Some aspects of numerical modeling of inviscid supersonic flow in a duct with a central wedge

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Abstract. On the example of the supersonic inviscid flow in a duct with a central wedge, the problem of increased errors of the solution arising in the vicinity of the fractures of a streamlined surface is investigated. The effectiveness of various ways to improve the solution quality is evaluated. Calculations based on the MUSCL approach for increasing the approximation order are performed using the finite-volume unstructured SINF/Flag-S code developed at the Peter the Great St. Petersburg Polytechnic University. The data obtained with this code are compared with the results of calculations performed using the ANSYS Fluent.

1. Introduction
It is well-known that transonic and supersonic flows may contain gasdynamic discontinuities, therefore special approaches in their numerical simulation are required. The main issue is how to approximate convective fluxes. Numerical scheme for convective flux evaluation should provide sufficiently accurate resolution of discontinuities in the absence of the spurious oscillations caused by solution discontinuities. Godunov-type schemes based on solving the local Riemann problem for a computational cell interface satisfy these requirements.

Usually, Godunov-type schemes are described in the literature with respect to calculation of fluxes at inner faces of computational cells. Because the evaluation of numerical fluxes at wall boundary faces requires pressure value at each boundary face centre, the method of wall pressure reconstruction has a significant effect on the solution, especially in the case when the streamlined surface contains a fracture.

The present paper covers description and application of different methods of wall pressure reconstruction in the framework of the first-order and second-order finite-volume method as applied to inviscid flow computations. Comparative analysis of quality of the solutions obtained with different approaches of wall pressure reconstruction are performed considering a representative test case that is supersonic flow in a duct with a central wedge. Since well-known analytical solution exists for this problem, basic characteristic of the flow are well defined, in particular, the position of the oblique shock wave and pressure distribution along the wedge. This test case is widely used in literature to assess the efficiency of various numerical schemes [1-3]. However, there is a rather limited amount of published data on the effect of numerical treatment of wall boundary condition on the solution quality.
2. Computational Method

2.1. Finite volume method and flux computations

Balance equations for the dynamics of an inviscid compressible gas in a finite-volume formulation can be written as:

$$\oint_{\Omega} \frac{\partial \tilde{\omega}}{\partial t} d\Omega + \sum_{m=1}^{N} \int_{S_m} \tilde{F} dS = 0,$$

where $\Omega$ is the control volume, $N$ – number of finite-volume faces, $S_m$ – area of the current face, $m=1,N$, $	ilde{\omega} = [\rho, \rho u, \rho v, \rho w, \rho H]$ – vector of conservative variables, $	ilde{F} = [\rho V_n, \rho u V_n + p n_x, \rho v V_n + p n_y, \rho w V_n + p n_z, \rho H V_n]$ – flux vector, $n_x, n_y, n_z$ – components of the normal to the face.

Convective flux at a finite volume face can be written as a sum of the central-scheme flux and an artificial dissipative flux: $\tilde{F}_f = \langle \tilde{F} \rangle - \tilde{D}$. In the case of the first-order scheme, the central-scheme flux is calculated as an average of values for the neighbouring (“left” and “right”) computational cells (control volumes), and the dissipative flux is evaluated by using the Roe’s approximate Riemann solver [4]:

$$\langle \tilde{F} \rangle = \frac{1}{2} \left( \tilde{F}(\tilde{\omega}_L) + \tilde{F}(\tilde{\omega}_R) \right),$$

$$\tilde{D} = \frac{1}{2} |\tilde{A}(\tilde{\omega}_R, \tilde{\omega}_L)| (\tilde{\omega}_R - \tilde{\omega}_L),$$

where Jacobian $\tilde{A} = (\partial \tilde{F} / \partial \tilde{\omega})$ on the face is calculated with the Roe’s average values of variables [4]. The absolute value of the Jacobian is computed as the product $|\tilde{A}| = R |\tilde{\Lambda}| R^{-1}$, where $|\tilde{\Lambda}|$ is the diagonal matrix composed of the absolute values of the matrix $\tilde{\Lambda}$ eigenvalues; $R$ is the matrix composed of right eigenvectors as columns.

The first-order accuracy is constructed under assumption of the piecewise-constant approximation in each control volume. To achieve the second-order spatial discretization, the MUSCL approach [5] is used. The fluxes are computed using reconstructed values of the variables at the cell faces. To prevent non-physical numerical oscillations arising in the vicinity of shock waves special limiter functions should be introduced while reconstructing of linear distributions. These limiters modify the slopes of variables distributions in the cells.

