МОДЕЛЮВАННЯ ТА ОПТИМІЗАЦІЯ В ТЕХНОЛОГІЇ КОНСТРУКЦІЙНИХ МАТЕРІАЛІВ

SIMULATION AND OPTIMIZATION IN TECHNOLOGY OF CONSTRUCTION MATERIALS

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APPLICATION OF INVERSE SPLINES IN THE MODIFICATION OF THE GODUNOV METHOD FOR CALCULATING COMPRESSIBLE GAS FLOWS

ЗАСТОСУВАННЯ ЗВОРОТНИХ СПЛАЙНІВ У МОДИФІКАЦІЇ МЕТОДУ ГОДУНОВА ДЛЯ РОЗРАХУНКУ ТЕЧІЙ СТИСЛИВОГО ГАЗУ

An implicit numerical algorithm for solving Navier-Stokes equations is proposed, taking into account the modification of the explicit Godunov method for calculating viscous flows. To avoid high computational costs, a modification of Godunov's method for calculating convective terms is proposed. The main idea of the modification is to approximate the original nonlinear dependence with an inverse cubic or parabolic spline. From a mathematical point of view, instead of finding the root of a nonlinear equation, it is sufficient to find the free coefficient of the inverse spline. The approach considered can be called "almost accurate" because it preserves the exact formulation of the gap decay and uses an approximate method for calculating only one quantity — the pressure value at the adjacent boundary between neighboring cells as a result of solving the Riemann problem. The proposed modification of the calculation of convective terms for compressible gas flows is implemented within the framework of our own computational aerodynamics software package, which has been developed and used for many years at the Institute of Transport Systems and Technologies of the National Academy of Sciences of Ukraine. The testing was performed on the problem of the interaction of an oblique compression jump with a turbulent boundary layer on a flat plate at a Mach number of 5 of an undisturbed flow. Comparison with experimental data on pressure distribution and coefficient, as well as experimental and numerical schlieren photographs, shows that the proposed method well reproduces both individual elements of the structure of the interaction under consideration and its general parameters.

***Keywords**: implicit numerical algorithm, gap decay, inverse splines.*

Розроблено неявну чисельну схему для розв'язання рівнянь Нав'є-Стокса, у якій використано модифікований підхід до явного методу Годунова для опису нев'язких течій. Класична реалізація методу Годунова базується на строгому розв'язанні задачі розпаду розриву між сусідніми контрольними об'ємами, що зумовлює необхідність багаторазового ітераційного визначення тиску шляхом застосування методу Ньютона на кожній грані скінченного об'єму. З метою зменшення обчислювальних витрат запропоновано альтернативну модифікацію обчислення конвективних складових. Її суть полягає у заміні вихідної нелінійної залежності апроксимацією за допомогою зворотного параболічного або кубічного сплайна. Такий підхід дозволяє звести задачу до визначення одного параметра сплайна замість прямого пошуку кореня нелінійного рівняння. Запропонований метод можна трактувати як «майже точний», оскільки строгий опис задачі Рімана зберігається, а наближення застосовується лише до обчислення тиску на спільній грані суміжних комірок. Реалізацію модифікованого алгоритму для розрахунку конвективних членів у задачах течії стисливого газу виконано в рамках авторського програмного комплексу з обчислювальної аеродинаміки, що тривалий час розробляється і використовується в Інституті транспортних систем і технологій НАН України. Перевірку ефективності підходу здійснено шляхом верифікації у складі раніше створеного неявного алгоритму для двовимірних нестаціонарних рівнянь Нав'є-Стокса, осереднених за Рейнольдсом, у загальних криволінійних координатах. Розрахунки проведено для задачі взаємодії косого стрибка ущільнення з турбулентним примежовим шаром на плоскій поверхні при числі Маха незбуреного потоку, рівному 5. Порівняльний аналіз чисельних результатів з експериментальними даними щодо розподілу тиску, відповідних коефіцієнтів, а також зі шлірен-зображеннями свідчить про здатність запропонованої методики адекватно відтворювати як локальні особливості структури взаємодії, так і її інтегральні характеристики.

