Generalized computational experiment in the problems of numerical methods verification

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This work is devoted to the application of a generalized computational experiment for a comparative assessment of numerical methods accuracy. The construction of a generalized computational experiment is based on the simultaneous solution using parallel computations in a multitasking mode of a basic problem with different input parameters, obtaining results in the form of multidimensional data volumes and their visual analysis. This approach can be effective in problems of verification of numerical methods. A comparative assessment of the accuracy for solvers of the open software package OpenFOAM is carried out. The classic inviscid problem of oblique shock wave is used as a basic task. Variations of the key parameters of the problem — the Mach number and angle of attack — are considered. An example of constructing error surfaces is given when the solvers of the OpenFOAM software package are compared. The concept of an error index is introduced as an integral characteristic of deviations from the exact solution for each solver in the class of problems under consideration. The surfaces of deviations from the exact solution in the L2 norm, constructed for each solver, together with the calculated error indices, make it possible to obtain a complete picture of the accuracy of the solvers under consideration for the class of problems defined by the ranges of variation of the Mach number and angle of attack.

Keywords: *generalized computational experiment, numerical methods, verification problems, error index*

1. Introduction

The tasks of numerical methods verification have always been of paramount importance throughout the history of the development of computational mathematics. Today, verification problems are of particular importance in the problems of computational gas dynamics. In mathematical modeling of practical problems in aerodynamics, the researcher must be sure of the accuracy of the numerical method used.

A comparative assessment of numerical methods accuracy is of particular importance at present. This is due to the wide distribution of software packages, both open and commercial, allowing to solve a wide range of problems. As a rule, a large number of numerical methods implemented in various solvers are integrated into such packages. When solving practical problems, it is not easy for the user to choose the most suitable solver for the studied class of problems.

The relevance of verification tasks is confirmed by the introduction in 2018 of the Federal Standard for the numerical simulation of supersonic inviscid gas flows and software verification [1]. Similar foreign standards have been around for quite some time [2,3]. Such standards will determine the direction of research in this area over the next decade. However, all these methodological documents are focused on verification in relation to a specific task with fixed values of key parameters.

At the present stage, researchers need more comprehensive estimates of the accuracy of numerical methods. For example, in assessing accuracy, not for a single task, but for a class of tasks. By a class of tasks is meant a basic task considered in the ranges of change in the set of key parameters. Such parameters in computational aerodynamics can serve characteristic numbers that determine flow velocity, viscosity, thermophysical properties of the medium, geometric parameters, etc. An opportunity of getting solution for a class of problems is provided by the construction of a generalized computational experiment.

The concept, basic methods and approaches of a generalized computational experiment, as well as a number of software tools for its implementation were developed in Keldysh Institute of Applied Mathematics RAS. The main aspects of constructing a generalized computational experiment and examples of its implementation are described in detail in [4–11].

This work is devoted to the application of a generalized computational experiment for a comparative assessment of numerical methods accuracy.

2. Generalized computational experiment

The emergence of the concept of a generalized computing experiment is associated with the development of high-performance computing clusters and parallel technologies. In problems of computational aerodynamics, parallel technologies usually provide the ability to quickly calculate on detailed grids. However, parallel technologies provide us with another important opportunity. This is the ability to simultaneously calculate on different nodes the same task with different input data. As a rule, such a calculation is performed in multitasking mode.

This opens up the possibility of implementing a generalized computational experiment. The key parameters of the problem under consideration are divided in certain ranges with a certain step, forming a grid partition of a multidimensional box in a multidimensional space of key parameters. The basic problem is solved using parallel technologies at each point of the grid partition. The obtained results represent multidimensional data volumes. Processing, analysis and visual presentation of this data is carried out using methods of visual analytics and scientific visualization. This computing technology is the most general description of a generalized computing experiment.

Obviously, such a concept can be applied to a wide range of tasks. This range includes parametric studies, optimization problems. A generalized computational experiment is an effective tool for solving inverse problems.

A large number of different applications of a generalized computational experiment are described in detail in [4-14]. The concept of a generalized computational experiment was applied to a wide range of both model and practical problems.

