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IMPROVEMENT OF THE ACCURACY OF THE LARGE-PARTICLE METHOD IN CALCULATION OF MOTIONS OF ENERGY-SATURATED MEDIA ON SUPERPOSED GRIDS

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A TVD-modification of the large-particle method with the algorithm of calculation on superposed grids with a set of cells differing in shape is presented.

One basic method of first order of accuracy is the large-particle method [1], which is widely used in computational practice [2, 3]. The large-particle method developed in the 1970s as applied to solution of the nonstationary problems of supersonic gasdynamics included a number of successful physically clear algorithmic solutions which made it possible to carry out its modifications necessary for practice.

Versatile investigations of many years into a number of modifications of the schemes of the large-particle method whose results are summed up in the collective monograph [3] have shown that it is expedient to construct improved-accuracy schemes of the large-particle method simultaneously for space and time coordinates with allowance for additional requirements on the total conservatism, entropism, and monotonicity of the schemes.

The suppression of oscillations, produced by the use of schemes of second order of accuracy or higher in the space coordinate in the large-particle method, was initially carried out by introducing specially selected terms of "artificial viscous" pressure or artificial dissipation at the final stage [3, Sections 4 and 9]. In passing it was found that for conservative schemes of first order of accuracy the mere rational control of the magnitude of the approximation viscosity by using the velocities, calculated at the first stage of the large-particle method, in determination of fluxes at the boundaries of the cells turned out to be quite sufficient for this purpose [3, Sections 9 and 15].

The overwhelming majority of modifications of the schemes of the large-particle method are mainly reduced to construction of stable monotone schemes of first order of accuracy in time $\sim O(\Delta t)$. However the use of the schemes of improved accuracy in the space coordinate with preservation of the accuracy $\sim O(\Delta t)$ in time is accompanied, as a rule, by the development of the phenomena of numerical instability as the solution moves in time, which was one determining factor of the employment of implicit and semiimplicit schemes in the large-particle method [3, Sections 5, 9, 15, and 22].

In [3, Section 15], it has been shown that the use of the semiimplicit schemes of the large-particle method makes it possible to determine the intermediate values of the pressure $\tilde{P}_i^{n+1}$ with an accuracy $\sim O(\Delta t^2)$ and to ensure the required stability of calculation. It has particularly been noted that a substantial (of about an order of magnitude) improvement in the accuracy and stability can be attained when one employs the pressure fields $(\tilde{P}_{i\pm 1/2}^{n+1})$ calculated at the boundaries of the cells rather than at their centers [3, Section 15, pp. 972–974]. Nonetheless, the total accuracy of calculation remained $\sim O(\Delta t, \Delta x)$ because of the employment of the linear schemes of first order of accuracy for convective terms.

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In investigating the unstable regimes of interaction of energy-saturated media [4] and detonation processes in cavities of different configurations [5–7], it has been found that one must carry out a modification of the large-particle method which would ensure an accuracy $\sim O(\Delta t^2, \Delta x^2)$ [8] corresponding better to results of the comparison of nonstationary calculated and experimental data [9]. In addition to the reports [8, 10], below we present in expanded form the obtained TVD-modification of the large-particle method and the algorithm of its calculation on superposed grids with a set of cells differing in shape.

It turned out that the splitting by physical processes and account (adequate to the accuracy $\sim O(\Delta t, \Delta x)$) for the directions of propagation and for the level of gasdynamic disturbances which are implemented in the algorithm of the large-particle method allow the TVD-modification of the large-particle method without fundamental changes in the algorithm in the case of introduction of a correcting step at the final stage of the method, which was done on obtaining the results of [5–10].

The presented TVD-modification of the large-particle method can be considered in another context as splitting of the original scheme of Harten [11–14] following the pattern of a generalized predictor-corrector scheme. Unlike the original scheme, the splitting makes it possible to determine the magnitude of the correcting fluxes $q_{i\pm 1/2}(U)$ from the values of the gasdynamic parameters from the intermediate upper time layer ($\tilde{\mathbf{U}}^{n+1}$) rather than from the lower layer ($\mathbf{U}^n$). To unambiguously understand the essence of the above we consider in retrospection the principles and technique of construction of the TVD-schemes of improved accuracy and the algorithm of TVD-modification of the large-particle method and the method of determination of a solution on superposed grids with a set of cells differing in shape.

