question of conservation of the total energy.

For convenience of performing the calculations for the net functions we will use the index-free notation [7]

$$y_i^j = y, \quad y_{i+1/2}^{j+1/2} = \bar{y}, \quad y_i^{j+1} = \hat{y}, \quad y_{i+1/2}^{j+3/2} = \hat{\bar{y}}, \tag{2.6}$$

$$\frac{\hat{y} - y}{\tau} = y_t, \quad \frac{y_{i+1} - y_i}{m} = y_x, \quad \frac{y_i - y_{i-1}}{m} = y_{\bar{x}}, \tag{2.7}$$

$$\sum_{i=1}^{N-1} y_i u_i m = (y, u), \quad \sum_{i=0}^{N-1} y_i u_i m = [y, u), \quad \sum_{i=0}^{N} y_i u_i m = [y, u]. \tag{2.8}$$

For the difference summation the following formula is valid:

$$[y, u_x] = -[y_x, u] + y_N u_N - y_{-1} u_0. \tag{2.9}$$

In the notation of (2.6), (2.7) the scheme (II) has a more compact form (scheme III):

$$v_t = -\bar{p}_{\bar{x}}, \tag{2.10}$$

$$r_t = \hat{v}, \tag{2.11}$$

$$\bar{\eta}_t = \hat{v}_x, \tag{2.12}$$

$$\bar{\varepsilon}_t = -\hat{\bar{p}}\,\hat{v}_x. \tag{2.13}$$

Using the notation of (2.8), we sum the energy equation (2.13) over the half-integral points and use formula (2.9):

$$[\bar{\varepsilon}_t, 1) = -[\hat{\bar{p}}, \hat{v}_x] = [\bar{p}_{\bar{x}}, \hat{v}] - \hat{\bar{p}}_N \hat{v}_N + \hat{\bar{p}}_{-1} \hat{v}_0, \tag{2.14}$$

where we understand by the formally introduced quantities $\bar{p}_N$ and $\bar{p}_{-1}$ the values of the pressure at the boundary nodes of the net.

From (2.10) after multiplying by $\hat{v}$ and summing over the nodes we have

$$[\hat{v}, v_t] = -[\bar{p}_{\bar{x}}, \hat{v}] = -[(\hat{\bar{p}} - 0.5\tau p_t)_{\bar{x}}, \hat{v}] = -[\hat{\bar{p}}_{\bar{x}}, \hat{v}] + 0.5\tau [\bar{p}_{t\bar{x}}, \hat{v}]. \tag{2.15}$$

Substituting (2.15) into (2.14) using the identity

$$\hat{v} v_t = 0.5 (v^2)_t + 0.5 \tau v_t^2 \tag{2.16}$$

and then summing the resulting equation with respect to time in the interval $[t^{j_1}, t^{j_2}]$, we arrive at the difference analog of the integral law of conservation of the total energy

$$[\bar{\varepsilon}, 1)|_{j_1}^{j_2} + 0.5\,[v^2, 1]|_{j_1}^{j_2} + \tau \sum_{j=j_1}^{j_2} \{\hat{\bar{p}}_N \hat{v}_N - \hat{\bar{p}}_{-1} \hat{v}_0\} = \Delta E, \tag{2.17}$$

$$\Delta E = 0.5\,\tau^2 \sum_{j=j_1}^{j_2} \{[\bar{p}_{\bar{t}\bar{x}}, \hat{v}] - [v_{\bar{t}}^2, 1]\}. \tag{2.18}$$

It is obvious from this that this law is infringed. The imbalance ΔE of the total energy accumulates in time and on smooth solutions is of order $O(\tau)$.

Here the balance of the internal energy is strictly satisfied:

$$[\bar{\varepsilon}, 1)_{\bar{t}} + \tau \sum_{j=j_1}^{j_2} [\hat{\bar{p}}, \hat{v}_{\bar{x}}) = 0,$$

which can be obtained by summing over time and space the energy equation (2.13).

We notice that the value of ΔE is independent of the step of the net relative to the mass m, hence the use of a finer spatial net does not lead to a noticeable decrease in the imbalance.

The appearance in the scheme (III) of an imbalance of the total energy is connected with non-divergence of the energy equation (2.13). However, the use in the scheme of a divergent energy equation, for example, in the form

$$\bar{\varepsilon}_{\bar{t}} + 0.25(v^2 + v(+1)^2)_{\bar{t}} = (\hat{\bar{p}}_* v)_{\bar{x}}, \quad v(+1) = v_{i+1}, \quad \bar{p}_* = 0.5(\bar{p}_{i+1/2} + \bar{p}_{i-1/2})$$

leads to similar difficulties. Of course, the law of conservation of the total energy will now be satisfied, but the balance of the internal energy is infringed, as is easily verified by performing calculations similar to (2.14) - (2.18).

