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TESTING OF NUMERICAL METHODS, CONVECTIVE SCHEMES, ALGORITHMS FOR APPROXIMATION OF FLOWS, AND GRID STRUCTURES BY THE EXAMPLE OF A SUPERSONIC FLOW IN A STEP-SHAPED CHANNEL WITH THE USE OF THE CFX AND FLUENT PACKAGES

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An unsteady supersonic flow of a nonviscous gas with a Mach number M = 3 in a step-shaped channel has been calculated. The accuracy of the forecasts made has been analyzed on the basis of the Roe dissipation model and the advective upwind splitting method with the use of convective schemes of the second and third orders of accuracy and algorithms for approximation of flows. Triangular and polyhedral grids have been tested. The mechanism of formation of an artificial physical instability on grid structures with a local-gradient adaptation has been considered. It is shown that the existence of a singular point — a right corner — in the computational region causes a large phase change in the evolution of the flow.

Keywords: *supersonic flow, shock wave, step-shaped channel, ideal gas, calculation, FLUENT and CFX packages.*

Introduction. Developers consider the universal gas-dynamic FLUENT and CFX packages as flexible and efficient instruments for numerical simulation of hydrodynamical and thermophysical processes, including those occurring in subsonic and transonic flows of viscous and nonviscous gases. In many respects this is explained by the fact that the use of nonstructured finite-element grids allows one to investigate the gas dynamics and the heat exchange in multidimensional regions of arbitrary geometry. Even though universal packages, such as the FLUENT package, practically do not impose limitations on the shape of an object being calculated, they call for the use of grids with cells in a quantity allowed by the available computational resources to provide an acceptable accuracy of numerical forecasts. This problem arises as a rule due to the necessity to represent different-scale complex flows on inadequate grid structures which, in many cases, is not taken into account by the developers of packages in full measure.

Formulation of the Problem. In the present work, which is a logical continuation of [1], numerical schemes of different orders of approximation and grid structures realized with the use of the FLUENT and CFX packages were analyzed by the example of calculation of a compressible flow of an ideal gas in a region of fairly simple geometry in which, however, nonstationary multielement shock-wave interactions can occur. The algorithms of the Roe splitting of flows [2], the advective upwind splitting (AUS) method [3, 4], and the monotone centered upwind scheme for conservation laws (MCUSCL) [5] were tested with the use of the artificial compressibility method as well as triangular and polyhedral grids.

For more than fifty years the problem on a supersonic flow with a Mach number M = 3 in a channel with a step has been used as a good test for comparison of the accuracy of different computational schemes. This test was published for the first time by Emery [6], then was repeatedly represented by Van Leer [5], and was popularized most widely by Woodward and Colella [7]. At this point, of special interest is the degree of resolution of complex gas-dynamic phenomena, such as nonstationary interactions of compression and rarefaction waves as well as Mach disks arising in the process of irregular interactions of waves with each other and with walls, with the use of a numerical algorithm selected.

The computational region represented a channel with a sharp narrowing, a unit height at the input, a length of 3, and a step of height 0.2 located at a distance of 0.6 from its left unput boundary.

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Brief Description of Numerical Methods. A peculiarity of the present problem is the existence of a singular point — a corner of a step, a rarefaction center. It was shown in [5–7] that a numerical simulation of a flow in this formulation leads to significant errors in its representation in the neighborhood of the singular point. In this case, a pseudoboundary layer appears above the step, with which shock waves interact. As a consequence, the pattern of the flow changes depending on the computational grids and numerical methods used [5–7]. Some results of determining the sensitivity of the indicated solution to the singular point are presented below.

In [1], a numerical investigation was performed in "forehead," i.e., in the computational region with a right corner. However, in the present work, to avoid numerical errors associated with the effect being considered, we changed the right corner for a facet with a rounding of radius 0.01. It should be noted that this method of solving the problem is not unique; for example, in [7] the density of the fluid in the cells positioned near the singular point was determined in such a way that the entropy field retained nonseparated. At the same time the mass velocity was corrected using the law of conservation of the kinetic energy and enthalpy in each time step.

The system of Euler equations for a perfect gas with an adiabatic index $\gamma = 1.4$ was solved by the finite-volume method on the basis of the artificial-compressibility procedure [8]. The serviceability and accuracy of numerical algorithms are conveniently estimated with the use of a set of parameters that, in the initial state, have unit values. Thus, in this case,

$$\rho = 1.4\,, \quad u_x = 3\,, \quad u_y = 0\,, \quad p = 1\,, \quad \gamma = 1.4\,. \tag{1}$$

The indicated parameters determine the local velocity of sound $a = \sqrt{\gamma p/\rho} = 1$; in this case, the Mach number becomes equal to the velocity of the incident flow $\mathrm{M} = u_x/a = u_x$.