Principles of Construction of TVD-Schemes of Improved Accuracy. We note that the very concept of a TVD-scheme (i.e., Total Variation Diminishing Scheme) was introduced by Harten [11–14] at the end of 1981 initially as the TVNI-principle (Total Variation Nonincreasing [11]) as applied to the two-layer numerical schemes approximating the conservation laws of the form

$$\mathbf{U}_t + \mathbf{f}\,(\mathbf{U})_x = 0\,, \tag{1a}$$

in particular, by explicit relations of the type

$$\mathbf{U}_i^{n+1} = \mathbf{U}_i^n - \frac{\Delta t}{\Delta x}\,(\tilde{\mathbf{f}}_{i+1/2}^n - \tilde{\mathbf{f}}_{i-1/2}^n)\,. \tag{1b}$$

Beginning in 1985, the concept of a TVD-scheme appeared in the titles of papers and became commonly used [15–19]. For the scalar functions U in (1) the total variation

$$\mathrm{TV} = \int_{-\infty}^{\infty} \left| \frac{\partial U}{\partial x} \right| dx \tag{2}$$

is preserved on smooth solutions and diminishes in the presence of discontinuities [11–15]. The schemes possess the TVD-property if the numerical analog of (2) $\mathrm{TV} = \sum_{j=-\infty}^{\infty} |U_{j+1} - U_j|$ does not increase, so that $\mathrm{TV}(U^{n+1}) \le \mathrm{TV}(U^n)$ for solutions at the subsequent time layer [11, 12]. Clearly, this property of the scheme keeps the nonphysical numerical oscillations from developing and ensures not only the stability of the numerical scheme but the monotonicity of the solution [11–19].

Distinctive features of the efficient difference schemes of direct calculation which were proposed in the middle of the 1990s account for the directions of propagation of disturbances by introducing certain ap-

proximate solutions of the one-dimensional Riemann problem of disintegration of an arbitrary discontinuity in the initial data into the algorithms of computational schemes and "good" localization of a conservatively introduced numerical dissipation in the vicinity of discontinuities of solutions. Historically, one can recognize two approaches here.

The first approach was discovered in the works of S. K. Godunov (1960s); these works initiated the creation of difference schemes with the employment of the so-called "disintegration" algorithm [20, 21]. It is significant that the order of approximation was increased here by replacement of the step distribution of parameters in the cells by a piecewise-linear distribution [22–24] and then by a piecewise-parabolic distribution [25], which actually meant the abandonment of the purely grid presentation of data in favor of a locally continuous presentation. The arising necessity of solving the non-self-similar problem of disintegration of a discontinuity in combination with a search for the answer to the nontrivial question of determination of increments in the parameters on elementary intervals of the lower layer was solved in [22] by using the *principle of minimum values of derivatives (or increments in parameters)* in construction of difference schemes [22–24].

In solving the Euler equations on strong (nonremovable) discontinuities, the scheme of [22] loses monotonicity. Because of this, at a later time [26–28], in accordance with [23, 24] and unlike [22], in increasing the order of approximation in Godunov-type schemes, in determination of increments one began to use the *monotone algorithm* (slope limiters [13, 23]) of the following form:

$$\Delta\mathbf{U}_{i-1/2} = \begin{cases} 0\,, & \Delta\mathbf{U}_i \cdot \Delta\mathbf{U}_{i-1} \le 0\,, \\ \min\left(2\,|\Delta\mathbf{U}_i|\,,\ 2\,|\Delta\mathbf{U}_{i+1}|\,,\ \dfrac{|\mathbf{U}_{i+1/2} - \mathbf{U}_{i-3/2}|}{2}\right) \operatorname{sign}(\Delta\mathbf{U}_i)\,, & \Delta\mathbf{U}_i \cdot \Delta\mathbf{U}_{i-1} > 0\,, \end{cases}$$

where $\operatorname{sign}(K) = K/|K|$ and $\Delta\mathbf{U}_k = \mathbf{U}_{k+1} - \mathbf{U}_k$, $k = i,\ i-1/2,\ i \pm 1$.

The second approach can be represented as generalization of the predictor–corrector scheme in which a monotone solution is found at the first step and is corrected at the second step with the aim of identifying discontinuous solutions satisfying the physical conditions. In realization of this approach, one first determines the values of the fluxes at the boundaries of computational cells introduced into consideration; this is done using one-sided differences in the algorithms of *first order* of approximation. Then these fluxes are corrected using finite-difference expressions that include the logic of elimination of numerical diffusion where this does not lead to the enhancement of the existing extrema or to the appearance of new ones.

This trend has been developed most effectively in the works of Boris and Book (Flux Corrected Transport Algorithms, i.e., FCT-algorithms [29, 30]) and also in the works of van Leer (Monotone Upstream-Centered Scheme for Conservation Laws, i.e., MUSCL-schemes [31]), who also made considerable effort to construct difference schemes of improved accuracy for "disintegration" algorithms [13, 24]. This approach was also supported in the former Soviet Union [32, 33].

The next two aspects can be recognized as the most significant in both approaches.

