On the estimation of the accuracy of numerical solutions in CFD problems

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Abstract. The task of assessing accuracy in mathematical modeling of gas-dynamic processes is of utmost importance and relevance. Modern software packages include a large number of models, numerical methods and algorithms that allow solving most of the current CFD problems. However, the issue of obtaining a reliable solution in the absence of experimental data or any reference solution remains relevant. The paper provides a brief overview of some useful approaches to solving the problem, including such approaches as a multi-model approach, the study of an ensemble of solutions, the construction of a generalized numerical experiment.

Keywords: mathematical modeling, computational fluid dynamics, accuracy estimation, multi-model approach, ensemble of solutions, generalized numerical experiment.

1 Introduction

The task of assessing accuracy in mathematical modeling of gas-dynamic processes is of utmost importance and relevance. A huge number of works devoted to this topic, for example [1]. Precisely, accuracy estimation played a key role in the entire history of the development of numerical methods in CFD. Throughout the history of CFD, the main criterion for accuracy and reliability has been a comparison with a physical experiment [2, 3]. The development of numerical methods followed the path of complicating the mathematical models under consideration. At the first stage, the Euler equations were used to model the inviscid flow. To calculate the friction coefficient on the body, the boundary layer equations were used, where the results of calculations of inviscid flow were used as boundary conditions at the upper boundary of the layer. In order to simulate viscous effects (vortices, separation zones), it was already necessary to consider the complete system of Navier-Stokes equations. To simulate turbulent flows, it was necessary to add turbulence models. The history of the development of numerical methods is presented in detail in [4].

At each stage of this development for the construction of numerical methods and algorithms for their implementation, the main criterion for accuracy and reliability was a comparison with a physical experiment. Having a numerical method with the necessary approximation, stability and convergence, it was possible to compare the

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numerical solution of the simulated problem with the experiment and verify the reliability of the method. However, each task is characterized by a whole set of defining parameters, such as the Mach number, the Reynolds number, the geometric parameters of the problem, and so on. Having achieved a satisfactory agreement with the experimental data for a specific set of determining parameters, it was assumed by default that with some reasonable variation of them, the solution is obtained quite accurately.

Modern software systems for solving CFD problems, both open and commercial, have now been greatly developed. Such complexes include a large number of numerical methods, turbulence models, methods for parallelizing algorithms. It would seem that now the problem of accuracy and reliability is solved. However, in practice there is a certain kind of paradox. With all the wealth of opportunities provided by modern computing software packages, in these packages there are a large number of tuning parameters. These parameters may vary in certain ranges. On the one hand, this is very good, since it gives the opportunity to customize the algorithms to match the experimental result. But in the absence of experimental data or any reference solution, there are serious problems in evaluation the accuracy of the solution obtained.

In this case, we are dealing with a complex type of uncertainty, where the total error consists of such components as model selection error, numerical method error, error of the algorithm’s numerical implementation method, computational grid construction error, and finally inaccuracies associated with setting numerous parameters characterizing the selected turbulence model. Analyzing and evaluating the accuracy for each of these components separately is quite difficult and ultimately inefficient. It is much more expedient to develop integrated approaches for obtaining a reference solution and an assessment of accuracy.

It should also be noted that the question of the method and standard of evaluation also plays a big role. The gas-dynamic fields obtained in the calculation can be compared with the experiment and the reference solution. For example, quite often numerical solutions are compared by the presence of oscillations in a shock wave and the degree of its smearing. The solutions obtained by monotonous schemes look best from this point of view. However, oscillating solutions may converge in the norms of L_1, L_2 better than monotone ones. Another way is to compare commonly used valuable functionals in practice, such as the drag coefficient of an object placed in a stream. Thus, the following question remains relevant: how can one obtain a relatively reliable solution in the absence of data from a physical experiment or a reference solution? The question is of special importance if we are not talking about a single calculation, but about the formulation of mass industrial calculations. Below some possible approaches to solving this problem are considered. The article presents three approaches to solving listed above problems that are developed simultaneously by our team at Keldysh Institute of Applied Mathematics (KIAM RAS). All the results presented in this article were developed at KIAM RAS as part of the development of these three approaches.