The flows through the faces of the control volumes were approximated on the basis of the Roe dissipation model [2] or by the modified AUS method of splitting [3, 4]. In the second case, the resulting Mach number, used for interpolation of the convective components of nonviscous flows, in each finite volume was calculated by the characteristic method. It should be noted that the AUS method offers a number of advantages over the Roe dissipation model: the contact discontinuities are calculated exactly, the scalar quantities remain positive, and nonphysical oscillations arising at the contact discontinuities are not reproduced.

In addition to the standard upwind scheme of the second order of approximation [9], the MCUSCL scheme of the third order of approximation [5] was used for integration of the convective components of the Euler equations. This scheme was proposed for the first time by Van Leer and represents a conjugation of the upwind scheme of the second order of approximation and the central-difference scheme. In contrast to the square Leonard QUICK scheme [9] that is mainly used with structured grids, the MCUSCL scheme can be applied to the measurements with arbitrary nonstructured grid structures. Potentially the indicated scheme allows one to substantially improve the accuracy of integration of the convective terms of equations over the space; however, this scheme, in its present form realized with the v6.3.26 FLUENT package [9], does not impose any limitations on flows. As a consequence, if a flow has any features, e.g., contact discontinuities, the indicated scheme begins to reproduce numerical errors caused by the nonmonotony of the solution. This effect is demonstrated in the present work.

The integration of the quantities being investigated with respect to the physical time was performed using the reverse Eulerian method [10] of the second order of approximation, and the integration of these quantities with respect to the pseudotime was carried out by the implicit marching method on the basis of the artificial compressibility [8].

The set of parameters (1) represents the input boundary conditions. The conditions of absence of flow were set for the impenetrable regions of the step-shaped channel. It was assumed that the parameters of the flow at its output cross section are not significant because the fluid flows through this section with a supersonic velocity. The initial conditions were as follows: the step-shaped channel is fully filled with a gas whose parameters are identical to the parameters of the fluid at its input boundary, which corresponds to an abrupt start of the motion of the channel with a supersonic velocity. The Courant number is taken to be equal to 0.8, and the numerical simulation of the nonstationary process is carried out with a fixed time step of 0.0025, which is reasonable in the case where an implicit scheme of the second order of approximation with respect to time is used. Note that the time step close in order and was equal to 0.00272 was used in [7]. Twenty local iterations were carried out in each step of the temporal integration.

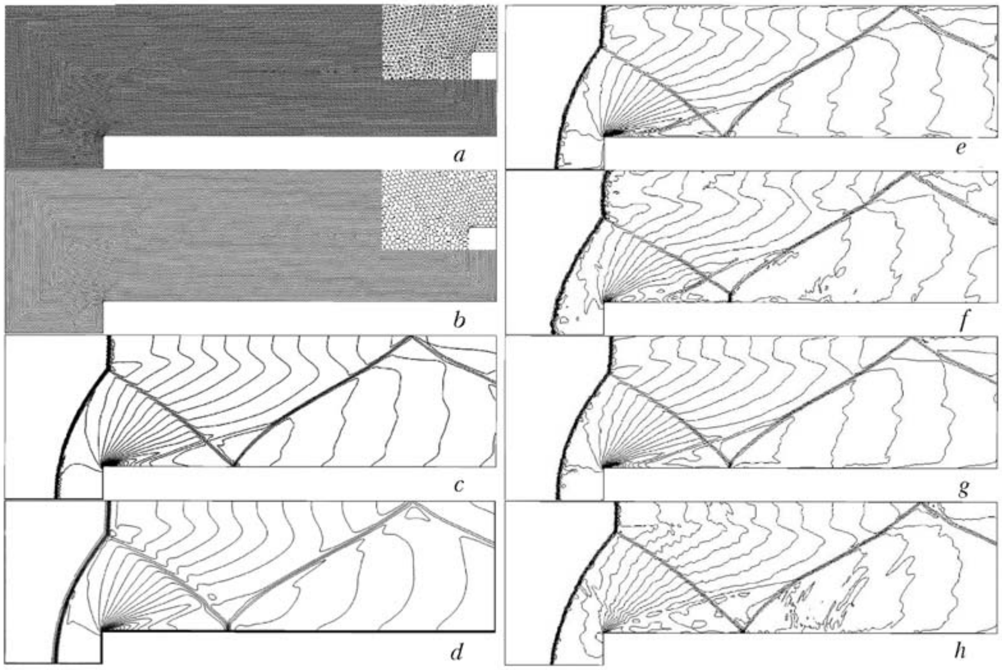

Fig. 1. Fields of the decimal logarithm of the isochores at the instant of time t = 4 obtained on the static triangular (a) and polyhedral (b) grids with the use of the gas-dynamic CFX (c) and FLUENT (d–h) packages as well as different combinations of difference schemes and algorithms of approximation of flows: the model of Roe dissipation and the standard convective scheme of the second order of accuracy (e), the model of Roe dissipation and the MCUSCL method (f), the AUS method and the standard convective scheme of the second order of accuracy (g), the AUS and MCUSCL methods (h). A step of the isolines is equal to 1/30, and the values of the density are varied from −1 to 1.

