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Comparative Evaluation of the Accuracy of Numerical Methods on Reference Solutions

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Abstract

When organizing a mass practical solution of computational problems of gas dynamics with the help of mathematical modeling, information on the comparative accuracy of the numerical methods used is now increasingly in demand. As a rule, calculators need information not only for a particular combination of the defining gas-dynamic parameters of the problem (characteristic Mach, Reynolds numbers, etc.), but also for the variation of these parameters in certain ranges. This work presents numerical studies devoted to a comparative assessment of the accuracy of numerical methods for a number of problems with reference solutions. The calculation of these problems is carried out for ranges of characteristic numbers using various numerical methods. The results obtained are compared with the reference solution and make it possible to estimate the error for each of the numerical methods. Calculations are carried out using the construction of a generalized computational experiment. A generalized computational experiment is a computational technology that combines the solution of mathematical modeling problems, parallel technologies and visual analytics technologies. The results of the generalized computational experiment are multidimensional arrays, where the dimension of the arrays corresponds to the defining parameters. Analysis and visual representation of the obtained results provide information on the comparative accuracy of the numerical method for the selected class of problems.

Keywords: numerical methods, comparative estimation of accuracy, generalized computational experiment, reference solutions, class of problems.

1. Introduction

This paper introduces numerical studies of a comparative analysis of the accuracy for various numerical methods and solvers, based on these numerical methods. The analysis is performed using reference solutions in the field of gas dynamics. The analysis considers not only solutions for specific combinations of key gasdynamic parameters that determine the flow (such as Mach numbers, Reynolds numbers, etc.), but also numerical solutions for classes of problems defined by variations in these key parameters. Such analysis is implemented numerically by constructing a generalized computational experiment, which combines mathematical modeling, parallel computing technologies, and visual analytics techniques.

Currently, research focusing on the comparative assessment of numerical methods' accuracy is becoming increasingly relevant and practical. When organizing large-scale practical solutions to computational gas dynamics problems using mathematical modeling, there is a growing demand for information regarding the comparative accuracy of the employed numerical methods. Typically, analysts require information not only for specific combinations of key gasdynamic parameters (such as Mach numbers, Reynolds numbers, etc.) but also for variations of these parameters within certain ranges. There are more and more international and domestic standards regulating the development and application of numerical methods in computational gas dynamics problems [1–3].

The growing demand for comparison analysis research on the accuracy of numerical methods in problem classes is also caused by several practical reasons:

- Some universal computing systems (for example, [4]) have a large number of integrated numerical methods and allow the incorporation of new numerical methods. The number of new numerical methods and their modifications is constantly increasing. It is far from always that the developers of these numerical methods perform an accuracy analysis for various types of problems. The one using these universal computational complexes has to have the required information about the accuracy for orientation. In other words, the mathematician needs to have certain knowledge about the accuracy of the numerical methods to be able to choose, which one to use in a certain case.
- Nowadays, in most cases, the accuracy of a numerical method is rated by a deviation from the reference solution. An accurate solution to a gas dynamics problem, a validated numerical solution, or experimental data might be used as a reference solution. As a rule, such comparison is considered at a single point in space of general defining problem parameters, as to say, with the fixed parameters of the fixed values of the fundamental gas dynamic parameters. Indeed, the approach, suggested in the current study, is oriented toward making a similar comparison not in a single point in space of the parameters, but for the usage of problem classes, determined by variations of the fundamental parameters.
- The results of comparative analysis of the accuracy of numerical methods for classes of problems provide the engineer with the necessary ideas about the accuracy of the methods used, and thus about their applicability, efficiency and reliability for a particular problem.

This paper presents the results of previous and ongoing research on comparative analysis of the accuracy of numerical methods and solvers developed on their basis. New methods and solvers, both previously developed and newly provided by authors, are constantly being added into the research. In the process of applying solvers to well-known problems with known reference solutions, quite unexpected results may be observed.

2. Previous studies

This study relies on several previous period studies, where various classes of gas dynamics problems that had reference solutions were examined. All the problems were examined for the supersonic flows.

The research focused on the comparison analysis of the solver accuracy in the flow around a circular cone at an angle of attack presented in the studies [5, 6, 7]. In this class of problems, the following fundamental defining parameters of the flow were varied: freestream velocity, half-angle of the cone, and angle of attack.