***Ключові слова**: неявний чисельний алгоритм, розпад розриву, зворотні сплайни.*

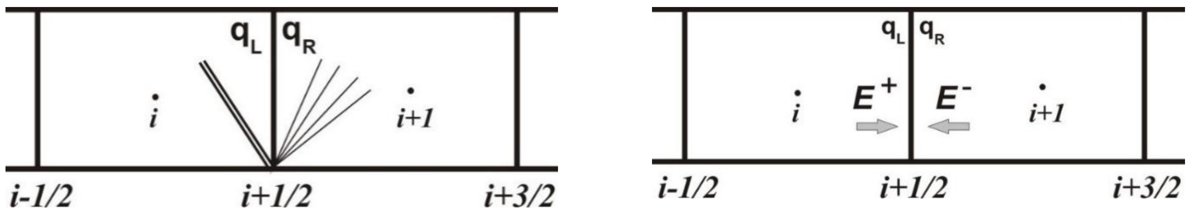
Problem`s Formulation

The supersonic and transonic velocity range is fundamental in the flow around aircraft, aircraft propellers and helicopter rotors, flows near aircraft engine air intakes, in diffusers and compressor grids, and in the flow section of gas turbines. In flows of this class, shock wave systems usually arise that interact with each other and with the boundary layers that develop on the outer surfaces.

From a mathematical point of view, compression jumps are infinitely thin rupture surfaces. In the 1970s and 1980s, the possibility of a thorough calculation of shock waves (without highlighting features) was demonstrated within the framework of the finite difference method (FDM) and the finite element method (FEM). At the same time, a number of theoretical questions remain open. In particular, for stable operation at discontinuities, such schemes require the introduction of additional components with artificial dissipation.

The finite volume method (FVM) is currently the most common approach to calculating compressible gas flows. A distinctive feature of the finite volume method is that it ensures the balance of physical quantities in the calculation cell without constructing a finite difference analogue of any individual derivative. FVM allows obtaining "weak solutions" in the sense of Lax, i.e., solutions that satisfy the initial equations written in integral form but cannot be obtained on the discontinuity surfaces for the differential form of the equations [1—7].

The main task in the numerical use of MCO is to determine convective and viscous flows at the boundary of adjacent cells (Fig. 1). For compressible flows, two basic models of gas particle interaction can be distinguished: wave interaction (Riemann approach) [1—3, 6, 7] and exchange of mass, momentum, and energy (Boltzmann approach) [4, 5].



a) Riemann's approach b) Boltzmann's approach

Fig. 1. Schemes for determining flows at the boundary of adjacent cells

Analysis of recent research and publications

The method of S.K. Godunov [1] is historically the first numerical algorithm that implemented Riemann's task (Riemann solver) within the CEA. It influenced the further development of the MCA to such an extent that the term "Godunov-type schemes" [3, 7] exists in the literature.

The advantage of S.K. Godunov's original method is that it fully formulates the wave problem of gap decay, but this leads to a complex procedure for finding parameters at the boundary of the control volume. The key point here is the solution of a nonlinear pressure equation in the inner region of the rupture decay, which uses Newton's iterative algorithm, leading to high computational costs. It was precisely the significant level of computer resource costs of S.K. Godunov's method that led to the emergence of approximate algorithms for calculating rupture decay. It should be noted that modifications of S.K. Godunov's method use simplified linearized formulations of the breakup problem without taking into account the increase in entropy on shock waves [2, 3, 6, 7]. Another disadvantage of the original method of S.K. Godunov [1] is its limitation as an explicit scheme of first-order accuracy for calculating viscous flows.

Formulation of the study purpose

Objective. To develop an effective implicit numerical algorithm of second-order accuracy for solving Navier-Stokes equations for compressible flow without linearizing the breakup problem when calculating convective terms. The main mathematical idea of the modification proposed in this work is to approximate the original nonlinear dependence for pressure with an inverse spline. This approach can be conditionally called "almost accurate" because it preserves the exact formulation of the gap decay problem and uses an approximate method to calculate only one value of the pressure at the boundary of neighboring cells as a result of solving the Riemann problem.

Complete nonlinear formulation of the gap decay problem. In [1], the sought values of the flow parameters are denoted by capital letters: P — pressure; R — density; U, V, W — components of the velocity vector. The key factor is the determination of the pressure P, after which the other values are found by analytical relations.

All possible configurations of wave gap decay are considered: two rarefaction waves; shock wave — rarefaction wave, two shock waves (Fig. 2). Theoretically, it is possible for a vacuum to form between two rarefaction waves (Fig. 2a). However, from the point of view of constructing a computational algorithm, this is an unacceptable situation caused by errors in the program or a non-physical initial approximation.