First, the use of the nonlinear function, i.e., the limiter in determination of the magnitude (average on the time internal) of the flux at the boundary of two cells, was the actual algorithmic realization of the TVD-property. Initially, this function was employed by Boris and Book in the FCT-algorithm in limitation of the magnitude of the flux $\mathbf{f}_{m+}^{\text{corr}}$ (flux limiters [29]) at the antidiffusion stage according to the formula

$$\mathbf{f}_{m+}^{\text{corr}} = s \max\left[0\,,\ \min\left[s\,(\delta\mathbf{F})_{m-}\,,\ |\mathbf{f}_{m+}|\,,\ s\,(\delta\mathbf{F})_{1+(m+)}\right]\right], \tag{3}$$

where $s = \operatorname{sign}(\mathbf{f}_{m+})$, $(\delta\mathbf{F})_{m\pm} = \pm\,\mathbf{f}_{i\pm1} \mp \mathbf{f}_i$, and $\mathbf{f}_{m+}^{\text{corr}}$ is the corrected value of the flux at the boundary between the cells i and $i+1$ [29, 30].

When some FCT-algorithms were modified, the modifications concerned the antidiffusion stage: selection of the form of correcting fluxes, the antidiffusion coefficients, and the form of limiters of the logic type that made it possible to ensure the monotonicity of the schemes in solutions with discontinuities [30–33]. However, one was unable to eliminate the drawbacks of the SHASTA basic scheme by modifications in just the antidiffusion algorithm. Finally, the idea of correction was extended to a number of existing schemes [19].

Second, at the end of 1981 Harten [11–15] successfully implemented in practice the idea dating back to the works of Lax and Wendroff, which were written in the 1960s [34–37]; these works were devoted to the employment, in (1), of the Jacobi matrix $A = \partial f(\mathbf{U})/\partial \mathbf{U}$ in algorithms of direct calculation to increase the order of approximation of two-layer difference schemes. Simultaneously with the introduction of the TVD-principle, one successfully employed the matrix of right-handed eigenvectors R for A to simultaneously solve several complex problems of construction of improved-accuracy schemes. Using the technique proposed in [11–17], it became possible to determine solutions with the second order of accuracy $\sim O(\Delta t^2, \Delta x^2)$ by calculating the magnitude of the convective flux $\tilde{\mathbf{f}}_{i+1/2}$ in (1) from relations of the following form:

$$\tilde{\mathbf{f}}_{i+1/2} = \frac{1}{2}(\mathbf{f}_i + \mathbf{f}_{i+1}) + \mathbf{q}_{i+1/2}, \tag{4}$$

$$\mathbf{q}_{i+1/2} = -\frac{1}{2}\,|\mathbf{A}|_{i+1/2} \cdot \Delta_{i+1/2}\,\mathbf{U} = \frac{1}{2}(\mathbf{R} \cdot \mathbf{\Phi})_{i+1/2}, \tag{5a}$$

$$\mathbf{\Phi}\,(\boldsymbol{\alpha})_{i+1/2} = (\mathbf{\Lambda} \cdot \mathbf{R}^{-1} \cdot \mathbf{\Delta U})_{i+1/2}, \tag{5b}$$

where the first two terms in (4) correspond to the scheme in central differences of second order of accuracy in space which is used in (1) to approximate $\mathbf{f}(U)_x$ and of first order of accuracy in time for $\mathbf{U}_t$. The last term in (4) is introduced just to ensure the second order of accuracy in time with the employment of a two-layer template and of the minimum local value of the numerical dissipation required to ensure stable calculation with simultaneous suppression of the sources of dispersion oscillations which are known to be inherent in central difference schemes [35, 36].

Thus, in constructing difference schemes of second order of accuracy, from the end of the 1980s one began to use a variable template and a nonlinear character of corrections in calculation of fluxes in order to ensure the monotonicity of solution and the second order of accuracy $\sim O(\Delta t^2, \Delta x^2)$ in both time and space.

Technique of Construction of TVD-Schemes of Improved Accuracy. The equations of Euler or Navier–Stokes do not have the form (1) because of both the nonzero right-hand side and the nonsingleness of the determining equation, and a "good" quality of a numerical solution for them has no substantiation and is only confirmed by results of numerous calculations. For example, in the general case, the TVD-principle (2) is inapplicable to calculation of single waves converging to the geometric centers of symmetry of fluxes because of the increase in the pressure in them or to calculation of fluxes with energy release, for example, with detonation waves.

Therefore, in developing schemes that preserve the "good" properties of TVD-schemes, one usually employs simple heuristic methods. They are reduced to addition of the terms of artificial dissipation q which correspond to a locally plane TVD-scheme in (4) either directly, as in [38], or by using the expansions of matrices determining the numerical viscosity of the schemes, for example, power expansion of the Jacobi matrix in quadratic or linear polynomials, as in [39, 40], in accordance with the ideas of [31, 41].

Much effort has been made to relate the corrections q to the centers of the cells rather than to their faces [8–10]. It was taken, for example, that $q_{i+1/2} = (q_i + q_{i+1})/2$, and it was assumed that, using the parameters for the centers of the cells, one can more accurately calculate the matrices in (5). By definition, q_i are the values averaged over the cell volume at a specific instant of time, and in such a calculation the vector of increments of the flux (average over the cell surface on the interval Δt) is split into certain components av-

eraged over the volumes of neighboring cells. A great number of difficulties and recommendations appeared because of the apparent necessity of ensuring the required accuracy for the chain of difference transformations $\Delta_{m+}\mathbf{f} = (\mathbf{A}\cdot\Delta\mathbf{U})_{m+} = (\mathbf{R}\cdot\Lambda\cdot\mathbf{R}^{-1}\cdot\Delta\mathbf{U})_{m+} = (\mathbf{R}\cdot\Phi(\alpha))_{m+}$.