Additionally, problems involving the formation of oblique shock waves when a supersonic flow impinges on a plate at a certain angle were examined [8, 9]. In these cases, the freestream velocity and the angle of incidence of the flow on the plate were the varied parameters.

Similarly, the problem of the formation of a rarefaction wave, occurring when a plate is subjected to flow at a certain angle was also examined [10]. In such a case, the varied parameters were the freestream velocity and the angle at which the plate is being subjected to flow.

Various numerical methods and solvers based on them were used in the accuracy analysis. Studies [7, 11] are dedicated to connecting new numerical methods with comparison accuracy analysis.

All the results are received by constructing a generalized computational experiment.

3. The generalized computational experiment

The research on comparison analysis of the numerical methods accuracy that is presented in the research article is based on constructing a generalized computational experiment. The conception of the generalized computational experiment has a wide spectrum of possible usage. First of all, for the problems of computational hydrodynamics, such an approach allows us to receive a solution not only for a single separate problem but also for the whole class of problems that is established in a certain range of the whole complex of the defining parameters. The generalized computational experiment implies a partition of each of the determining parameters of the problem in a certain range. This way, a grid decomposition for a multidimensional parallelepiped composed of the defining parameters of the gas dynamics problem under consideration is formed. For each point of this grid, a problem is calculated in the space of the determining parameters. The practical implementation of the approach becomes possible when using parallel calculations in a multitasking mode. The calculation result is a multidimensional volume of data that can be processed using data analysis tools and visual analytics. It should also be noted that the usage of this approach allows performing of research calculations on coarse grids for a problem class with the following clarification for the sets of determining parameters of great interest. The conception and implementation of the generalized computational experiment were made under the guidance of A. E. Bondarev for the Keldysh Institute of Applied Mathematics, Russian Academy of Sciences. The main characteristics and elements of the generalized computational experiments are described in detail in the papers [12–14].

4. Numerical methods and solvers based on them, involved in comparison

The open source software package OpenFOAM [4] was used for comparative analysis of the accuracy of numerical methods and solvers implemented on their basis. It offers a wide range of built-in solvers, as well as the function of creating one's own. Four solvers were used for comparative analysis: rhoCentralFoam, pisoCentralFoam, sonicFoam and QGDFoam.

The sonicFoam solver uses the PISO (Pressure Implicit with Splitting of Operator) algorithm [15] to link pressure and velocity. The pressure field obtained using the discretized momentum and continuity equations is corrected using two difference equations. This approach is used because the velocity field corrected in the first correction step does not satisfy the continuity equation.

The rhoCentralFoam solver uses the central-anti-threading scheme proposed by Kurganov et al. (KT/KNP) [16, 17] and implemented for OpenFOAM by Greenshields [18]. This method using interpolation of flows between neighboring cells, which allows for good modeling of discontinuous solutions [6]. It is shown in [19] that this solver gives the best results of the two for transonic and supersonic flows, showing better approximation to analytical solutions and more stability than sonicFoam. However, rhoCentralFoam cannot successfully model subsonic regimes. KT/KNP schemes have demonstrated good accuracy in solving subsonic/supersonic flows, but they fail in modeling viscous flows at low Mach numbers ($M < 0.3$).

Alternatively, hybrid schemes have been developed that combine the PISO algorithm for subsonic flow modeling with the KT/KNP scheme for accurate calculation of discontinuities occurring in supersonic regimes [19]. Moreover, the solvers are enhanced by the ability to incorporate external iterations of the SIMPLE (Semi-Implicit Method for Pressure Linked Equations) algorithm to obtain more accurate solutions [20]. The combined collection of all these hybrid solvers is not embedded in OpenFOAM, but can be found in the authors' public repository [21]. The solver pisoCentralFoam is a semi-implicit pressure-based solver for a compressible ideal gas.

The QGDFoam solver [22, 23] is based on a system of quasi-gasdynamic equations [24] developed by a research team led by B.N. Chetverushkin. The mathematical model generalizes the system of Navier-Stokes equations by adding additional dissipative terms in the form of second spatial derivatives with a small parameter in the form of a coefficient [25]. The fundamental difference between quasi-gas-dynamic and quasi-hydrodynamic systems and the system of Navier-Stokes equations is the space-time averaging for determining the main gas-dynamic quantities. The controlled parameter at dissipative terms gives this solver the function of adjustable scheme viscosity, which makes it possible to suppress unwanted oscillations at discontinuities.