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2 Approaches to obtaining a reference solution

2.1 Multi-model approach

This approach is in a sense historical. It was widely distributed at the end of the twentieth century. The approach allowed to carry out with sufficiently high accuracy mass industrial and scientific calculations in a wide class of problems of modeling flows around objects. This computing technology was complex and combined several mathematical models. Each of the models used the results obtained using a different model as boundary conditions. It is here that the body drag coefficient in the flow was used as a valuable functional. This technology was especially effective for elongated bodies of rotation. Here aerodynamic drag coefficient was computed as a sum of three components: coefficient for inviscid flow, coefficient for viscous friction and coefficient for near wake. The results for inviscid flow were used as boundary conditions for computing of viscous friction coefficient. Then the results for viscous friction were used as boundary conditions for computing of near wake problem. This approach was widely used for analyzing the aerodynamic properties of different bodies with high efficiency.

Currently, there are successful attempts to implement this approach at the modern level using parallel computing in the form of a computational pipeline, where data is automatically transferred from the model to the model [5, 6]. To simulate a non-viscous flow around an open software package OpenFOAM (Open Source Field Operation And Manipulation CFD Toolbox) [7] is used. This package has a large number of solvers, both standard and developed by various teams. For a comparative assessment of the accuracy of these solvers, a series of calculations were carried out on the test problem of a flow around a cone at an angle of attack. During the test calculations, the Mach number, the angle of the cone, and the angle of attack were varied. The results allowed to make conclusions about the most appropriate solvers in terms of accuracy [6].

To determine the friction coefficient on the body placed in a flow, a computational technique [5] is implemented, based on an approximate semi-empirical model combining the results of experimental studies and the well-known effective length method. This technique uses the results of calculations of non-viscous flow as input data and allows one to obtain a drag friction resistance coefficient and characteristic boundary layer thicknesses in a wide range of Mach and Reynolds numbers both for the laminar and turbulent regime. To determine the coefficient for near wake pressure, the Navier-Stokes equations are used, where the results obtained in the previous stages are used as boundary conditions.

This approach is not universal. It works well for classes of problems where friction coefficient and coefficient for near wake pressure are small compared with coefficient for inviscid flow. Nevertheless, for many classes of problems, this technology allows obtaining results that can be used as a reference solution in the absence of experimental data.

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2.2 Use of ensemble solutions

If there is a set of numerical solutions (for example, obtained using various finite-difference schemes) and *a priori* information about the error ranking of these solutions, then we can estimate the neighborhood of the approximate solution containing the exact solution *(exact solution enclosure)*. If an ensemble of numerical solutions can be divided into clusters of “accurate” and “inaccurate” solutions, then the error ranking of values can be performed using an a posteriori analysis of the distances between the numerical solutions. This can serve as a computational proof of the existence of an exact solution in the case of nonlinear problems. This approach is described in detail in [8], where the results of tests for supersonic flows within the framework of the Euler model are presented. A set of solvers with different approximation orders was used. The comparison considered a set of finite-difference schemes with accuracy order from the first up to forth. The results of comparison demonstrated the exact solution enclosure

This approach can be considered as perspective. Nevertheless, it has evident drawback. For using of this approach one should have a set of solvers with different accuracy order.

2.3 Construction of generalized numerical experiment

This approach is the most interesting from the point of view of the author. The modern development of high-performance computing clusters and the wide distribution of parallel computing technologies open up a number of new opportunities for solving problems of mathematical modeling in computational gas dynamics. These new features include high-grade parametric research and solving optimization analysis problems. Parametric studies suggest multiple solutions to the direct problem of mathematical modeling with variations in the defining parameters of the problem. The defining parameters of the problem include characteristic numbers, such as the Mach number, Reynolds number, Strouhal number, etc., and the geometric parameters of the problem. Each of the defining parameters varies in a certain range of variation with a certain partitioning step. The tasks of optimization analysis are more complex from a computational point of view. At each split point of the space of defining parameters, such problems assume the solution of the inverse problem, which aims to find the extremum of one or another valuable functional (optimal form, minimal drag coefficient, etc.). Parametric studies and optimization analysis tasks are the basis of a generalized computational experiment. A generalized computational experiment allows one to obtain in discrete form a solution not only for one single task, but for a whole class of problems. Here the class of problems is determined by the ranges of change of defining parameters.