We also note that we have tested the technique [41] of splitting of the vector of the flux on cell faces depending on the signs of eigenvalues, which reflects the influence of grid-characteristic procedures, particularly, of generalized variants of the λ-schemes of Moretti [19]. However the additional body of computations for different methods of splitting in calculation of q was not a marked advantage. More economical schemes with a smaller body of matrix computations turned out to be more attractive.

The computational practice of the past three decades has shown that elimination of the characteristic transformations in the algorithms makes the calculations much cheaper (by three- to fivefold [24, 27]). And determination of fluxes according to (4) ensures acceptable accuracy (of second order); as it has turned out, this accuracy on the whole differs insignificantly [15–17, 42–45] from specific schemes of determination of q constructed at the end of the 1990s on the basis of different initial hypotheses in the works of Roe (1981, Approximate Riemann Solvers [37]), Steger and Warming (1981; Flux Vector Splitting [41]), van Leer (1982, MUSCL [31]), and a number of other researchers [16–19]. In special cases, for example, at points where the values of the eigenvalues change their sign, one has revealed the presence of glitches [41] or even the occurrence of nonphysical shock waves ("carbuncle" shocks) [17]. The practice also revealed other differences, in particular, excessive numerical diffusion even in the existence domains of physically meaningful shear stresses [31], which became one stimulating factor of further perfection of these systems [28, 40, 46–48].

Unlike the remaining schemes, a distinctive feature of the Harten schemes [11, 12] was the application of limiter functions not directly to conservative variables, as in (3), but in computation of the difference analogs of the Riemann invariants (i.e., the components α^1 of the vector function $\mathbf{\Phi}(\alpha)$ in (5b)) in the characteristic-variable space [11, 14, 15, 21] in such a manner that the total variations of precisely the grid analogs of the Riemann invariants and the entropy function do not increase with time. In so doing, the consistency of all the parameters that are physically meaningful in the evolution of a discontinuity and the accuracy $\sim O(\Delta t^2)$ are ensured. Here the matrix $\mathbf{R}$ is used to transform the vector function of the increments $\mathbf{\Phi}(\alpha)$ from the space of characteristic variables to the space of conservative physical variables $\mathbf{U}$, thus determining the specific values of the correcting fluxes $q_{i+1/2}$ in (5a) and (4).

According to [14, 15], construction of the TVD-schemes of improved accuracy as applied to the equations (formally coincident with (1)) of one-dimensional gasdynamics of a perfect gas, now is as follows:

$$\mathbf{U} = [\rho,\ \rho u,\ \rho E]^{\mathrm{t}},\quad \mathbf{f}(\mathbf{U}) = [\rho u,\ \rho u^2 + P,\ (\rho E + P)\,u]^{\mathrm{t}};$$

$$\boldsymbol{\alpha} = \mathbf{R}^{-1}\cdot\Delta\mathbf{U} = \left[\frac{1}{2}\left(\frac{\Delta P}{c^2} + \frac{\rho}{c}\Delta u\right),\ \Delta\rho - \frac{\Delta P}{c^2},\ \frac{1}{2}\left(\frac{\Delta P}{c^2} - \frac{\rho}{c}\Delta u\right)\right]^{\mathrm{t}} \sim \left[\Delta u + \frac{\Delta P}{\rho c},\ \Delta S,\ \Delta u - \frac{\Delta P}{\rho c}\right]^{\mathrm{t}}, \tag{6}$$

where ΔS is the entropy change corresponding to the increment in the entropy function (coefficient α^2) in the vector α; this vector results from the expansion of the solution $\mathbf{U}$ in eigenvectors. In this case, the matrices $\mathbf{R}$ and $\mathbf{R}^{-1}$ have the following form [15–17, 44]:

$$\mathbf{R} = \begin{bmatrix} 1 & 1 & 1 \\ u + c & u & u - c \\ E + \dfrac{P}{\rho} + uc & \dfrac{u^2}{2} & E + \dfrac{P}{\rho} - uc \end{bmatrix},\quad \mathbf{R}^{-1} = \begin{bmatrix} \left(b_1 - \dfrac{u}{c}\right)/2 & \left(-b_2 u + \dfrac{1}{c}\right)/2 & \dfrac{b_2}{2} \\ 1 - b_1 & u b_2 & -b_2 \\ \left(b_1 + \dfrac{u}{c}\right)/2 & \left(-b_2 u - \dfrac{1}{c}\right)/2 & \dfrac{b_2}{2} \end{bmatrix}, \tag{7}$$