In the process of organizing calculations on comparative evaluation of the accuracy of numerical methods on reference solutions, new solvers were added to the selected solvers. Among them, one can single out the author's solvers based on the numerical WW method [26, 27] and the discontinuous particle method [28-30].

Considered numerical WW method is based on hybrid implicit finite-difference scheme (WW scheme). The scheme can be referred to class of two-parametrical finite-difference schemes. Having second order accuracy for time and space and unconditional stability the scheme has also internal artificial viscosity regulated by the choice of weight parameters. The feature of controlled artificial viscosity allows one to avoid undesirable oscillations in solution. Being simple and effective the method is applied to some practical CFD problems such as: jets interaction, separation problems, optimizing analysis. The presence of adjustable artificial viscosity is a common feature with the QGDF solver.

Particle methods belong to a different class than classical difference methods, since they use the Lagrangian approach [28], an example of the particle method is the SPH method [29]. In the discontinuous particle method [30] we write the problem in the form of a system of ODEs, then we introduce the distribution density represented as a sum of delta functions, which, in turn, for the convenience of calculations, we approximate by rectangle functions. Thus, the model of a continuous medium is replaced by a discrete model - a set of particles. Each particle, based on the initial conditions, is assigned a set of attributes, such as mass, velocity, and position in space.

First, the particles are moving according to the numerical solution of the ODE system. Then pairs of interacting particles are chosen, thus the two-dimensional problem is reduced to a set of one-dimensional ones. The mass between the coordinates of the particles is equal to the half-sum of the particle masses and, in the absence of diffusion, it must also remain constant. The distances between the particles change after the shift, resulting in changes in the areas of the trapezoid. Therefore, in the corrector step, we need to change the heights of the particles so that the mass between the particles remains constant (Figure 1). The next step of the algorithm is to take into account the pressure forces. The difference of pressures to the left and right of the particle leads to a change in the momentum and energy of the particle, i.e., to an increase in the volume of the corresponding particles. As a result, we recognize the values of the sought quantities at a new time step.

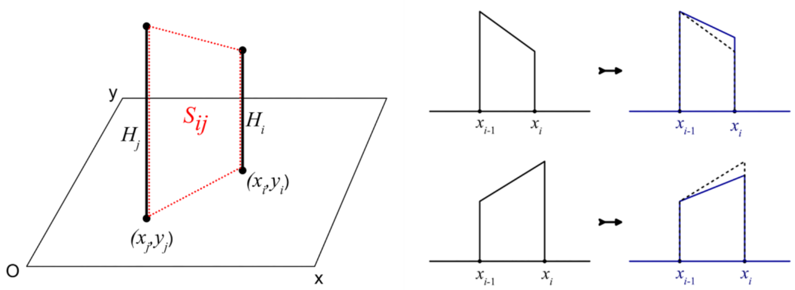

Fig.1. Transition from two-dimensional to one-dimensional problem and particle correction based on area constancy.

5. The problems with reference solutions

Three classical problems for a non-viscous gas with a reference solution, either exact or tabulated, were chosen for solver comparison.

The first problem is the streamline of a cone with a half-angle β at an angle of attack α at different Mach numbers of the advancing flow. In this case, a shock wave appears in front of the cone in the form of a conical surface with angle θ. A flow is formed between the surfaces of the cone and the shock wave, the flow parameters of which remain constant along the straight lines drawn from the cone apex. There is a tabular solution of the problem [31]. The parameters varied here were the angle of attack α, Mach number, and cone half-angle β. The ranges of variation of the varied parameters and the step of variation were chosen as follows: angle of attack α = 0°, 5°, 10°, Mach number M = 3, 5, 7, cone half- angle β = 10°, 15°, 20°. The streamline scheme is presented in Figure 2.

The second problem is the modeling of an oblique shock wave. A supersonic gas flow with Mach number M falls on a flat plate at an angle β. An oblique shock S appears in front of the plate. This problem is considered in the framework of the system of Euler equations and has an exact analytical solution [32, 33]. The general flow scheme is presented in Figure 3.