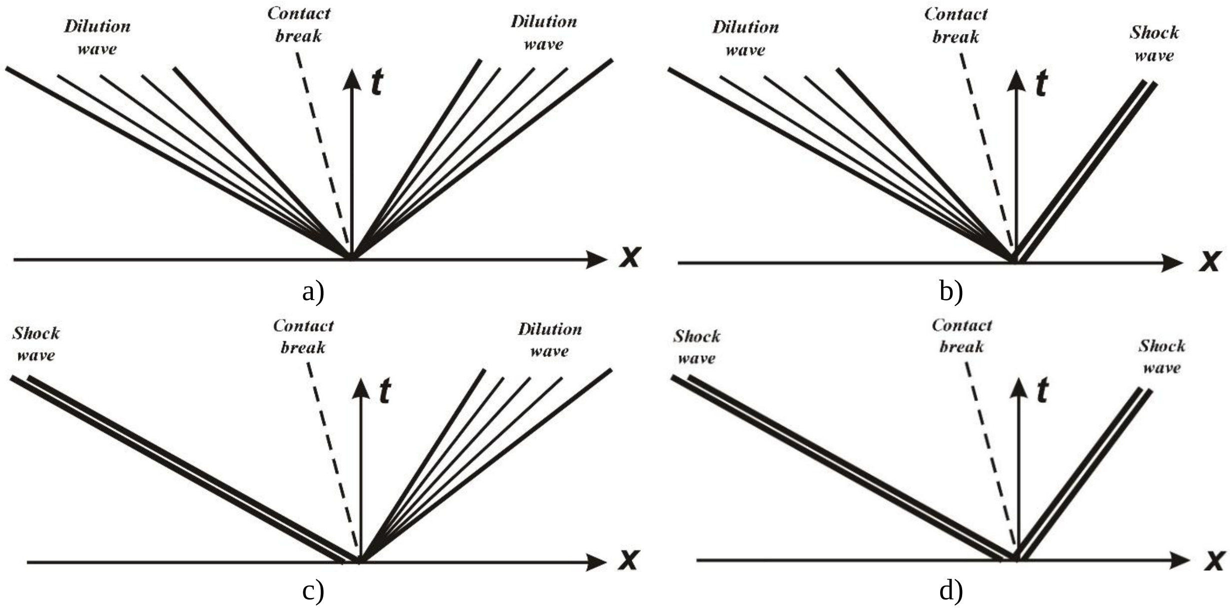


Fig. 2. Possible configurations of gap decay

For the "two rarefaction waves" configuration, there are exact analytical relationships [1] that do not require further modification.

In the "rarefaction wave – compression jump" configuration (Fig. 2b), the desired pressure value at the boundary P is in the range $p_L<P<p_R$. The functional dependence $F=F(P)$ has the form:

$$F(P)=\frac{2}{\gamma-1}\left\{a_L\left[\left(\frac{P}{p_L}\right)^{\frac{\gamma-1}{2\gamma}}-1\right]+\frac{P-p_R}{\rho_R a_R\sqrt{\frac{\gamma+1}{2\gamma}\frac{P}{p_R}+\frac{\gamma-1}{2\gamma}}}\right\}-\left(u_L-u_R\right). \quad (1)$$

Here, p is pressure; ρ is density; u is the gas velocity normal to the boundary; a is the speed of sound; γ is the adiabatic index. The indices "L" and "R" refer to the parameters of the flows to the left and right of the edge (Fig. 1a). According to the recommendations [1], adjacent cells are labeled so that $p_R - p_L \geq 0$.

The pressure value at the edge P is found as the root of the nonlinear equation $F(P)=0$ (Fig. 3). Since the dependence $F=F(P)$ is a convex function, Newton's iterative algorithm was used in the original work [1].

In the "two compression jumps" configuration (Fig. 2d), the pressure value at the edge $P \geq p_R$, i.e., outside the range $[p_L , p_R]$. The function $F(P)$ is written as:

$$F(P)=\frac{2}{\gamma-1}\left\{\frac{P-p_L}{\rho_L a_L\sqrt{\frac{\gamma+1}{2\gamma}\frac{P}{p_L}+\frac{\gamma-1}{2\gamma}}}+\frac{P-p_R}{\rho_R a_R\sqrt{\frac{\gamma+1}{2\gamma}\frac{P}{p_R}+\frac{\gamma-1}{2\gamma}}}\right\}-\left(u_L-u_R\right). \quad (2)$$

Function (2) also has a convex character, but unlike (1), $F(p_L) < F(p_R) < 0$ since $P > p_L > p_R$. To solve equation (2) $F(P) = 0$, it is also necessary to use Newton's iterative algorithm [1].