where $b_1 = b_2 u^2/2$ and $b_2 = (E + P/\rho - u^2/2)^{-1}$. For the TVD-schemes of Harten [11, 12] it is common practice to calculate the elements of the vector $\mathbf{\Phi}(\alpha)$ in (5) from the formulas [44]

$$(\mathbf{\Phi}^l_{i+1/2})^{\text{upwind}} = \boldsymbol{\sigma}\,(\boldsymbol{\lambda}^l_{i+1/2}) \cdot (\mathbf{g}^l_{i+1} + \mathbf{g}^l_i) - \boldsymbol{\Psi}\,(\boldsymbol{\lambda}^l_{i+1/2} + \boldsymbol{\gamma}^l_{i+1/2}) \cdot \boldsymbol{\alpha}^l_{i+1/2}\,, \tag{8a}$$

$$(\mathbf{\Phi}^l_{i+1/2})^{\text{symmetry}} = 2\boldsymbol{\sigma}\,(\boldsymbol{\lambda}^l_{i+1/2})\,\boldsymbol{\Theta}^l_{i+1/2} - \boldsymbol{\alpha}^l_{i+1/2}\,\boldsymbol{\Psi}\,(\boldsymbol{\lambda}^l_{i+1/2})\,, \tag{8b}$$

where

$$\begin{vmatrix} \boldsymbol{\alpha}^{(1)}_{i+1/2} \\ \boldsymbol{\alpha}^{(2)}_{i+1/2} \\ \boldsymbol{\alpha}^{(3)}_{i+1/2} \end{vmatrix} = \begin{vmatrix} (aa + bb)/2 \\ \Delta_{m+}\,\rho - aa \\ (aa - bb)/2 \end{vmatrix}, \qquad \begin{aligned} aa &= b_2 \cdot \left(\frac{u^2}{2}\,\Delta_{m+}\,\rho - u \cdot \Delta_{m+}\,\rho u + \Delta_{m+}\,\rho E \right) \equiv \frac{\Delta P}{c^2}\,, \\ bb &= \frac{1}{c}\,(\Delta_{m+}\,\rho u - u \cdot \Delta_{m+}\,\rho) \equiv \frac{\rho}{c}\,\Delta u\,, \quad (m+) = i + 1/2\,, \end{aligned} \tag{8c}$$

$$\boldsymbol{\gamma}^l_{i+1/2} = \boldsymbol{\sigma}\,(\boldsymbol{\lambda}^l_{i+1/2}) \cdot \begin{cases} \dfrac{\mathbf{g}^l_{i+1} - \mathbf{g}^l_i}{\boldsymbol{\alpha}^l_{i+1/2}}, & \boldsymbol{\alpha}^l_{i+1/2} \neq 0\,, \\ 0\,, & \boldsymbol{\alpha}^l_{i+1/2} \equiv 0\,; \end{cases} \qquad \boldsymbol{\sigma}\,(z) = \frac{1}{2}\left[\boldsymbol{\Psi}\,(z) - \frac{\Delta t}{\Delta x}\,z^2 \right]; \quad \boldsymbol{\Psi}\,(z) = \begin{cases} |z|\,, & |z| \geq \delta\,, \\ \dfrac{(z^2 + \delta^2)}{2\delta}, & |z| < \delta\,; \end{cases}$$

$\lambda^{(1)}_{i+1/2} = (u + c)_{i+1/2}$, $\lambda^{(2)}_{i+1/2} = (u)_{i+1/2}$, and $\lambda^{(3)}_{i+1/2} = (u - c)_{i+1/2}$. Here λ represents the eigenvalues of the Jacobi matrix. Finally, the remaining quantities in (8a) and (8b) are determined from the expressions

$$\boldsymbol{\Theta}^l_{i+1/2} = \mathbf{g}^l_i + \mathbf{g}^l_{i+1} - \boldsymbol{\alpha}^l_{i+1/2}\,; \quad \mathbf{g}^l_k = \min\text{mod}(\boldsymbol{\alpha}^l_{k-1/2}\,, \boldsymbol{\alpha}^l_{k+1/2}) \quad \text{for } k = i,\ i+1 \text{ and } l = 1, 2, 3\,. \tag{8d}$$

The limiter function in (8d) for $a = a^l_{i-1/2}$ and $b = \alpha^l_{i+1/2}$ acquires the form min mod (a, b) (minimum modulus) and corresponds to formula (3), i.e., is equal to the smallest argument with a "b" sign if all the arguments are positive or is equal to zero if there is a negative argument. This is not the only form of nonlinear functions that ensure the monotonicity of the scheme and its stability. The limiters acting as (8d) for (8a) and (8b) can be represented as follows [42, 48]:

a) $\mathbf{g}^l_i = \min\text{ mod }(2a, 2b, (a + b)/2)$; b) $\mathbf{g}^l_i = \min\text{ mod }(2a, 2b, 2c, (a + c)/2)$;

c) $\mathbf{g}^l_i = \sup\ b\,(a, b) = s\,\max[0, \min(2\,|b|\,sa), \min(|b|, 2sa)]\,, \quad s = \text{sign}\,(b)$;

d) $\mathbf{g}^l_i = \dfrac{(a^2 + \delta)\,b + (b^2 + \delta)\,a}{a^2 + b^2 + 2\delta}\,, \quad 10^{-7} \leq \delta \leq 10^{-5}\,.$