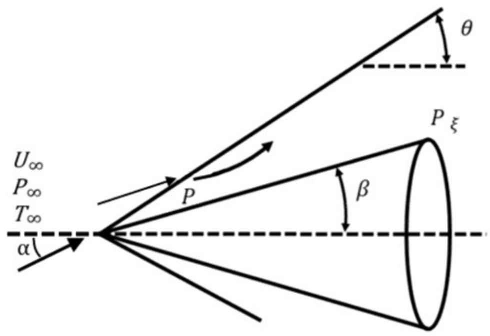

Fig. 2. Flow diagram of cone flow at angle of attack

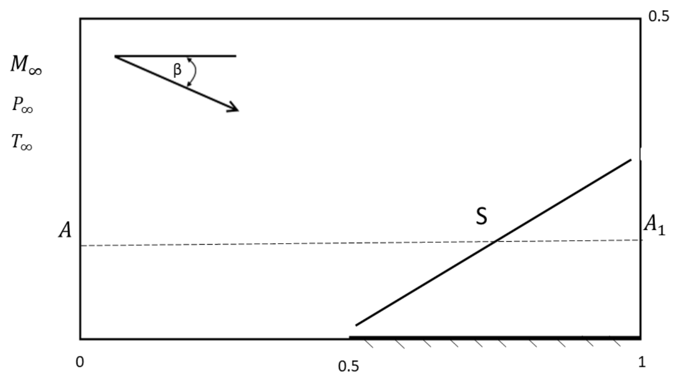

Fig. 3. Flow diagram of oblique shock wave

At the inlet boundary, the parameters of unperturbed incoming flow at Mach number M and a certain value of β are set. On the part of the lower boundary corresponding to the flat plate, the no-flow condition is set. On the outlet boundary, the boundary conditions of zero equality of derivatives of gas-dynamic functions along the normal to the boundary are set. At the upper boundary for the velocity components, the boundary conditions are set similarly to the conditions for the inlet boundary. For other gas dynamic functions of the upper boundary, the conditions are set similarly to the conditions for the output boundary. Variable parameters were: angle of incidence β = 6°, 10°, 15°, 20°. Mach number M from 2 to 4 with a step of 0.5.

As the third problem, we considered the well-known classical problem of the formation of a two-dimensional rarefaction wave when a flat plate is streamlined by a non-viscous gas flow at an angle of attack. The scheme of such a flow is presented in Figure 4. A supersonic flow of a non-viscous compressible gas flows over a flat half-plate at an angle of attack β, as shown in the figure. A rarefaction wave fan is formed at the end of the plate. This problem is commonly known as the Prandtl-Meyer flow. This problem has an exact solution, the description of which can be found in [32, 34, 35]. The exact solution in our case acts as a benchmark. The parameters to be varied here were: flow deflection angle β = 6°, 10°, 15°, 20°. Mach number M from 2 to 4 with a step of 0.5.

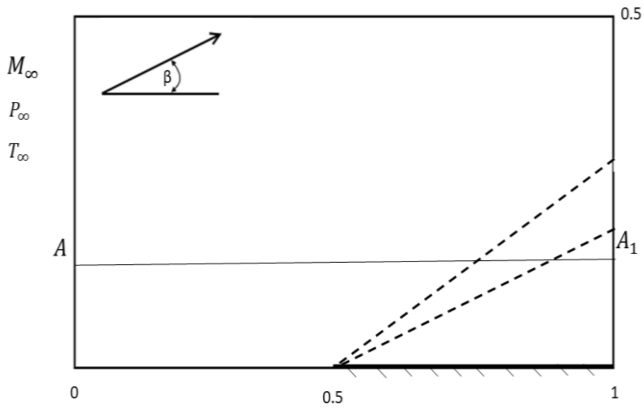

Fig. 4. Prandtl-Meyer flow diagram

6. Results

Let us consider the comparative analysis of accuracy on the example of the three-dimensional problem of cone flow with supersonic flow of a non-viscous gas at the angle of attack. The exact solution was taken from [31].

To get an idea of the behavior of the error *Err* as a function of angle of attack α, half- angle β, and Mach number M, we first estimate the contribution of the three variables to the variance. For fixed values of the half- angle β and Mach number M, the variation of the angle of attack α provides the smallest variance. Let us represent the *Err* function as *Err* = *Err*(0°, β, M) for a fixed angle of attack α = 0°. Thus, we obtain a representation of the surface form *Err*(0°, β, M). Let us now present in a similar way the results of calculations in the form of a group of surfaces, i.e. as three surfaces at values of angle of attack α = 0°, 5°, 10° for the solvers rhoCentralFoam (Fig. 5), pisoCentralFoam (Fig. 6), sonicFoam (Fig. 7). These were the solvers used in the comparison for this task.