These tasks include the analysis of the interaction of a viscous supersonic flow with a jet barrier, the flows in the wake of the body, the problems of the interaction of jets, the problem of flowing around a cone at an angle of attack, the problem of oblique shock waves, and many others. The approach to constructing a generalized computational experiment was applied to the problem of finding the optimal three-dimensional shape of the blades assembly for a power plant in terms of power loads.

Also, this approach was applied to the problems of verification of numerical methods. A comprehensive comparative analysis of a number of solvers of the OpenFOAM open software package [15] was carried out in [12–14, 20, 21]. As basic tasks, we used problems that have a reference solution (exact solution or experimental data). These tasks include the problem of a supersonic inviscid flow around a cone at an angle of attack and the problem of an oblique shock wave formation. In both cases, a class of problems was considered, formed by key parameters variations of the problem in question.

3. The problems of numerical methods verification

As already mentioned above, verification problems have been an important section throughout the history of the development of computational mathematics and mathematical modeling. As a rule, a comparison of the numerical results was carried out with some reference solution, in the role of which the exact solution was used if available or the available experimental data.

If there is a reference solution, the accuracy of the numerical method can be estimated for the solution element or for the entire calculation domain. For example, for problems containing discontinuities (shock waves), previously, the width of the "smearing" of the solution at discontinuity was traditionally considered as a characteristic of the numerical method accuracy. In this case, a comparison with the reference solution over the entire flow field was also applied. For an objective assessment of numerical method accuracy, it seems appropriate and reliable to apply both approaches. In the presence of a reference solution, the construction of a generalized computational experiment allows us to compare not only for one problem with fixed key parameters, but also for problems in the entire field of variation of key parameters.

If the class of problems is determined by two key parameters, then for each numerical method involved in the comparison, the dependence of the error on these parameters is constructed in the form of an error surface. In the case of three key parameters, scientific visualization methods are used to analyze a three-dimensional figure representing the dependence of the error on key parameters. In the case when the number of key parameters is more than three, then methods of visual analytics should be used to analyze the results. In some cases, approaches to lowering the dimension of the multidimensional space of key parameters under consideration are useful.

A separate problem is the estimation of the accuracy of numerical methods in the absence of a reference solution. Here, to assess the accuracy, foreign standards recommend to apply Richardson method [2,3]. However, for practical problems of computational aerodynamics this is very difficult due to the enormous computational costs. The computational costs are due to the fact that the implementation of Richardson method requires multiple calculations with a decrease in the step of the spatial grid decomposition. One of the alternatives in this case is the estimation of accuracy on the ensemble of solutions. The ensemble of solutions obtained by various numerical methods on the same grid allows us to estimate the location of the exact solution and to divide the obtained numerical solutions into clusters of different levels of accuracy. This direction is being actively developed at present and is presented in [16-19]. A natural drawback of this approach is the need for researcher to have at his disposal a certain number of solvers that implement numerical methods with different computational properties.

4. The example of verification problem

This section provides an example of constructing a generalized computational experiment for a comparative assessment of numerical methods accuracy. As an example, we use the numerical results described in detail in the authors' works [20,21]. In these papers, a class of computational gas dynamics problems is considered that describe the incidence of an inviscid supersonic gas flow onto a flat plate at an angle of attack.

With such an incidence, an oblique shock wave is formed. The Mach number and angle of attack are used as key parameters. These values vary in certain ranges. This problem has an exact solution. With the exact solution, a comparison is made at each point of the calculation domain, and for each combination of key parameters, an error is evaluated in the norm of L1 and L2. The results obtained make it possible to construct an error surface as an error function of two key parameters of the problem.

Carrying out similar calculations for several numerical methods implemented in the solvers of the open software package OpenFOAM, makes it possible to build several such surfaces on one drawing. This opens up the possibility of a deep and clear comparative analysis of the accuracy of the studied numerical methods. The construction of such a generalized computational experiment involves the creation of computational technology from solving a direct problem up to visual analysis of the results. One of the most expressive and visual forms of visualization is the construction of stereo animations of the results of numerical studies. A similar construction of stereo images for this task was carried out and described in [22].

Fig. 1 presents the results of constructing error surfaces for four OpenFOAM solvers with variations in the Mach number from 2 to 4 and variations in the angle of attack from 6 to 20 degrees [21]. It should be noted that error surfaces for the class of problems for the comparative analysis of the accuracy of numerical methods were constructed in [21] for the first time. Four error surfaces for OpenFOAM solvers are presented - rhoCentralFoam (rCF), pisoCentralFoam (pCF), sonicFoam (sF) and QGDFoam (QGDF).