With this approach second-order Roe’s scheme can be written as:

$$\langle \tilde{F} \rangle = \frac{1}{2} \left( \tilde{F}(\tilde{\omega}_L) + \tilde{F}(\tilde{\omega}_R) \right),$$

$$\tilde{D} = \frac{1}{2} |\tilde{A}(\tilde{\omega}_R, \tilde{\omega}_L)| (\tilde{\omega}_R - \tilde{\omega}_L),$$

where $\tilde{\omega}_{L/R}$ denotes results of piecewise-linear reconstruction of the solution in the left/right cells.

Piecewise-linear reconstruction of the solution in each cell is performed using gradients of variables at the cell centre. Variable on the face is evaluated as

$$\tilde{u}_{L/R} = u_{L/R} + \varphi_{L/R} (\nabla u)_{L/R} \cdot \tilde{r}_{L/R},$$

where $u$ stands for any of the variables, $\varphi_{L/R}$ – value of the scalar limiter in the left/right cell, $\tilde{r}_{L/R}$ – vector from the left/right cell center to the face center. For the calculations presented below, we used the scalar limiter proposed by Venkatakrishnan [6] and modified in [7].
2.2. Boundary conditions for pressure on the wall

In order to evaluate numerical fluxes at boundary faces belonging to the wall, it is necessary to reconstruct pressure at each boundary face centre. In this section, possible variants of wall pressure reconstruction are given.

Figure 1 illustrates a variable arrangement for the near wall computations. Here, \( p \) stands for value of pressure in the center of the first inner cell adjacent to the boundary, \( P \) is a restored value of pressure at boundary face center, \( V_n \) is the normal component of velocity.

The simplest approach to get evaluation of wall pressure is to use the first-order extrapolation from the near wall cell center:

\[
P = p
\]  

However, this approach does not take into account the effect of normal-to-wall momentum that can be of great importance \([8]\). Indeed, if the value of \( V_n \) is negative (opposite to the wall normal vector), there is a compression wave towards the surface. Therefore, the pressure at the face should be greater than in the cell center. If \( V_n \) is positive then there is a rarefaction region near the wall and pressure value should decrease in comparison with the value at the cell center.

The approach based on the Riemann problem of discontinuity breakdown allows to get a more physical value of reconstructed wall pressure. With this approach, the values of the variables at the dummy outer cell (marked by dash line in figure 1) are defined first. In the case of zero boundary value of normal velocity component, the dummy cell velocity value of \( V_n \) has the opposite sign to the value of the inner near-wall cell, whereas the dummy cell pressure and density values can be taken same as in the inner cell. The boundary value of pressure is determined from solution of the discontinuity breakdown problem as the value on the contact surface, which is assumed to be located on the boundary face. That gives the following expressions \([8]\):

\[
P = p \left(1 - k \frac{1 - V_n}{c} \right)^{\frac{2k}{k+1}}, \quad \text{if } V_n > 0
\]  

\[
P = \sqrt{\rho \left(\frac{k+1}{2} p + \frac{k-1}{2} V_n^2 \right)} = -V_n, \quad \text{if } V_n < 0
\]  

Both the above given approaches are of the first-order accuracy. A second-order boundary condition can be obtained by replacing value of \( V_n \) in (9), (10) by a reconstructed value, denoted as \( \overline{V}_n \). To calculate this value, reconstruction procedure (7) is used, either without introducing the limiter (the third variant of wall pressure reconstruction) or with the limiter (the forth variant).

The fifth and the sixth variant consists in using a weighted scheme for evaluation of \( V_n \):

\[
\overline{V}_n^{\text{weighted}} = d \cdot V_n + (1-d) \cdot \overline{V}_n, \quad d \in [0,1],
\]  

where \( d \) – weight.
Denotation of the above described variants of wall pressure reconstruction are given in Table 1.

Table 1 Variants of wall pressure reconstruction

| №  | denotation | calculation of P                        |
|----|------------|----------------------------------------|
| 1  | P1         | formula (7)                            |
| 2  | R1         | formulas (8), (9)                      |
| 3  | R2         | formulas (8), (9) with reconstructed value of $\tilde{V}_n$ ($\varphi=1.0$) |
| 4  | R3         | formulas (8), (9) with reconstructed and limited value of $\tilde{V}_n$ |
| 5,6| R2(d), R3(d) | formulas (8), (9) with weighted value $\tilde{V}_n^{\text{weighted}}$ |

2.3. CFD codes used
All the variants have been implemented in the in-house unstructured-grid CFD-code SINF/Flag-S that is under permanent development at the St.-Petersburg Polytechnic University. Using this code, calculations of inviscid supersonic flow in a duct with a central wedge were carried on the base of an implicit scheme of the stepping method (in increments) with the stabilizing operator discretized by the first-order scheme with scalar dissipation.