TVD-Modification of the Large-Particle Method. In constructing the difference schemes of the large-particle method, the transition from one time layer to another is carried out in two stages [1, 2]. At the first stage, use is made of a certain scheme in Lagrange variables. At the second stage, the parameters are converted to the initial Euler grid, which corresponds to one of several possible interpretations of the method. As has been shown in [3, Section 19], the difference operator of convective terms in the large-particle method can be represented in the form

$$\langle \text{div}\,(\mathbf{U} \cdot \mathbf{W}) \rangle^n_i\,\Delta V = \sum_k \left\{ \frac{(\mathbf{U}\,\mathbf{W}_k)_{i+1}\,F_{(m+)_k} - (\mathbf{U}\,\mathbf{W}_k)_{i-1}\,F_{(m-)_k}}{2} + (\mathbf{W}_k)_i\,\frac{(\mathbf{U})_{i+1}\,F_{(m+)_k} - (\mathbf{U})_{i-1}\,F_{(m-)_k}}{2} - \right.$$

$$-\frac{((\mathbf{W}_k)_{(m+)_k+m_k} F_{(m+)_k} + (\mathbf{W}_k)_{(m-)_k+m_k} F_{(m-)_k})}{2} \cdot ((\mathbf{U})_{(m+)_k+m_k} - (\mathbf{U})_{(m-)_k+m_k})\Bigg\}, \tag{9}$$

where $(m\pm)_k = i \pm 1/2$, $m_k = -\text{sign}\,(\mathbf{W}_k)/2$, $\mathbf{W}_k$ is the projection of the velocity vector $\mathbf{W}$ onto the x_kth coordinate direction, ΔV is the cell volume, and F_m is the area of the mth face of the cell. The last two terms of the difference operator (9) govern, in essence, the presence of the dissipative terms of the large-particle method which ensure not only the stability of calculation but the accuracy $\sim O(\Delta x)$ as well. Transforming (9) to the form (4), we obtain the following expression for the flux $\tilde{\mathbf{f}}_{i+1/2}$ in the large-particle method:

$$\tilde{\mathbf{f}}^n_{i+1/2} = \frac{1}{2}\left(\mathbf{f}_{i+1} + \mathbf{f}_i - |\mathbf{W}_k|_{(m+)_k+m_k} (\mathbf{U}_{i+1} - \mathbf{U}_i)\right), \tag{10}$$

whence for the correcting flux we have

$$\mathbf{q}^n_{i+1/2} = -\frac{1}{2} |\mathbf{W}_k|_{(m+)_k+m_k} (\mathbf{U}_{i+1} - \mathbf{U}_i)\,. \tag{11}$$

It is clear from the comparison of (11) and (5) that to ensure the accuracy $\sim O(\Delta t^2, \Delta x^2)$ in (9), one must replace in (10) the value of the correcting flux (11) by (5). This replacement has been carried out with allowance for the logic of the algorithm of the large-particle method. For the sake of definiteness it is also assumed that we have (1) and (6) for the kth direction; then to calculate the correcting flux (5) we can use relations (7) and (8). Finally we obtain a modified algorithm of the large-particle method; this algorithm acquires the following form:

I. Eulerian stage (unchanged)

$$(\tilde{\mathbf{U}}_i{}^n)^I = (\mathbf{U}_i{}^n)^I - \frac{\Delta t}{\rho^n_i} \sum_k \frac{(\mathbf{f}^n_{i+1})^I - (\mathbf{f}^n_{i-1})^I}{2\Delta x_k}, \tag{12a}$$

where $\mathbf{U}^I = [u, E]_t$ and $\mathbf{f}(\mathbf{U})^I = [P, Pu]_t$.

II. Lagrangian stage (changed)

$$(\Delta\mathbf{M})^n_{(m+)_k} = \frac{(\tilde{\mathbf{f}})^n_i + (\tilde{\mathbf{f}})^n_{i+1}}{2} F_{(m+)_k}\,. \tag{12b}$$

III. Final stage

(a) (unchanged)

$$\text{a) (unchanged)}\quad \tilde{\mathbf{U}}_i{}^{n+1} = \tilde{\mathbf{U}}_i{}^n - \frac{\Delta t}{\Delta V_i} \sum_k \left((\Delta\mathbf{M}^n_{(m+)_k} - \Delta\mathbf{M})^n_{(m-)_k}\right), \tag{12c}$$