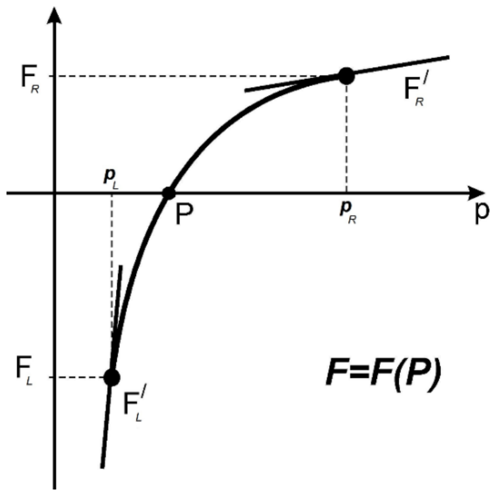


Fig. 3. Direct dependence *F(P)* according to the method of S.K. Godunov [1]

Presenting main material

Calculation of the gap decay using inverse splines. The main idea of the modification proposed in this work is to approximate the nonlinear dependencies (1) and (2) with an inverse spline $P=P(F)$. If we consider the inverse functional dependence $P(F)$ (Fig. 4) on the interval $[F_L, F_R]$ for function (1) and select an approximating parabolic or cubic spline, then the task of determining the value of P will be reduced to finding the value $P=P(0)$. From a mathematical point of view, the value $P(0)$ corresponds to the free coefficient of the inverse spline. Thus, instead of an iterative procedure that is expensive in terms of computational costs, we will have an effective, albeit approximate, method for determining the pressure value at the gap breakdown. This approach can be conditionally called "almost accurate" because it preserves the exact formulation of the gap collapse problem and uses an approximate method to calculate only one quantity — the pressure value at the cell boundary as a result of solving the Riemann problem.

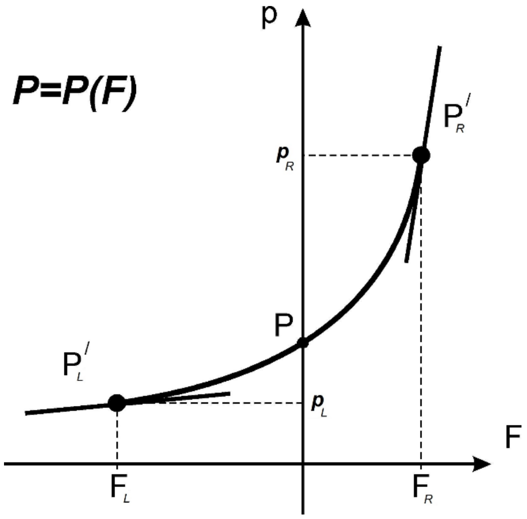


Fig. 4. Inverse dependence *of* $P(F)$ for equation (1)

In [1], analytical expressions for the derivatives $F'(P)$ for equations (1) and (2) are given, which allows cubic splines to be constructed. However, as test calculations have shown, a cubic spline is not a monotonic function and can lead to non-physical numerical errors. Therefore, parabolic splines with the calculation of additional values of functions $F=F(P)$ were chosen as the interpolation polynomial.

For equation (1), the average value $F_C=F(0.5(p_L+p_R))$ was calculated. Constructing an inverse spline to function (2) leads to extrapolation, since $P \geq p_R > p_L$, which can lead to an increase in numerical error. However, this can be avoided by selecting a point P_H on the curve $F(P)$ such that $p_R < P < P_H$. For this configuration, the value *of* P_H can be obtained from an approximate calculation of the "strong break" [1] using the quadratic equation

$$\frac{P-p_L}{\sqrt{\theta \rho_L P}} + \frac{P-p_R}{\sqrt{\theta \rho_R P}} = u_L - u_R \,, \tag{3}$$

where $\theta = (\gamma+1)/2$. The larger root of equation (3) is selected as P_H.

After calculating the pressure value at the boundary, other parameters (density, velocity components) at the adjacent boundary are determined according to the original method of S.K. Godunov [1].