For the sake of comparisons, numerical solutions of the problem were obtained also by the ANSYS Fluent 16.2 choosing the second-order Roe scheme and the modified Venkatakrishnan limiter, same as implemented in SINF/Flag-S.

3. Results and discussion
Inviscid supersonic flow in a duct with a central wedge was calculated for different wedge angle tangent: $\text{tg}(\alpha)=0.3(3); 0.5; 0.6$ (figure 2(a)). It is assumed that supersonic flow enter the duct with the inlet Mach number $M_{in} = 3.0$. The outflow is also supersonic. For all cases, the quasi-structured computational mesh used consists of 4800 quadrangle elements (figure 2(b)).

Figure 3 illustrates Mach number maps calculated for $\text{tg}(\alpha)=0.3(3)$ and 0.6. As seen, the flow consists of interacting shocks and expansion waves. In the case of $\text{tg}(\alpha)=0.6$ the shock front begins to bend near the upper wall due to interaction with rarefaction waves (figure 3(b)).

![Figure 2. Geometry of the computational domain (a) and mesh (b).](image-url)

![Figure 3. Fields of Mach number for the case $\text{tg}(\alpha)=0.3(3)$ (a) and $\text{tg}(\alpha)=0.6$ (b).](image-url)
In order to investigate effect of approaches for wall pressure reconstruction on regions near fractures of boundary surface (points A and B in figure 2), pressure distributions on the wedge of surface are analyzed. Figure 4 presents the pressure distributions computed for the case of tg(α)=0.3(3) with different variants of wall pressure calculations.

As seen, even in the case of the first-order scheme, figure 4 (a), the simplest approach (variant P1) results in nonmonotonic solution in the vicinity of the fractures. In the case of the R1 approach, there are no nonmonotonicities near the surface fractures, and the SINF/Flag-S solution is closer to the analytical results than the solution obtained with the ANSYS Fluent.

Results obtained with different wall pressure reconstruction approaches based on the second-order scheme for flux computations are compared in figure 4 (b). Same as in the case of the first-order flux scheme, the P1 approach leads to appearance of regions with strong nonmonotonicity in the pressure distribution, while the R1 technique provides monotone solution in the vicinity of both point A and point B.

Figure 4 (b) shows also that the attempt to increase the order of accuracy in the wall pressure reconstruction approach based on the Riemann problem of discontinuity breakdown (variant R2) leads to a nonmonotonicity in the pressure distribution, although it is much less expressed than in the case of the simplest approach (variant P1). Appearance of these non-physical oscillations is prevented via introducing the limiter together with employment of the weighted scheme setting a small weight of the first order scheme (variant R3(d)). For instance, completely monotone solution in the vicinity of both point A and point B is obtained in the case of R3(d=0.3). Using the “pure” weighted scheme leads to worse result (see variant R2(d=0.5)). Figure 5 illustrates the scalar limiter field from computations with the R2 approach. As seen, the limiter is «turned on» not only along the shock, but also in the region between the shock and the wedge, and it is «turned off» near other walls.

Figure 6 presents an additional comparison of the ANSYS Fluent data with results obtained for tg(α)=0.3(3) and 0.6 with the best choice from the wall pressure reconstruction variants implemented in the in-house code. Choosing variant R3(d=0.3) for tg(α)=0.3(3) and R3 for tg(α)=0.6, it is possible to get the best quality of the solutions.
4. Conclusions

Numerical solutions of inviscid supersonic flows can contain areas with non-monotone solution in the vicinity of the boundary surface fractures. The quality of the solution strongly depends on wall pressure reconstruction.

Several variants of wall pressure reconstruction, implemented in the in-house finite volume code, have been described. Comparative analysis of quality of the solutions obtained with different approaches of wall pressure reconstruction has been performed considering a representative test case being supersonic flow in a duct with a central wedge.

First-order wall pressure reconstruction based on the solution of the Riemann problem of discontinuity breakdown results in monotone solution in the vicinity of the surface fractures, both for the first-order and the second-order scheme for convective fluxes at inner faces of computational cells.

An attempt to increase the order of accuracy in the Riemann-problem-solution wall pressure reconstruction, without introducing any limitation procedure, has resulted in appearance of pressure distribution nonmonotonicity in the vicinity of the surface fractures. This undesirable effect can be fully suppressed by introducing a limiter in combination with the weighted scheme. Finally, all this allows getting high quality results for the whole flow region.

References

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