Figure 5 allows us to see three closely overlapping surfaces of the same type. As the angle α increases, the error increases.

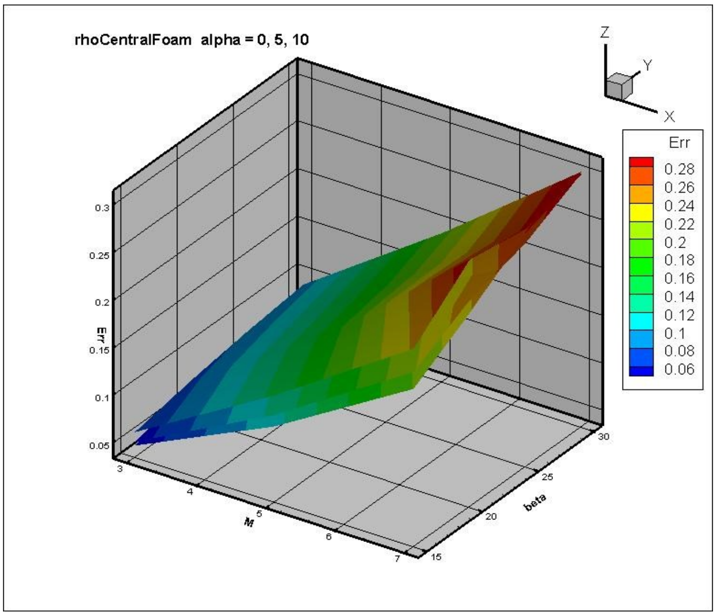

Fig. 5. Error dependencies on M and β at α = 0°, 5°, 10° for the rhoCentralFoam solver

Similar surface groups are shown in Figures 6 and 7 for the pisoCentralFoam and sonicFoam solvers. As for the rhoCentralFoam solver, the error increases as the angle α increases. Figures 5, 6, 7 give a complete picture of the behavior of the error under variation of the defining parameters for all the solvers involved in the comparative accuracy assessment.

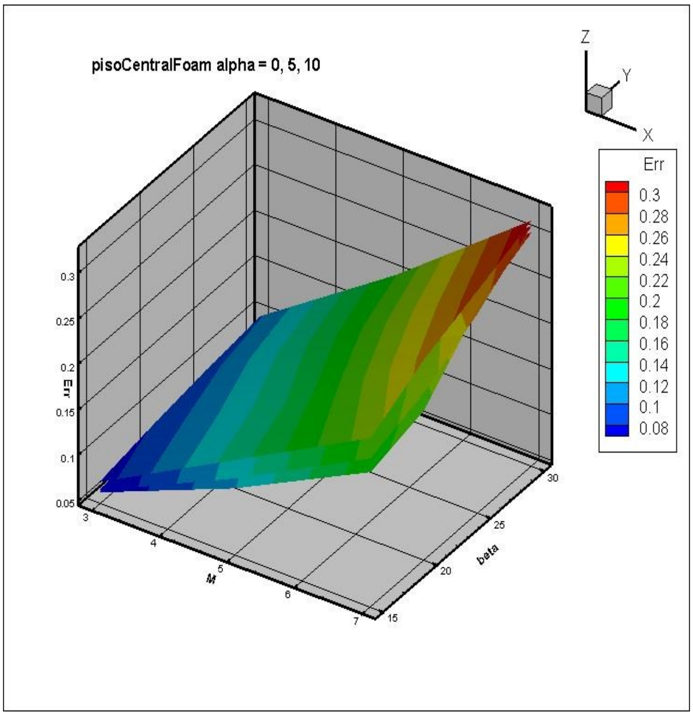

Figure 6. Error dependencies on M and β at α = 0°, 5°, 10° for the solver pisoCentralFoam