These surfaces allow a thorough visual comparison of deviations from the exact solution in the class of problems under consideration. It can be seen that all 4 surfaces behave in a very similar way. The deviation from the exact solution increases with the growth of key parameters - the angle of attack and the Mach number. Fig. 1 also shows that the best accuracy in the class of problems is provided by the rCF and pCF solvers, for which the error surfaces almost coincide.

Thus, the construction of a generalized computational experiment allows us to conduct a full-fledged comparative accuracy assessment for four solvers of the OpenFOAM software package in the class of problems. The class of tasks in this particular case is determined by the basic task (oblique shock wave) and the ranges of variation of the key parameters of the problem - the Mach number and angle of attack.

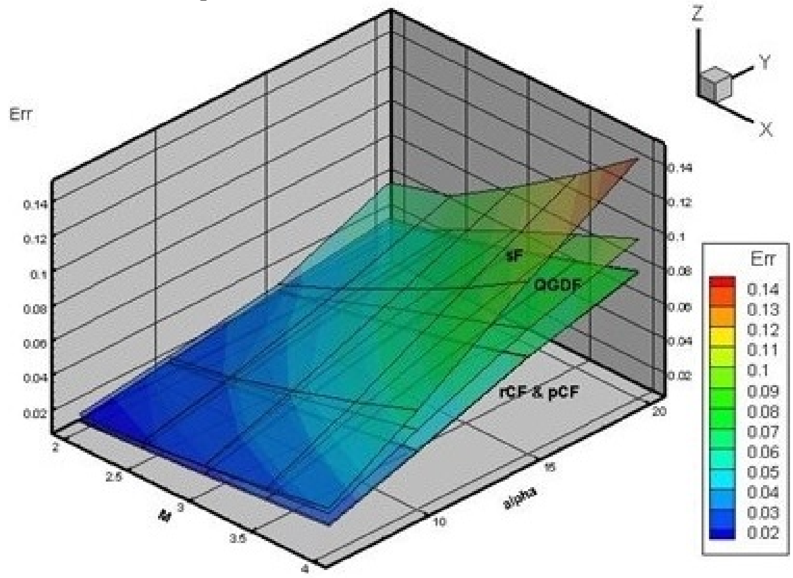

Fig. 1. Image of the surface deviation from the exact solution for 4 OpenFOAM solvers with variation of the Mach number and angle of attack for the oblique shock wave [21]

The image of error surfaces presented in Figure 1 gives a fairly clear idea of the comparative accuracy of OpenFOAM solvers in the class of problems. However, for a more complete assessment, an integral characteristic for each surface can be introduced.

We call this characteristic the Error Index (EI).

The error index is defined as follows. Let $i = 1, M$ and $j = 1, N$ be the grid partitions of key parameters, and A_{ij} - the deviation from the exact solution at each point of the grid partition. Then the error index is defined as:

$$EI = \sum_{ij} A_{ij}/(M * N).$$

Then the error index values for the surfaces shown in Fig. 1 can be calculated and written in the form of table 1.

Table 1. Error Index Values for 4 OpenFOAM Solvers

Solver	rCF	pCF	QGDFOAM	sF
Error Index	0.037734	0.038751	0.0453406	0.058216

Table 1 shows that the values of the error index EI completely correspond to the relative positions of the surfaces in Figure 1. Therefore, the calculated error index can serve as a characteristic of the accuracy of numerical methods in the selected class of problems.

5. Conclusion

The application of a generalized computational experiment to the problems of comparative estimation of the accuracy of numerical methods is considered. An example of constructing a generalized computational experiment for a class of problems is described. The class of tasks is formed on the basis of the basic problem (the oblique shock wave) and variations of the determining parameters of the problem - the Mach number and angle of attack. An example of constructing error surfaces is given. The concept of a numerical method error index for a class of problems is introduced.

The construction of a generalized computational experiment can serve as an effective tool for verification problems.

Acknowledgments

This work was supported by RFBR grants 19-01-00402 and 20-01-00358.

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