The main advantage of a generalized computational experiment is that it allows one to obtain a solution not for one specific problem, but for a class of problems. However, the discrete solution itself cannot provide an understanding of the results

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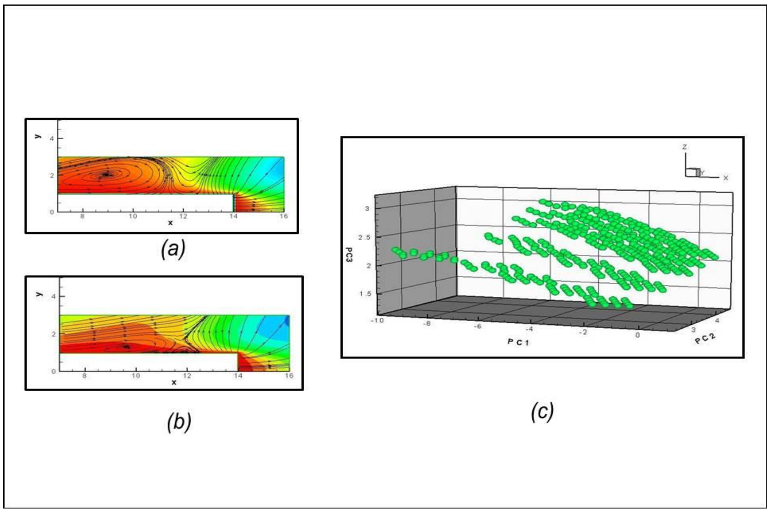
obtained. It requires a wide and creative use of the tools of scientific visualization and visual analytics. When visualizing the results of a generalized computational experiment, it is necessary to combine the use of classical methods of visualization and animation of three-dimensional scalar and vector fields with visual analytics tools designed for analyzing multidimensional data. Various aspects of the construction of a generalized computational experiment and its formal description are described in detail in [9].

Let's consider some examples of this approach applied to some practical problems. It is applied in some variations due to different aims for each class of problems [6, 9-11].

The first example is presented in [9]. We consider a nozzle in supersonic viscous flow. Underexpanded supersonic jet exhausts from the nozzle. Jet propagation creates an obstacle in the main flow. For standard case we have flow structure presented in Figure 1(a). If we increase velocity of pressure ratio growth in the jet, then we obtain a new flow structure presented in Figure 1(b). This crucial value of the velocity is used as control parameter. We consider four characteristic numbers (Mach number, Reynolds number, Prandtl number, Strouhal number) as coordinates in the space of defining parameters. Each of these parameters within the range is divided with some specific step. So we have a set of points in a four-dimensional space created by four defining parameters. For each point of this four-dimensional space, we find the value of the crucial velocity at which the flow structure changes. Then one can construct the space of three first principal components for computed data and make visual presentation for crucial velocity in a new system of coordinates (Figure 1(c)). The form of dependence in question allows to approximate the dependence by plane. So the construction of generalized numerical experiment allowed to obtain desired dependence in an analytical form [9].



(a)

(b)

(c)

Fig. 1. Two types of flow structure ((a) and (b)) and control parameter in the space of 3 first principal components (c).