In [1], fairly close results were obtained with the use of different-topology (triangular and quadrangular) grids, which allows the conclusion that the forecasts made by us are reliable to some degree and the computational algorithm used is adequate. In the present work, the accuracy of the numerical estimations was determined using the nonstructured triangular (Fig. 1a) and polyhedral (Fig. 1b) grids constructed on the basis of the triangular grid with elements of uniform size equal to 0.0125; these grids are equivalent to some degree to the structured grid used in [7] with elements of size $1/\Delta x = 1/\Delta y = 1/80$. Compared to the grid used in [1], the number of nodes in the grid used in the present work was increased from 8 to 20 thousand. An insignificant bunching of the grid nodes was made in the region of the rounding of the right corner. The triangular grid was also used as the initial grid for calculations with a dynamic local adaptation [11, 12] to the density gradient with two levels of fragmentation. In the process of solving the problem, the number of nodes was no more than 400 thousand; in this case, the fragmentation and bunching thresholds were taken to be equal to 0.01 and 0.02, respectively. The restructuring was carried out with an interval in five time steps.

Analysis of the Results Obtained. The accuracy of the solutions obtained was estimated by the following structured elements of the flow: the spatial position of the triple point — the point of intersection of the upper Mach disk with the leading shock wave, the length of the upper Mach disk, and the interaction of the shock waves with the upper walls of the step and the channel. In this case, the solution obtained in [7] was postulated as a standard solution. We used a field of isochores to analyze the nonmonotonicity of this solution and the decimal logarithm for its better visualization. In the problem being considered, the density is a parameter that is most difficult to calculate because of the existence of a weak contact discontinuity — a Mach disk, arising as a result of the interaction of the leading arched shock wave with the upper wall.

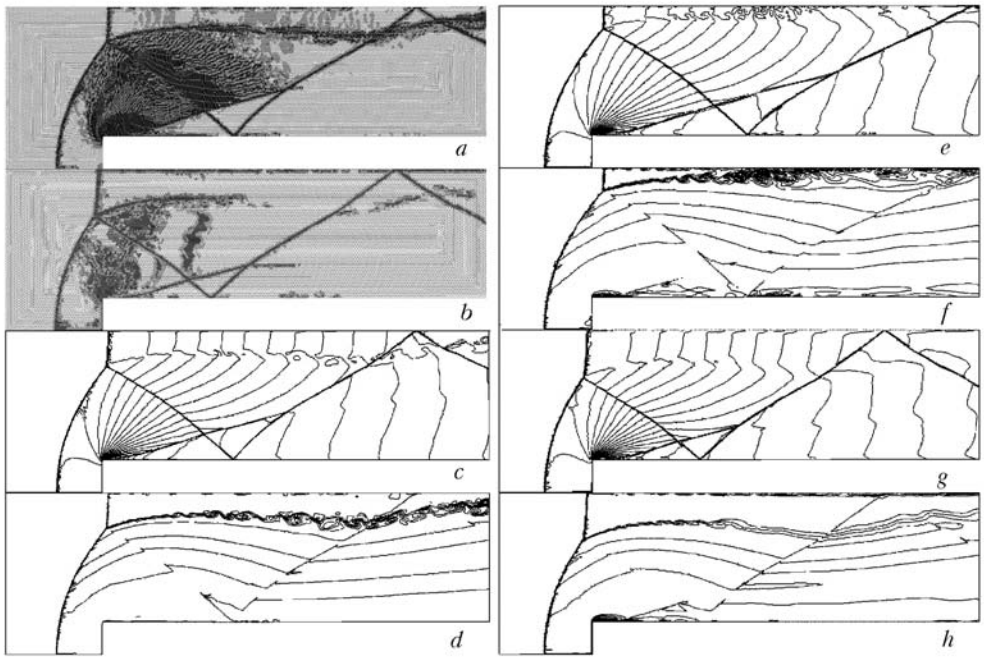

Fig. 2. Results of the numerical simulation with a dynamical local-gradient adaptation obtained in the computational regions with a filleted right corner (a) at the instant of time t = 4 (c, d) and with a right corner (b) at the instant of time t = 4 (e, f) and t = 7 (g, h): the fields of isolines of the decimal logarithm of isochores (c, e, g) and the fields of isolines of the entropy function A (d, f, h). A step of the isolines is equal to 1/30, and the values of the density and the entropy function are varied from −1 to 1 and from 0.3 to 1.7 respectively.