(b) (supplemented)

$$\text{b) (supplemented)}\quad \mathbf{U}_i{}^{n+1} = \tilde{\mathbf{U}}_i{}^{n+1} - \Delta t \sum_k \frac{\mathbf{q}^n_{(m+)_k} - \mathbf{q}^n_{(m-)_k}}{\Delta x_k}\,. \tag{12d}$$

Let us make a few comments. The employment of the velocities with "waves" for (Pu) in "disintegration" tests at the Eulerian stage leads to the appearance of the "precursor" of shock waves and thereby to an excessive "smearing" of discontinuities. Conversely, the employment of them at the Lagrangian stage

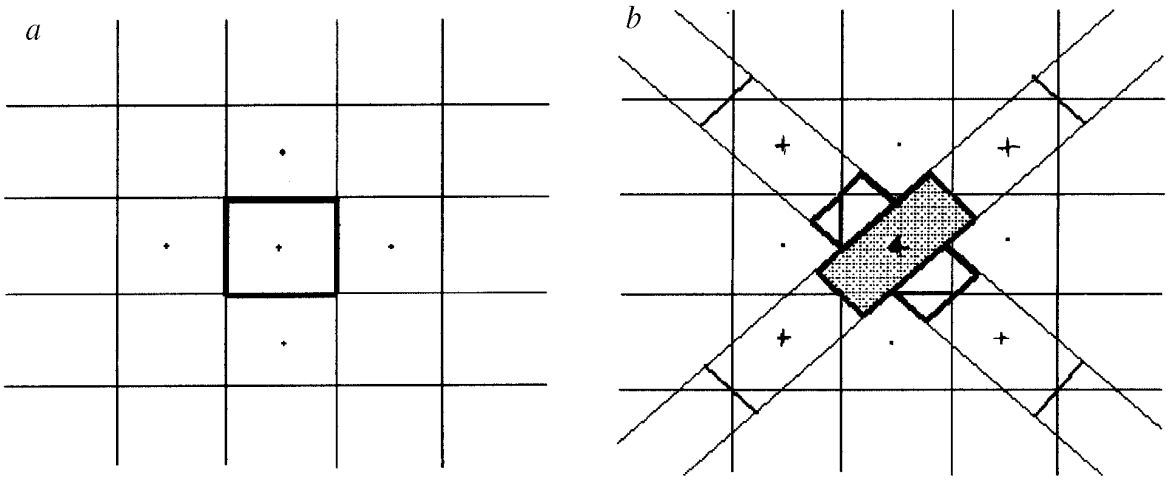

Fig. 1. Fragment of a regular grid (a) (points denote the nodes ordinarily employed for a five-point 2D template); the same fragment with additionally drawn diagonal strips (b) (two of them are shown in the figure; a number of cells with centers superposed on the nodes of the primary cell are constructed along the strips; the nodes for employment of the same five-point 2D template but on the cells of diagonal strips now are marked by a + sign).

markedly decreases the effect of dispersion oscillations that are known to be inherent in central difference schemes [2]. In determining the values of q_m, one should employ the increments and parameters (in computation of the matrices (5)) after the completion of step (12c) and not from the lower layer (as is the convention in the Harten schemes [11–15]). In this case, instead of $\mathbf{q}(\mathbf{U}^n)^n_{m+}$, one computes the values of $\mathbf{q}(\mathbf{U}^{n+1})^n_{m+}$ in accordance with (5)–(8), including the pressure $P(\tilde{\mathbf{U}}^{n+1})^n_{m+}$. All ensures the "smearing" of moving discontinuities by only one to two cells [6, 9].

Improvement of the Accuracy of Solution on a Sequence of Superposed Grids with a Set of Cells Differing in Shape. It is well known [18, 19, 49] that in computing balance relations in (1) the highest error occurs in the case of motion of a medium in the direction of one top of the cell around a calculational grid node. The narrowing of the cells does not eliminate this problem basically. However it is solved if another cell or a set of other cells constructed on the same grid nodes are introduced into calculation in addition to a primary cell separating a certain space around the node.

For illustration we employ a fragment of a regular 2D grid forming the simplest square cells, as is shown in Fig. 1a. It is clear that the mass of points forming the grid can basically be selected quite arbitrarily. The same is permissible in selecting the topology of 2D (3D) cells, which was reflected in the appearance of algorithms implementing finite-difference methods on three-, four-, and six-faced 2D cells. A demand for cells has arisen in construction of difference relations by integro-interpolation methods [50] that do not impose in themselves any special requirements on their shape. For the sake of definiteness we also assume that we are dealing with the employment of numerical schemes on three-point 1D templates.

Let us now fix the position of grid nodes and then draw diagonal strips (two of which are shown in Fig. 1) across the space. Thus, we obtain a series of new rectangular cells along the diagonals of the primary cells. Let us employ these new cells and the same three-point 1D template to calculate the same parameters determined at the nodes of the same grid but now along its diagonals. How does one stand to gain?