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The following example of constructing a generalized computational experiment is presented in [10], where the problem of finding the optimal shape for a three-dimensional blade assembly is considered. The blade assembly has a rather complicated configuration and is located in the stream. Note that this blade assembly belongs to the power plant. The target functionals here were chosen the value of the total aerodynamic force acting on the blade, and the amount of torque. As the defining parameters were set two angles, which set the slope of the blade and the transverse width of the blade. These three parameters varied in certain ranges. For the numerical implementation of this generalized computational experiment, a computational technology was constructed that simulates the load on the blade assembly, placed in the air flow at various flow rates. The task was complicated by the fact that the modeling of the flow around and the variation of the geometric parameters were carried out taking into account quantitative restrictions on the moment of inertia and the mass of the blade assembly. These characteristics should not exceed certain boundary values when changing geometric parameters. This problem was solved using parallel computing. Figure 2 shows the resulting shape of the blade assembly. The figure also shows the pressure distribution over the surface of the blade assembly.

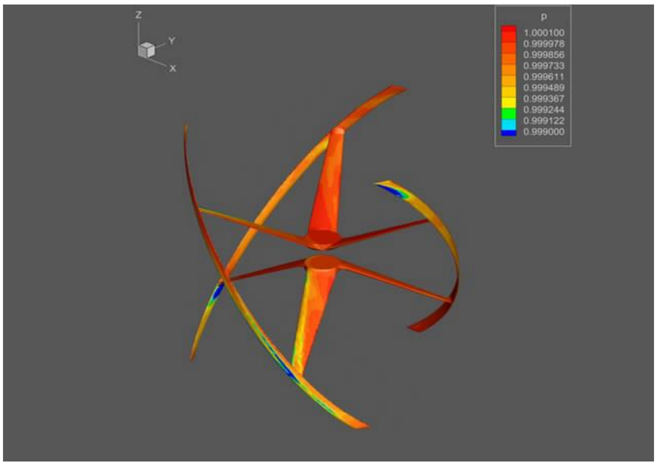

Fig. 2. 3D blade assembly shape and pressure distribution on its surface [10].

The next example considers the problem of the evaluation of the accuracy for different numerical methods. The problem of inviscid compressible flow around a cone at zero angle of attack is used as a base one. The results obtained with the help of various OpenFOAM solvers are compared with the known numerical solution of the problem with the variation of cone angle and flow velocity [6]. Cone angle β changes from 10° to 35° in steps of 5°. Mach number varies from 2 to 7. For comparison, four solvers were selected from the OpenFOAM software package: *RhoCentralFoam, SonicFoam, RhoPimpleFoam, RhoPimpleFoam*. The results of such kind of numericsl experiment were presented as errors in the form of an analog of the L2 norm for all solvers. Fig.3 illustrates the results in a form of a change in deviation from the exact

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solution for pressure depending on the cone angle and the velocity for the solver *rhoCentralFoam*. Such changes were obtained for all solvers.

Figure 3 shows a multidimensional dataset for pressure obtained as a result of parametric calculations in the space of the first three principal components. Yellow shows the results for *rhoCentralFoam* solver, red for *pisoCentralFoam*, green for *sonicFoam* and blue for *rhoPimpleFoam*. Figure 3 shows that the errors for *rhoCentralFoam* and for *pisoCentralFoam* can be roughly approximated by a plane reflecting the dependence of the error on the Mach number and cone angle. The results for *sonicFoam* and especially for *rhoPimpleFoam* are significantly separated from the results for the first two solvers due to their particular numerical characteristics. This methodical research can serve as a basis for selecting the OpenFoam solver for calculating the inviscid supersonic flow around the elongated bodies of rotation. The results of solvers comparison can also be useful for developers of OpenFoam software content.

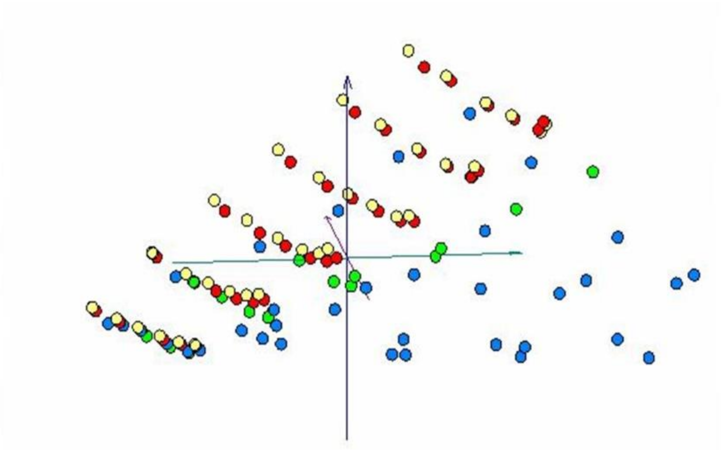

Fig. 3. Errors for different OpenFOAM solvers in the space of principal components