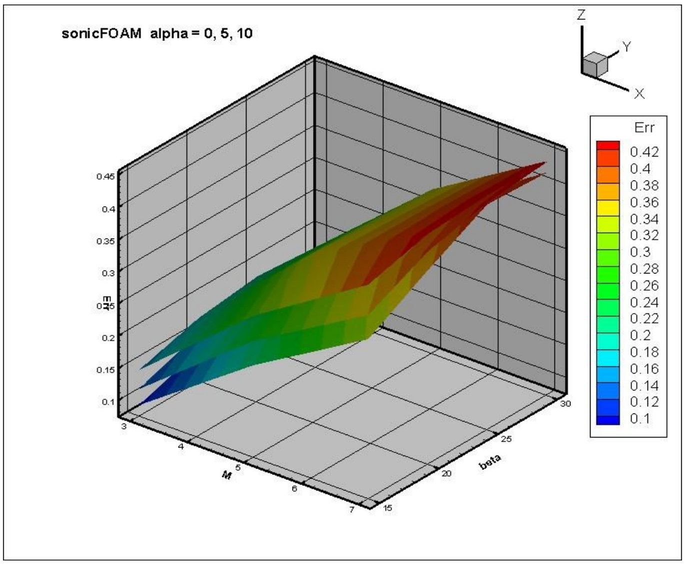

Fig. 7. Error dependencies on M and β at α = 0°, 5°, 10° for sonicFoam solver

Let us proceed to the problem of the oblique shock. For this problem, we construct estimates of the deviation from the exact solution for the entire computational domain in the L_2 norm. For this purpose, we define the relative error Err for the norms L_1 and L_2 as follows

$$Err = \sum_m |y_m - y_m^{exact}|\, S_m / \sum_m |y_m^{exact}|\, S_m. \tag{1}$$

$$Err = \sqrt{\sum_m |y_m - y_m^{exact}|^2\, S_m} / \sqrt{\sum_m |y_m^{exact}|^2\, S_m}. \tag{2}$$

Here y_m is the pressure p, S_m is the cell area. The y_m^{exact} values are obtained from the exact solution of the problem. The sonicFoam, QGDFoam, rhoCentralFoam, and pisoCentralFoam solvers participated in the comparative accuracy analysis. Figure 8 shows the relative error surfaces Err for all the solvers under the variation of the flow incidence angle and Mach number of the impinging flow. It can be seen that the sonicFoam solver is the coarsest, the QGDFoam solver is more accurate, the rhoCentralFoam and pisoCentralFoam solvers are almost indistinguishable. The increase of deviation with increasing of these defining parameters is clearly shown.

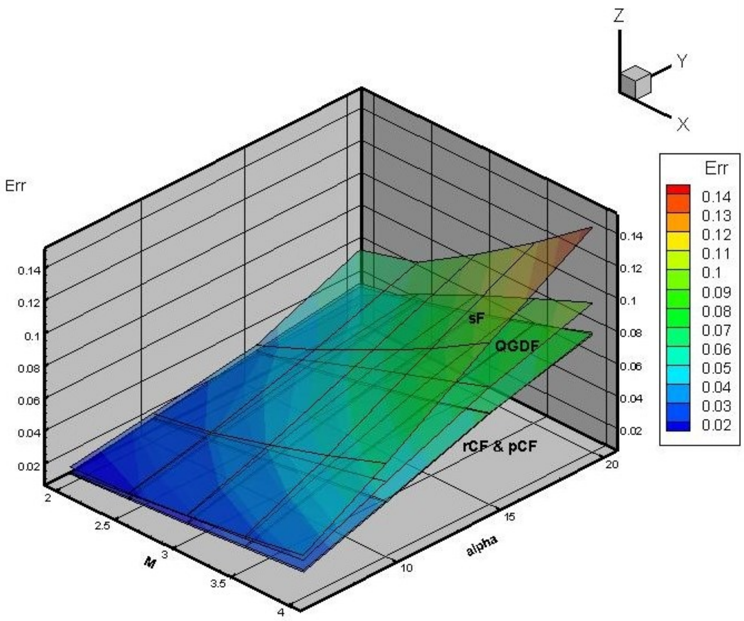

Fig. 8. Variation of the deviation from the exact solution for pressure as a function of Mach number and flow incidence angle for all solvers in the L_2 norm

A similar comparison of relative error surfaces for the particle method (PM) and solvers rhoCentralFoam, pisoCentralFoam and QGDFoam is also presented in Figure 9.