We will briefly analyze the solutions obtained using the stationary triangular grid (Fig. 1a) and polyhedral grids (Fig. 1b). Figure 1c and d shows the fields of the decimal logarithm of the isochores at the instant of time t = 4, obtained with the use of the CFX [13] (Fig. 1c) and FLUENT packages (Fig. 1d) on the polyhedral grids. A distinguishing characteristic of these two solutions is the absence of nonmonotonicity. The average disagreement between the standard solution [7] and the solution obtained in the topology of all the elements of the flow did not exceed 3%. Further analysis of Fig. 1 shows that the use of the MSUSCL scheme of the third order of approximation gives a solution with a large nonmonotonicity (Fig. 1f and h) as compared to the standard scheme of the second order of approximation (Fig. 1e and g). In turn, the existence of a nonmonotonicity in the solution leads to a fairly strong distortion of the topology of the flow: 1) in Fig. 1f, the length of the Mach disk is overstated by 24% and the triple point is displaced by 8% to the left in the longitudinal direction; 2) in Fig. 1h, the length of the Mach disk is underestimated by 9% and the triple point is shifted by 9% to the right in the longitudinal direction; in this case, the points of interaction of the oblique shock waves with the upper walls of the step and the channel are shifted by 8 and 6% respectively. The solutions obtained using the standard upwind scheme of the second order in combination with the AUS method have a much smaller nonmonotonicity (Fig. 1e and g) even though they represent the topology of the flow with certain errors. For example, the length of the Mach disk represented in Fig. 1e is overstated by 12% and the triple point in Fig. 1g is shifted by 6% to the right.

It should be noted that the flow being considered has some nonphysical features arising due to the numerical errors. Among them are the appearance of a weak rarefaction wave arising as a result of the interaction of a fan of waves propagating from the corner of the step with its upper wall and the development of the Kelvin–Helmholtz instability propagating from the triple point along the upper wall of the channel. Even though the last mentioned instability has a physical origin, it is most likely due to the computational circumstances in this case. The main reason for the appearance and development of this instability is that small oscillations of the entropy are generated by the numerical schemes at the triple point. The indicated features of the flow are independent of both the computational grids and different numerical algorithms.

The further improvement of the solution and investigation of the above-listed features of the flow were carried out with the use of adopted grids (Fig. 2a and b). By analogy with [7], we analyzed the mechanism of the instability with the use of the so-called adiabatic index $A = p/\rho^{\gamma}$ representing an entropy function. The influence of the numerical errors, arising due to the existence of the singular point in the computational region, on the evolution of the flow is presented in Fig. 2e and h. Analysis of the entropy field (Fig. 2f and h) shows that the existence of a singularity leads to the formation of a pseudoboundary layer at the upper wall of the step. The interaction of the shock-wave structure with this boundary layer causes a delay (a phase shift) in the development of the flow. Figure 2e–h presents data obtained for the computational region with a right corner: the fields of the isolines of the decimal logarithm of the isochores (Fig. 2c, e, and g) and the entropy (Fig. 2d, f, and h) at the instants of time $t = 4$ and 7. It is seen that the phase error is equal to $t \sim 3$.

A Kelvin–Helmholtz instability develops on the grid structures with a local gradient-dynamic adaptation (Fig. 2a and b) independently of the existence of a singularity in the computational region. Analysis of the entropy field (Fig. 2d, f, and h) shows that this instability is due to the small oscillations of the entropy in the zone of the contact discontinuity originating from the triple point — the point of intersection of the upper Mach disk with the leading shock wave (Fig. 2b and c) — and propagates along the upper wall of the channel.

Conclusions. Convective schemes of the second and third order of approximation and algorithms of splitting of flows (the Roe dissipation model and the AUS method), realized on the basis of the finite-volume procedure of artificial compressibility on different grid structures, have been tested by the example of a supersonic flow in a step-shaped channel. It is shown that:

a) the solutions obtained on the polyhedral grids are nonmonotone to the least degree and correspond most exactly (the disagreement is ~3%) to the standard solution (all other things being equal);

b) in the case where the flow in the cells positioned near the computational region with a singular point is not corrected (the right angle is not rounded), in this region there arises a large phase change ($t \sim 3$) in the evolution of the flow as a result of the interaction of the shock waves with the pseudoboundary layer at the upper wall of the step;

c) a further increase in the resolution of the computational grids or the use of a local dynamicadaptation leads to the appearance of a hydrodynamic Kelvin–Helmholtz instability, arising mainly due to the small oscillations excited in the entropy field at the triple point.

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NOTATION

a, local velocity of sound; A, entropy function or "numerical noise;" M, Mach number; p, pressure; t, time; u_x, longitudinal component of the velocity vector; u_y, transverse component of the velocity vector; γ, adiabatic index; Δx, Δy, dimension of the structured computational grid along the horizontal and vertical directions, respectively; ρ, density.

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