The following example is devoted to improving the computational properties of finite-difference schemes. The problem of mathematical modelling of the flow in the far wake behind the body is solved. In the general case, in a rectangular computational domain, a viscous compressible heat-conducting gas flow is considered, described by a complete system of time-dependent Navier-Stokes equations. At the input boundary, the distributions of gas-dynamic parameters are given, obtained from calculations of the flow around an axisymmetric body and a portion of the track behind it. The main goal of the generalized computational method was to thoroughly study the properties of artificial viscosity incorporated in the hybrid difference scheme. For this purpose, we studied the properties of the weight coefficients of the hybrid scheme on the example of the problem of flow in the far wake and determined the limitations for the weight coefficients. In this task, the following defining parameters were varied, such as the steps of the grid decomposition in the x and y directions, the weighting coefficients of the difference scheme, the Reynolds number of the problem.

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As a result of the generalized computational experiment, a limiting surface was constructed for the dependence of the weight coefficient on the other determining parameters of the problem. An example of the limiting surface is presented in Fig. 4. When choosing the value of the weighting factor below the surface, in the numerical solution, non-physical oscillations arise, which can lead to the collapse of the solution. Such surfaces are constructed for non-viscous and viscous flow. In the case of viscous flow, laminar and turbulent regimes are considered.

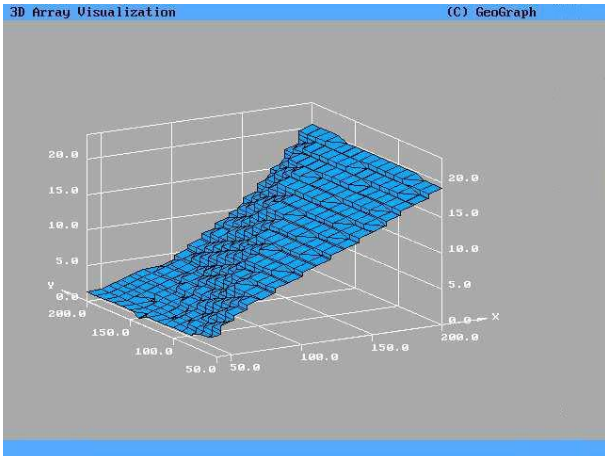

Fig. 4. Limiting surface for inviscid case.

From the point of view of accuracy assessment, the application of this approach allows us to deal with valuable objective functionals constructed for a multidimensional data volume, rather than with gas-dynamic fields. The construction of such a functional as a function of several variables (defining the parameters of the problem) in some cases gives the possibility of representing the function in an analytical form. This will be the solution that interests us for a class of problems, a certain set of external parameters and ranges of changes of these parameters. If inside the multidimensional volume of defining parameters there are some points for which there are experimental data, then we can calculate the average deviation for the resulting objective functional and consider from this point of view the suitability of the constructed functional for practical use.

It should be noted that you need to stay within the framework of the model used. As a rule, there are no clear boundaries of applicable models, there are transition zones. The amendment to these zones requires additional uncertainty in terms of the applicability of the selected model.

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3 Conclusion

Evaluation of the accuracy of mathematical modeling problems solutions in CFD is important and relevant. This importance especially increases when it is necessary to carry out calculations in the absence of experimental data for comparison or a reference solution. Three approaches that may be useful in this situation are presented - the multi-model approach, the use of an ensemble of solutions and the construction of a generalized computational experiment. All these approaches are not universal and have their drawbacks, but for different classes of tasks they can be used to complement each other.

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