Construction of an implicit algorithm for Navier-Stokes equations. The Institute of Transport Systems and Technologies of the National Academy of Sciences of Ukraine has been developing and applying its own computational aerodynamics software package for many years [8—11]. For two-dimensional unsteady Reynolds-averaged Navier-Stokes equations in arbitrary coordinates

$$\frac{\partial \hat{\mathbf{q}}}{\partial t}+\frac{\partial \hat{\mathbf{E}}}{\partial \xi}+\frac{\partial \hat{\mathbf{F}}}{\partial \eta}=\frac{1}{\mathrm{Re}}\left\{\frac{\partial \hat{\mathbf{E}}_v}{\partial \xi}+\frac{\partial \hat{\mathbf{F}}_v}{\partial \eta}\right\}, \tag{4}$$

an implicit numerical algorithm of second order accuracy in space and time has been constructed [9]. In the system of equations (4) $\hat{\mathbf{q}}$ is the vector of conservative gas-dynamic parameters; $\hat{\mathbf{E}}$, $\hat{\mathbf{F}}$, $\hat{\mathbf{E}}_v$, $\hat{\mathbf{F}}_v$ are vectors of convective and viscous flows, written in arbitrary coordinates, taking into account metric coefficients and the Jacobian of the coordinate transformation. Convective terms were calculated according to the Roe scheme [6]:

$$\hat{\mathbf{E}}_{i+1/2}=\frac{1}{2}\left[\hat{\mathbf{E}}(\mathbf{q}_L)+\hat{\mathbf{E}}(\mathbf{q}_R)-\left|\tilde{A}\right|\cdot(\mathbf{q}_R-\mathbf{q}_L)\right], \tag{5}$$

where $\mathbf{q}_L$, $\mathbf{q}_R$ — are the parameters of the flows on the left and right sides of the adjacent boundary *i+1/2*, located between the neighboring control volumes with numbers *i* and *i+1* (Fig. 1a). The Jacobian matrix $\tilde{A}=\partial\hat{\mathbf{E}}/\partial\mathbf{q}$ was calculated using the Roe averaging procedure [6, 9]. Equation (5) is a linearization of the gap decay problem.

When applying the calculation for the complete formulation of the gap decay problem, there is no need for relations of type (5). Convective and viscous flows through the adjacent edge of neighboring finite volumes are calculated directly through the functional expressions $\hat{\mathbf{E}}$, $\hat{\mathbf{F}}$, $\hat{\mathbf{E}}_v$, $\hat{\mathbf{F}}_v$.

The general principle of constructing an implicit algorithm is based on differentiating the discrepancy $\hat{\mathbf{R}}$ of the discrete analogue of equations (5) using Taylor series [2, 9]. This leads to a cumbersome form of the implicit operator and certain difficulties in its software implementation. The procedure for constructing an implicit operator can be simplified by using a modified Steger-Warming scheme for the increment of convective terms [5], i.e.

$$\Delta\hat{\mathbf{E}}_{i+1/2}=\hat{A}^{+}(Q_{i+1/2})\cdot\Delta\mathbf{q}_i+\hat{A}^{-}(Q_{i+1/2})\cdot\Delta\mathbf{q}_{i+1}, \tag{6}$$

where $Q_{i+1/2}=(R,U,V,P)$ is the vector of non-conservative gas-dynamic variables at the boundary *i+1/2*, defined using the modified method of S.K. Godunov, $\hat{A}^{+}(Q^n_{i+1/2})$, $\hat{A}^{-}(Q^n_{i+1/2})$ are Jacobian matrices corresponding to positive and negative eigenvalues (Fig. 1b). The increment of viscous flow vectors and the general procedure for numerical implementation of the constructed implicit algorithm correspond to [9].

Testing the developed methodology. In this work, to test the developed implicit algorithm for solving the Navier-Stokes equations, we chose the problem of the interaction of an oblique density jump with a boundary turbulent layer on a flat plate (Fig. 5). This choice of test problem is due to the fact that it includes all the characteristic features of viscous-inviscid interactions: density jumps, rarefaction waves, growth, and separation of the boundary layer. In addition, there is a wide selection of scientific literature for these problems, and the physical features of the analyzed processes are well studied, which allows for an unambiguous interpretation of the results obtained.