First of all, the total template for a 2D grid has been augmented to include nine points instead of five and the seven-point template has become a 27-point one for a 3D grid in calculating the parameters at each node of the primary cell. Solution at the node continues to be determined from the balance relations for each

coordinate direction but already with allowance for the rotation of a coordinate system. There is no need to compute the matrices of mixed derivatives to determine diagonal fluxes, which is of special importance in the implementation of methods of high order of accuracy [49–52].

When a primary cell forming regular square cells is selected the orthogonality of the coordinate directions holds for the diagonal strips. And for the rectangles the value of the cell volume related to the calculational node remains constant, despite the change in the shape and orientation of the cells upon change of the coordinate directions. Therefore, the mass of a substance and all specific parameters assigned to the node of superposed grids of such type coincide, and unlike the approaches of [51–53], the same array of data is used to improve the exactness of the grid solution. For superposed grids forming arbitrary rectangular cells, the constancy of the volume of the enclosed cells can be another criterion (among others) in constructing a grid [53].

Next, one can act as follows. Let us introduce the parameter a_k ("weight" related to the kth set of cells, $k = 1, 2$ for 2D) so that $a_1 = \cos^2(2\alpha)$, $a_2 = 1 - a_1$, and α is the angle between the velocity vector $\mathbf{W}$ and its projection $\mathbf{W}_1$ onto the first coordinate direction. The final value of the quantities at the node will now be determined as follows: $\mathbf{U}_i^{n+1} = a_1 \cdot (\mathbf{U}_i^{n+1})_1 + (1 - a_1) \cdot (\mathbf{U}_i^{n+1})_2$.

When the velocity at the node coincides with one singled-out coordinate direction (and/or along the strips) the calculational error of the motion will be the lowest and correspond to the calculational 1D scheme which has been implemented for this set of cells. Whereas the calculation of the motion along the diagonal of the primary cell has the highest error, here we have $a_1 = 0$ and $a_2 = 1$, and the error is minimized since now it coincides with the motion along the normal to the face of a new cell and is determined by the solution $(\mathbf{U}_i^{n+1})_2$.

In the general case, the quantities a_k are, apparently, other than 0 and 1, and they are basically free parameters; one can select the optimum values of these parameters for a sequence of superposed grids, taking into account the special properties and conditions of exactness improvement for the solution of a specific problem. In particular, application of a sequence of superposed grids to space-time cells differs from the approach of [54] and has a number of distinctive features; they will be reported additionally in the next publication.

We also note that some sets of cells can be obtained by drawing diagonal strips in such a manner that their intersections form squares inscribed or circumscribed about the squares of primary cells. But this corresponds to the ordinary procedure of narrowing (refinement) of primary cells or making them (twofold) coarser employed in the methods of improvement of the exactness of solutions on a sequence of grids [49–53]. In these previous methods, either it has been necessary to introduce new nodes (in the case of narrowing of the cells) or part of the information is lost (in the case of their coarsening). However, additional gain from the employment of a sequence of superposed grids is quite obvious here, too.

As far as the specification of boundary conditions is concerned, we report that in the calculations of [5–9], we used the same conditions as in a primary cell (nonflow or "streamwise drift") for a new set of 2D cells.

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NOTATION

Δt, time step; Δx, step of the space grid along one coordinate direction; ΔV_i, volume of the ith cell; F_m, area of the mth face of the cell; q, correcting flux; $\mathbf{U}$ and $\mathbf{f}(\mathbf{U})$, independent variables and stream functions in (1), (6), and (12); $\tilde{\mathbf{f}}_{i\pm1/2}^n$, certain approximation of the fluxes on the lateral faces of neighboring cells; $\mathbf{W}_k$, projection of the velocity vector $\mathbf{W}$ onto the x_kth coordinate direction; P, pressure; ρ, u, and E, density, velocity, and total energy of unit volume respectively; $c = \sqrt{\gamma P/\rho}$, velocity of sound for a perfect gas with

an adiabatic exponent γ; $\mathbf{A} = \partial f(\mathbf{U})/\partial(\mathbf{U})$, Jacobi matrix in (1) and (6); $\mathbf{R}$, matrix of the right-handed eigenvectors (such that $\mathbf{A} = \mathbf{R}\cdot\Lambda\cdot\mathbf{R}^{-1}$ or $\mathbf{R}^{-1}\cdot\mathbf{A}\cdot\mathbf{R} = \Lambda$); Λ, diagonal matrix composed of the eigenvalues λ of the Jacobi matrix. Subscripts and superscripts: n, index of the time grid with a time step Δt, $n = 0, 1, 2, ...$; i, index of the space grid with a step Δx containing I cells, $i = 1, 2, ..., I$; m, index of any lateral face; $(m\pm) = (m\pm)_k = i \pm 1/2$, indices of the lateral faces of three neighboring cells with indices i and $i \pm 1$ along the singled-out coordinate direction k; $m_k = -\text{sign}\,(\mathbf{W}_k)/2$; $[...]_t$, index of the transposed matrix; $l = 1$, 2, and 3.

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