Visualization of the Influence of Changes in the Controlled Dissipative Properties on the Accuracy of the QGDFoam Solver

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Abstract

This work is devoted to the study of the influence of variation of the controlled dissipative properties on the accuracy of the QGDFoam solver and the visual representation of this influence. The work continues a series of studies on the comparative assessment of the accuracy of various numerical methods and solvers built on their basis. To carry out a comparative assessment, a generalized computational experiment for classes of problems with a reference solution is constructed and implemented. A generalized computational experiment based on the synthesis of solutions of mathematical modeling problems, parallel technologies and visual analysis tools makes it possible to obtain solutions not only for individual problems, but for whole classes of problems determined by the specified ranges of key parameters. Accordingly, a comparative assessment of the accuracy of numerical methods is also carried out for a class of problems. Earlier, a similar computational experiment was carried out for a comparative assessment of the accuracy for solvers of the OpenFOAM open source software package on the well-known classical problem of an oblique shock wave formation. One of the solvers participating in the calculations, namely the QGDFoam solver, was the only one of all to have controlled dissipative properties. New generalized computational experiment was implemented to study the effect of variation of the parameter that controls the dissipative properties. The target was to reduce the error in comparison with the reference solution. The research results are presented in this work.

Keywords

Generalized computational experiment, visualization, QGDFoam solver, comparative assessment of the accuracy

1. Introduction

This work develops an approach to constructing a generalized computational experiment for comparative analysis of the accuracy of numerical methods and solvers implemented on their basis. The work continues a series of studies devoted to the comparative assessment of the accuracy for solvers of the open source software package OpenFOAM [1,2]. These studies are described in detail in [3-8].

The general essence of the research carried out can be described as follows. Problems are selected that have a reference solution in certain ranges of key parameters. The region of the key parameter space is meshed. At each point of the grid partition, the problem under consideration is solved using several solvers and compared with the exact solution. The target functional here is the error of each solver - a deviation from the reference solution. The data obtained are investigated using visual analysis and give a sufficient idea of the comparative accuracy of the considered solvers in a specific class of problems [3-8].

Previously, a similar study was carried out for 4 solvers of the OpenFOAM open source software package for the problem of oblique shock wave formation. A shock wave was formed when a supersonic flow fell on a plate at an angle of attack. Results have been obtained that allow a comparative assessment of the accuracy [6, 7]. However, one solver from the comparison, namely the QGDFoam solver, has

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unique properties. This solver has a parameter that allows one to control the dissipative properties of the implemented numerical method, that is, to regulate the artificial viscosity. Therefore, we had an idea to investigate the issue of improving the accuracy of this solver by varying this parameter. These studies are summarized in this paper.

2. Background – previous studies

This work is based primarily on the use of a generalized computational experiment. A generalized computational experiment is a computational technology based on the synthesis of solutions to problems of mathematical modeling, parallel technologies and visual analysis tools. This technology makes it possible to obtain solutions not only for individual problems, but for entire classes of problems, determined by the specified ranges of changes in key parameters. As a rule, the purpose of constructing a generalized computational experiment is to study the dependence of a certain target functional on changes in the defining parameters of the problem under consideration. The result of such an experiment is multidimensional data, the study of which requires the use of visualization and visual analytics methods.

This work continues the research cycle. Previous papers contain a description of the main approaches to the construction of a generalized computational experiment and the visualization problems arising in this case. Papers [3-5, 8] consider the problem of comparative assessment of the accuracy of OpenFOAM solvers when considering an inviscid flow around a cone at an angle of attack. Three defining parameters vary here - the Mach number, the cone half-angle and the angle of attack. Papers [6, 7] use a similar approach for the problem of the formation of an oblique shock wave when a supersonic flow falls on a plate. Here, the variable parameters are the Mach number and the flow deflection angle. It was this task that became the basis for the research presented in this work.