The calculations were performed under the conditions of an experiment conducted in the DLR Göttingen Ludwieg Tube wind tunnel [12]. The model was a wedge with a windward length of 300 mm, located at an angle $\theta=10^0$ to the undisturbed flow. The front sharp edge of the wedge was located at a height of 115 mm above the flat plate and 23 mm downstream. The turbulent boundary layer developed from the sharp edge of the flat plate, with the transition ending at a distance of ~120 mm from the edge. The undisturbed flow was characterized by Mach numbers M_∞=5 and Reynolds numbers Re=3.7·10^7 1/m, temperature T_∞=68.79 *K*. The distance from the leading edge of the plate to the point of fall of the jump in the viscous flow was ~350 mm. The temperature of the plate was T_W=300 *K*. This experiment has been recognized by NASA as a verification for two-dimensional problems of shock wave interaction with a turbulent boundary layer [13]. To calculate the turbulent viscosity, the Spalart-Allmaras differential model was used with an additional component that takes into account the supersonic velocity in the flow [14].

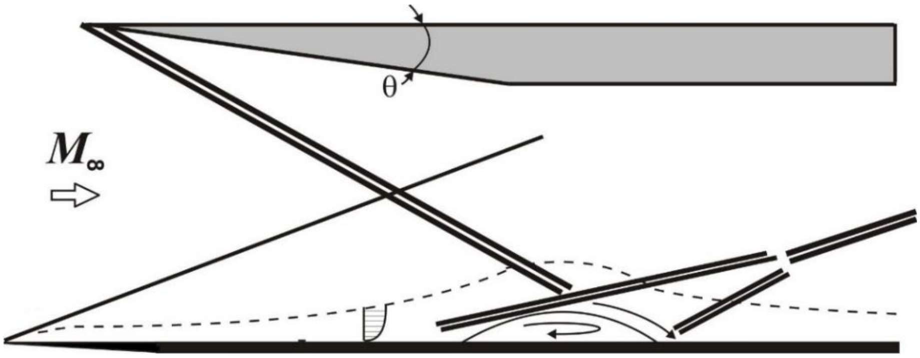
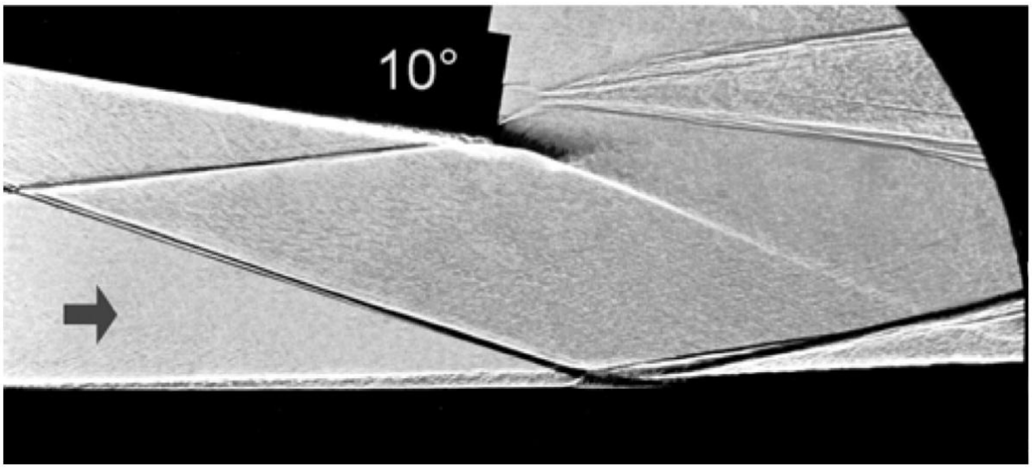
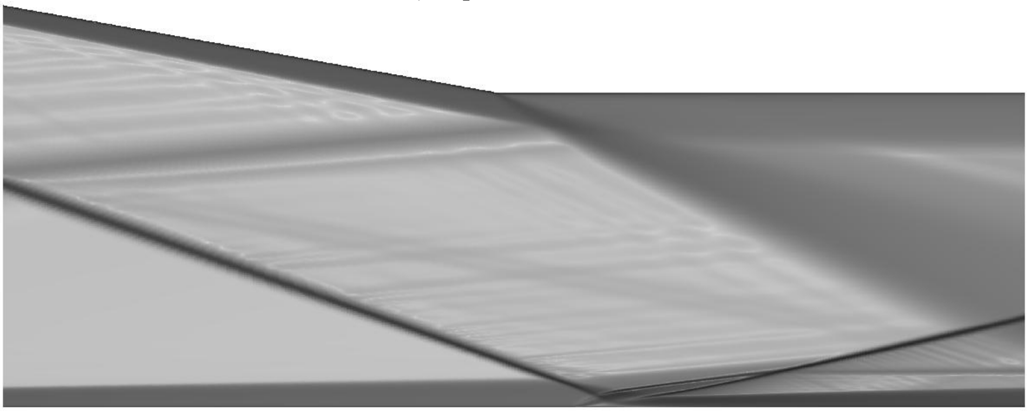