Despite the conservation of the total energy, the balance of the internal energy, and consequently also of the kinetic energy separately is not observed. In particular, this means that in the scheme (III) the temperature is badly approximated. The latter fact may be vital, if for example, in the problem considered processes are present which are strongly dependent on the temperature (electrical conductivity, thermal conductivity etc).

The presence in the difference scheme of an energy imbalance can be treated as the presence in the scheme of sources and sinks of energy of a purely

difference origin. On smooth solutions the "power" of these sources is small and their influence on the course of the process studied is small. However, the integral contribution of these fictitious sources on strongly varying solutions may become comparable with the total energy and considerably distort the nature of the phenomenon.

Effects connected with imbalances also appear in other difference schemes extensively used for the calculations of problems in gas dynamics, for example, [2, 3].

3. We consider a family of difference schemes approximating to the system of equations (I) of gas dynamics (scheme (IV)):

$$v_t = -p_{\overline{x}}^{(\sigma_1)}, \tag{3.1}$$

$$r_t = v^{(\sigma_2)}, \tag{3.2}$$

$$\eta_t = v_x^{(\sigma_3)}, \tag{3.3}$$

$$\varepsilon_t = -p^{(\sigma_1)} v_x^{(\sigma_4)}. \tag{3.4}$$

We use the notation $f^{(\sigma)} = \sigma \hat{f} + (1-\sigma) f$, $f = f_i^j$, $\hat{f} = f_i^{j+1}$. All the net functions are taken on the same time layers. As before, the functions r, v related to the nodes of the net, and p, ϵ, η, to the half-integral points.

The parameters $0 \leqslant \sigma_k \leqslant 1$, $k = 1, 2, 3, 4$, are weighting factors, by means of which it is possible to perform some kind of time interpolation for the corresponding terms of the difference equations.

We study the problem of for what values of the parameters σ_k in the scheme (IV) difference analogs of the gas dynamics conservation laws will be satisfied.

A. Law of conservation of mass.

We perform the difference differentiation with respect to x of equation (3.2) and use the obvious relation

$$f^{(\alpha)} = f^{(\beta)} + (\beta - \alpha)\tau f_t.$$

We obtain the equation

$$r_{tx} = v_x^{(\sigma_2)} = v_x^{(\sigma_3)} + (\sigma_3 - \sigma_2)\tau v_{xt} = \eta_t + (\sigma_3 - \sigma_2)\tau v_{xt},$$

which implies that the relation $\eta = r_x$ ensuring the observance of the law of conservation of mass, is only valid provided that $\sigma_3 = \sigma_2$.

B. The satisfaction of the law of conservation of momentum follows directly from the divergent form of writing the equation of motion (3.1).

C. To illustrate the question of the law of conservation of the total energy we repeat one after another the calculations performed in section 2:

$$[\varepsilon, 1)_t = -[p^{(\sigma_1)}, v_x^{(\sigma_4)}) = [p_{\overline{x}}^{(\sigma_1)}, v^{(\sigma_4)}] - p_N^{(\sigma_1)} v_N^{(\sigma_4)} + p_{-1}^{(\sigma_1)} v_0^{(\sigma_4)}. \tag{3.5}$$

From equation (3.1) after multiplying by $v^{(\sigma_4)}$ and summing over the nodes we have

$$-[p_{\overline{x}}^{(\sigma_1)} v^{(\sigma_4)}] = [v^{(\sigma_4)}, v_t] = 0.5[v^2, 1]_t - (0.5 - \sigma_4)\tau[v_t^2, 1]. \tag{3.6}$$

Substituting (3.6) into (3.5), we obtain for the time interval $[t^{j_1}, t^{j_2}]$ the following balance of the total energy:

$$[\varepsilon, 1)|_{j_1}^{j_2} + 0.5[v^2, 1]|_{j_1}^{j_2} + \tau \sum_{j=j_1}^{j_2} \{p_N^{(\sigma_1)} v_N^{(\sigma_4)} - p_{-1}^{(\sigma_1)} v_0^{(\sigma_4)}\} = \Delta E_1, \tag{3.7}$$

$$\Delta E_1 = (0.5 - \sigma_4)\tau^2 \sum_{j=j_1}^{j_2} [v_t^2, 1]. \tag{3.8}$$

Therefore, in order to ensure in the scheme (IV) strict satisfaction of the law of conservation of the total energy, it is necessary to impose the requirement $\sigma_4 = 0.5$.