3. QGDFoam solver and control of dissipative properties

The system of quasi-gas dynamic (QGD) equations was created in the eighties by a group of scientists from the Keldysh Institute of Applied Mathematics under the leadership of B.N. Chetverushkin [9, 10]. Later, quasi-gas dynamic equations were presented in the form of conservation laws, investigated in detail, and theoretically substantiated [11-15]. Monographs dedicated to the derivation of the equations and their applications to numerical modeling problems were also written [16, 17]. A fundamental and essential difference of the QGD approach from the Navier-Stokes theory was the use of a space-time averaging procedure to determine the basic gasdynamic quantities. Thus, additional terms appear. More precisely, the mass flux density vector, the viscous stress tensor and the heat flux vector are represented as a sum of the corresponding quantities in the Navier-Stokes form and small additions of a significantly nonlinear form, proportional to a small parameter having the time dimension.

Many calculations have been carried out based on the QGD system of gas dynamics equations. However, all of them were performed using individual programs. In order to extend the application of the QGD approach to a wider range of problems, the OpenFOAM solver [18-20] was developed under the guidance of T.G. Elizarova at the Keldysh Institute of Applied Mathematics of the Russian Academy of Sciences.

One of the most important properties of this approach is the possibility to control the dissipative properties. In the framework of the Euler equations the dissipative coefficient can be written out as:

$$\tau = \alpha \frac{h_x}{c_x}, \tag{1}$$

where α is a dimensionless parameter, h_x is the spatial grid step, c_s is the sound speed. The presence of a controllable parameter with dissipative terms allows one to successfully suppress undesirable oscillations in numerical simulations of problems with discontinuities.

4. QGDFoam solver and control of dissipative properties

During numerical experiments, the problem formulation fully corresponded to that described in [6, 7]. We considered a two-dimensional problem of oblique shock wave formation. A supersonic flow of inviscid gas falls on a half-plate at the angle of attack. An oblique shock wave is formed at the end of the plate. The problem was considered with a variation of the defining parameters, where the Mach number varied from 2 to 4 in 0.5 step, and the angle of attack varied from 6° to 20°. The deviation from the known exact solution in different norms, L_1 and L_2, was calculated. Using the obtained data, the error surfaces were plotted for all solvers involved in the calculations.

In the past studies [6, 7] the parameter α was taken equal to 0.1 for the solver QGDFoam. But we need to find the optimal values of this parameter to minimize the error in the norms L_1 and L_2. Taking into account that a single uniform grid is used for all calculations, we have to solve the inverse problem. We need to find such a value of the parameter α at which the value of the error is minimal in both norms. Then the problem of finding such values can be formulated as follows:

$$\text{Argmin } Err_{L1}(\alpha)\,,\ \ Err_{L1}(\alpha) = \frac{\sum_m |y_m(\alpha) - y_m^{exact}|}{\sum_m |y_m^{exact}|} \quad \text{for norm L1} \tag{2}$$

$$\text{Argmin } Err_{L2}(\alpha)\,,\ \ Err_{L2}(\alpha) = \frac{\sqrt{\sum_m (y_m(\alpha) - y_m^{exact})^2}}{\sqrt{\sum_m (y_m^{exact})^2}} \quad \text{for norm L2} \tag{3}$$

The search for optimal values of α was carried out for fixed values of the defining parameters M=2, β=6°. This variant was chosen as a basic one in [6, 7]. To begin with, the minimum possible value of the parameter was found, at which the solver worked. For this problem the value was α=0.031. Further a numerical calculation with variation of parameter α was carried out and an error for the pressure field in norms L_1 and L_2 was found. The minimum values of the norm are highlighted in bold. The results are presented in Table 1.

Table 1

Search results

	α=0.2	α=0.125	α=0.1075	α=0.1	α=0.031
L_1	0.002406	**0.002178**	0.002211	0.002245	0.004427
L_2	0.015647	0.014443	**0.014373**	0.014393	0.019517

The values of the parameter α that provide the minimum error in the norms L_1 and L_2 were found. These values differ from the previously used value α = 0.1. For norm L_1 the optimal value is α = 0.125, for norm L_2 – α = 0.1075. It was decided to carry out a generalized computational experiment for each norm separately with a fixed value of α at variations in Mach number and angle of attack. It would be natural to solve such an inverse problem for each point of the grid partitioning of the area of the defining parameter space, but this is too computationally expensive. Numerical solutions with parameter α computed from the point for the base case should provide insight into the effect of variation in parameter α on the accuracy of the solver under consideration. The results are presented in Tables 2-11.