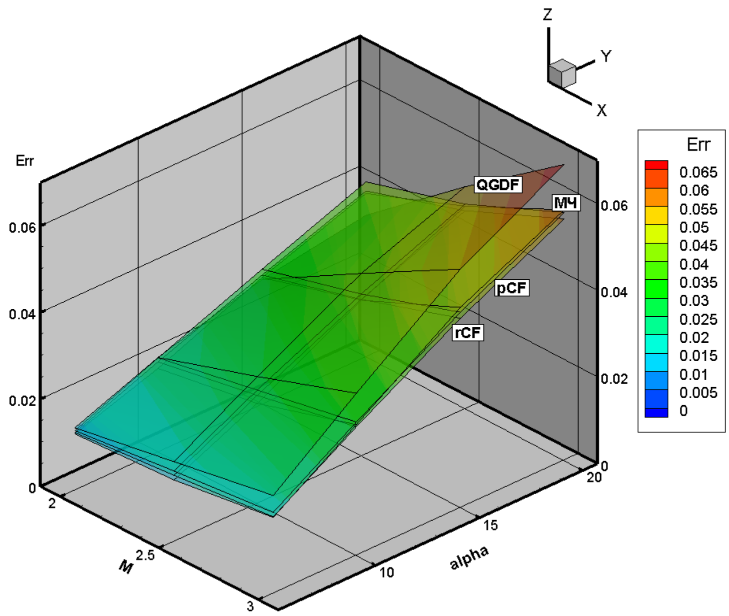

Fig. 9. Variation of the deviation from the exact solution for pressure as a function of Mach number and flow incidence angle for all solvers in L2 norm involving the particle method

At β = 10° and M = 3, the particle method is less accurate than the rhoCentralFoam solver. At β = 15°, the particle method is less accurate than the QGDFoam solver at M = 2 and less accurate than the rhoCentralFoam and pisoCentralFoam solvers at M = 3. At β = 20°, the particle method gives lower accuracy than the rhoCentralFoam and pisoCentralFoam solvers at M = 3. In other cases, the discontinuous particle method is more accurate than the other compared methods. Thus, the proposed approach allows a comparative analysis of the accuracy of numerical methods even of different nature of origin.

Let us consider the problem of two-dimensional rarefaction wave formation. We implement a generalized computational experiment, from the results of which we calculate the error for each solver at each combination of (M, β). This gives us the opportunity to construct the error for both norms as a function of two variables $Err(x_1, y_1)$where x_1 = M and y_1 = β. These notations will be used in all subsequent figures.

Now let us consider the comparison of all four solvers in different error norms. Figure 10 shows the deviations from the exact solution in the L_1 norm for all solvers in the ranges of variation of the defining parameters. Similarly, Figure 11 shows the deviations from the exact solution in the L_2 norm for all solvers.

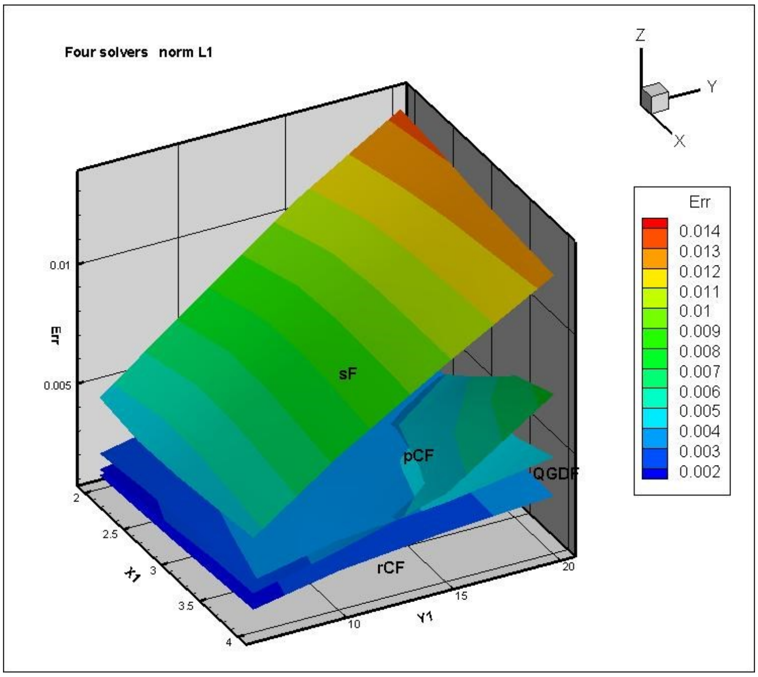

Fig. 10. Representation of deviation from the exact solution in the L_1 norm for all solvers in the ranges of variation of the defining parameters

As can be seen from Figures 10 and 11, qualitatively similar results are obtained for both norms. The solver rhoCentralFoam provides the smallest deviation from the exact solution. The QGDFoam solver is next in terms of deviation from the exact solution. Slightly worse results are provided by the pisoCentralFoam solver. It should be noted that in the selected ranges of Mach number and flow deflection angle, the error surfaces for the QGDFoam and pisoCentralFoam solvers are close to each other. The largest deviation from the exact solution is observed for the sonicFoam solver.