Moreover, from the very process of deriving (3.8) it is clear that the time interpolations of the net pressure function in equations (3.1) and (3.4) must be identical. Otherwise an additional imbalance term occurs in (3.7).

D. The balance of the internal energy is observed because of the use in the scheme (IV) of the non-divergent form of the energy equations.

We call a difference scheme, approximating the system of equations of gas dynamics, completely conservative, if the laws of conservation of mass, momentum, total energy, and also the detailed energy balance, that is, the balance for the individual forms of energy, internal and external, are satisfied for it.

For the scheme (IV) to be completely conservative it is sufficient for the

following conditions to be satisfied:

$$\sigma_4 = 0.5, \qquad \sigma_3 = \sigma_2. \tag{3.9}$$

Therefore, a two-parameter family exists (with the free parameters σ_1, σ_2) of completely conservative schemes IV. All these schemes have the approximation $O(\tau + m^2)$.

There is only one completely conservative scheme of the second order of approximation in τ and m. It is defined by the conditions (3.9) and the conditions

$$\sigma_1 = 0.5, \qquad \sigma_2 = 0.5. \tag{3.10}$$

4. In IV we replace the last equation in the condition (3.9) by the divergent energy equation

$$\varepsilon_t + 0.25(v^2 + v(+1)^2)_t = -(p_*^{(\sigma_1)} v^{(0.5)})_x, \tag{4.1}$$

where the notation $f(+1) = f_{i+1}$, $f(-1) = f_{i-1}$, $p_{*\,i} = 0.5(p_{i+1/2} + p_{i-1/2})$ has been used.

The difference equation (4.1) is completely equivalent to the difference equation (3.4) and can be reduced to it by using the remaining equations of the scheme (IV). Indeed, multiplying (3.1) by $v^{(0.5)}$, we have

$$-p_{\underline{x}}^{(\sigma_1)} v^{(0.5)} = v^{(0.5)} v_t = 0.5\, v_t^2, \tag{4.2}$$

$$-p_{\underline{x}}^{(\sigma_1)} (+1)\, v^{(0.5)}(+1) = 0.5\, v_t(+1)^2. \tag{4.3}$$

Taking half the sum of the equations (4.2) and (4.3) and adding them to (4.1), we obtain equation (3.4).

It is also easy to see that the scheme (IV), where (3.4) is replaced by (4.1) will also be completely conservative.

(Note added in proof. A similar scheme was obtained by V. Ya. Gol'din and N. N. Kalitkin from other considerations. A scheme based on the "predictor-corrector" idea presented in [4], p. 426 reduces to a similar completely conservative scheme).

The formal requirement imposed on completely conservative schemes for solving the gas dynamic equations is that by means of the remaining equations of the scheme the non-divergent energy difference equation is transformed into

divergent form, and conversely.

(Note added in proof. similar observations were made by Harlow with reference to the method of particles in cells [8]).

The divergent equation (4.1) can be obtained by means of the integro-interpolational method [1]. The essence of this method is that the difference equations are constructed from integral relations expressing the laws of conservation for an elementary cell of the net. Then a definite interpolation of the required solution and of the coefficients of the equation is introduced on the net, and by varying this the various difference schemes are obtained.

The formal requirement formulated above can be considered as a rule for selecting completely conservative schemes from the class of schemes given by the integro-interpolational method.

In particular, the integro-interpolational method enables two more divergent difference equations to be constructed:

$$(\varepsilon + 0.5v^2)_t = -(p^{(\sigma_1)}(-1)v^{(0.5)})_x, \tag{4.4}$$

$$(\varepsilon + 0.5v(+1)^2)_t = -(p^{(\sigma_1)}v^{(0.5)})_x, \tag{4.5}$$

which are equivalent to (3.4).

The equivalence of (4.4) and (4.5) to equation (3.4) implies an interesting fact: equations (4.4) and (4.5) have a second order of approximation in the space $O(m^2)$, while the other terms of these equations are approximated to the first order.

5. To judge the quality of the difference schemes for the equations of gas dynamics the model equations of acoustics are often used. We notice that effects connected with completely conservative schemes cannot be exhibited in this approximation because it does not, in fact, include the energy equation.

We will not discuss the investigation of the stability of the schemes obtained, because the stability of these schemes is obvious from their implicitness.

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