Fig. 5. Flow diagram for the interaction of a shock wave with a turbulent boundary layer



a) experiment [12]



b) calculation of this work based on the modified implicit method of Godunov and Steger-Warming

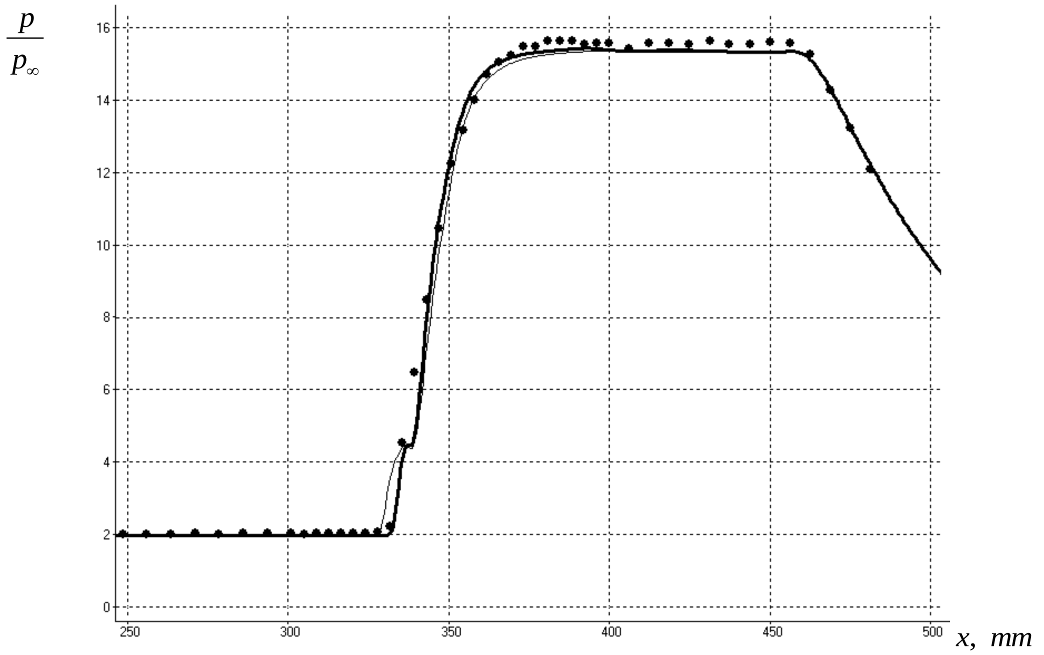
Fig. 6. Schlieren photographs of the interaction region of the shock wave with the turbulent boundary layer

The calculations were performed on a grid with a dimension of 885×650 nodes, approximately 55 % of which were located in the boundary layers on the wedge and plate.

The general structure of the strong interaction of the shock wave with the boundary turbulent layer is conveyed by schlieren photographs (Fig. 6). The calculated distribution of gas-dynamic parameters is in good agreement with the experimental picture of the flow in the interaction region. The boundary layer is clearly visible; a jump caused by a sharp leading edge; a falling shock wave; a separation zone, separation and reattachment jumps; a contact break; a reflected compression jump formed above the reattached turbulent boundary layer.

The intensity of the falling compression jump is large enough to cause the separation of the turbulent boundary layer. The pressure increase resulting from the falling compression jump is transmitted upward along the flow through the subsonic part of the boundary layer, causing its thickening and subsequent separation. The separation point is located above the flow from the point of the oblique jump in the viscous flow. As a result of the flow separation, a separation jump is formed, then the flow passes through an expansion wave and is compressed again in the connection jump. Further, the jumps merge into a reflected compression jump with the formation of a triple point and a contact break surface.