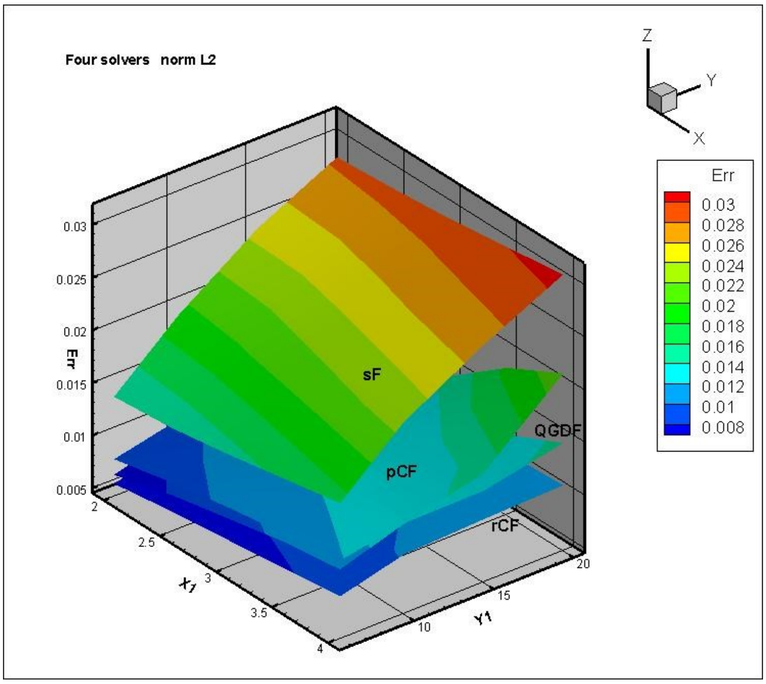

Fig. 11. Representation of the deviation from the exact solution in L_2 norm for all solvers in the ranges of variation of the defining parameters

All obtained surfaces can be represented in analytical form according to the method proposed and described in [36]. To approximate curvilinear surfaces, we will use second-order polynomials, where the error for the considered surface can be represented as a function of the following form:

$$Err = Ax_1 + By_1 + Cx_1^2 + Dy_1^2 + Ex_1y_1 + F. \tag{3}$$

Here x_1 is the Mach number M, y_1 is the flow deflection angle β, Err is the error of comparison with the exact solution in L_1 or L_2 norm. The coefficients A, B, C, D. E, F are calculated for a particular surface.

For example, for the QGDFoam solver in the L_2 norm, approximating the desired surface by a second-order polynomial using the least squares method, we obtain the following values of the coefficients:

A = 0.0007426759754917806
B = 0.0005021159520976077
C = 0.00020442857142857106
D = - 0.000012584191705984598
E = - 0.0000167566591422123
F = 0.0038062569399619252

For a more general comparative evaluation, an Error Index (EI) is calculated, similar to that proposed in [37]. Error Index (EI) represents the average value for each error surface.

The results for each solver in the L_2 norm according to Figure 10 are summarized in Table 1.

Table 1. Error Index values for the problem of rarefaction wave formation

Solver	rCF	QGDF	pCF	sF
Error Index	0.00894	0.01134	0.01182	0.02285

Table 1 shows that the EI values are fully consistent with the relative positions of the numerical results presented in Figure 10.

Thus, the obtained results in the form of visual representations of error surfaces, their analytical representations and calculated error indices allow the user of these solvers to get a complete idea of their accuracy in the class of rarefaction wave formation problems.

Conclusion

This study presents the results of the performed research in comparing the accuracy of various numerical methods and based on these methods solvers for gas dynamic problems that have a reference solution. The calculations are done by constructing a generalized computational experiment. The generalized computational experiment is a computational technology, connecting the mathematical modeling problem solutions with parallel technologies and visual analytics technologies. The results of the generalized computational experiment are multidimensional arrays, where the dimensionality of the arrays corresponds to the number of determining parameters. The defining parameters in the examined problems could be characteristic Mach and Reynolds numbers, geometric problem parameters, etc. The analysis of the obtained multidimensional arrays allows to organize a comparison with the reference solution not only in a single point in space but also in ranges of their change.

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