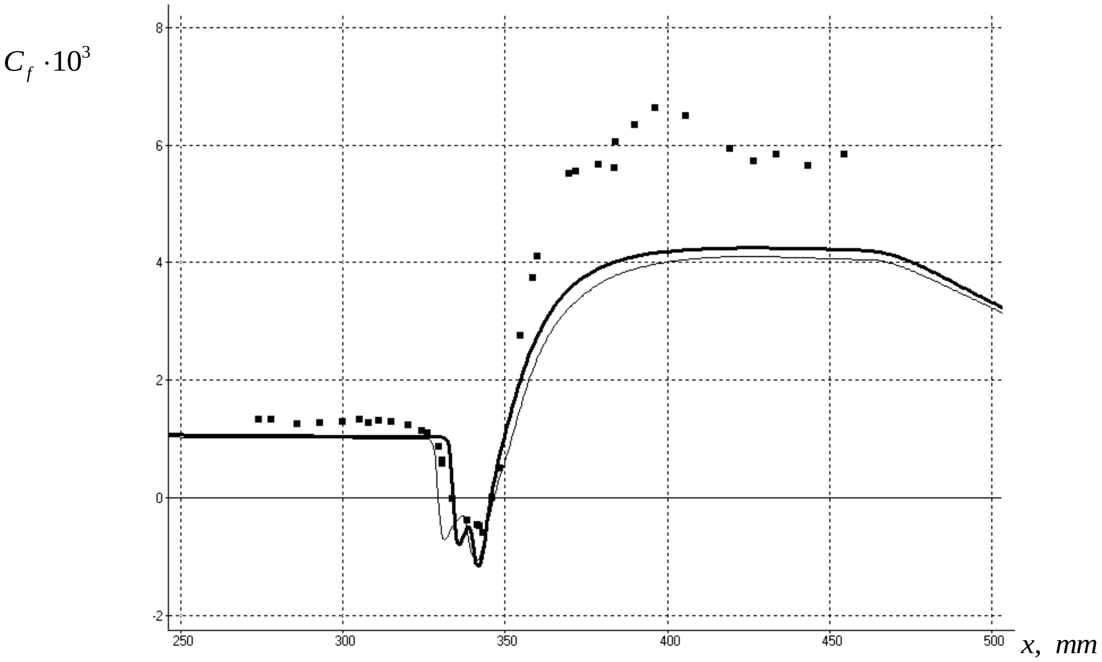
The pressure distribution on the plate surface (Fig. 7) shows good agreement between the experimental and calculated data, both for the Roe scheme and for the proposed algorithm. The pressure drop in the junction area of the boundary layer is due to the action of rarefaction waves behind the generator of the main compression jump.



— — calculation according to the Roe scheme; ▬ — calculation according to the proposed algorithm; ● — experimental data [12]

Fig. 7. Pressure distribution on the plate surface

The distribution of the friction coefficient (Fig. 8) shows the agreement between the experimental and calculated data regarding the position of the separation point. The results for the developed implicit algorithm based on the Godunov and Steger-Warming methods show a slightly smaller upward influence on the flow and better agreement with experimental data compared to the Roe scheme. The nonlinear nature of the friction change in the reverse flow conveys the influence of rarefaction and compression waves formed above the separation zone. A certain discrepancy between the results of numerical calculations and experimental data is observed in the area of flow reattachment. The boundary layer is restored with some "delay," which is a property of the Spalart-Allmaras turbulence model.



— – calculation according to the Roe scheme;
▬ – calculation according to the proposed algorithm;
● – experimental data [12].

Fig. 8. Distribution of the friction coefficient of the plate surface

Conclusions

An implicit numerical algorithm for solving Navier-Stokes equations for compressible gas is proposed, taking into account the modification of the explicit Godunov method for inviscid flows. The modification of the calculation of convective terms consists in approximating the original pressure dependence by a reverse cubic or parabolic spline instead of finding the root of a nonlinear equation by Newton's iterative algorithm. The approach considered can be called "almost accurate" because it preserves the exact formulation of the Godunov gap decay and uses an approximate method for calculating only one value on the adjacent boundary between neighboring cells. The proposed approach was verified on the problem of the interaction of an oblique compression jump with a turbulent boundary layer on a flat plate at a Mach number of 5 of undisturbed flow. Comparison with experimental data shows that the proposed method accurately reproduces both individual elements of the interaction structure and its general parameters.

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