Table 2

M=2, norm L_1

β	rCF	pCF	sF	QGDF, 0.1	QGDF, 0.125
6	**0.001755**	0.001902	0.003182	0.002245	0.002178
10	**0.002505**	0.002834	0.004005	0.003228	0.003019
15	**0.003510**	0.004154	0.005226	0.004155	0.003833
20	0.004572	0.005442	0.007977	0.004483	**0.004143**

Table 3

M=2.5, norm L_1

β	rCF	pCF	sF	QGDF, 0.1	QGDF, 0.125
6	**0.001907**	0.002176	0.003258	0.003065	0.002843
10	**0.002977**	0.003354	0.004888	0.004827	0.004338
15	**0.004239**	0.004820	0.007497	0.006846	0.006061
20	**0.005526**	0.006390	0.010739	0.008477	0.007468

Table 4

M=3, norm L_1

β	rCF	pCF	sF	QGDF, 0.1	QGDF, 0.125
6	**0.002172**	0.002473	0.003823	0.003762	0.003459
10	**0.003491**	0.003906	0.006385	0.006165	0.005487
15	**0.005160**	0.005800	0.010299	0.009171	0.008049
20	**0.006916**	0.007866	0.014886	0.011836	0.010334

Table 5

M=3.5, norm L_1

β	rCF	pCF	sF	QGDF, 0.1	QGDF, 0.125
6	**0.002454**	0.002801	0.004542	0.004321	0.003956
10	**0.004096**	0.004542	0.008074	0.007368	0.006546
15	**0.006302**	0.006842	0.013586	0.011245	0.009859
20	**0.008689**	0.009521	0.019913	0.014933	0.013034

Table 6

M=4, norm L_1

β	rCF	pCF	sF	QGDF, 0.1	QGDF, 0.125
6	**0.002764**	0.003063	0.005408	0.004905	0.004488
10	**0.004709**	0.005101	0.009991	0.008538	0.007593
15	**0.007639**	0.007975	0.017449	0.013293	0.011671
20	**0.010738**	0.011271	0.025992	0.018022	0.015756

Table 7

M=2, norm L_2

β	rCF	pCF	sF	QGDF, 0.1	QGDF, 0.125
6	**0.013287**	0.013744	0.017505	0.014393	0.014373
10	**0.020839**	0.021740	0.024742	0.021850	0.021718
15	0.029893	0.031227	0.034439	0.028868	**0.028660**
20	0.036691	0.038737	0.055141	0.032726	**0.032514**

Table 8

M=2.5, norm L_2

β	rCF	pCF	sF	QGDF, 0.1	QGDF, 0.125
6	**0.015357**	0.016346	0.019139	0.018502	0.018304
10	**0.025023**	0.026259	0.030647	0.029376	0.028918
15	**0.036192**	0.037452	0.049236	0.042189	0.041430
20	**0.045692**	0.047210	0.070880	0.051230	0.050282

Table 9

M=3, norm L_2

β	rCF	pCF	sF	QGDF, 0.1	QGDF, 0.125
6	**0.017717**	0.018736	0.023005	0.022639	0.022320
10	**0.029721**	0.030812	0.040618	0.037448	0.036733
15	**0.043788**	0.045160	0.066691	0.055111	0.053956
20	**0.055751**	0.057216	0.093369	0.068286	0.066812

Table 10

M=4, norm L_2

β	rCF	pCF	sF	QGDF, 0.1	QGDF, 0.125
6	**0.020624**	0.021802	0.027651	0.026308	0.025902
10	**0.034941**	0.036279	0.051637	0.045070	0.044138
15	**0.052408**	0.053305	0.085221	0.067027	0.065553
20	**0.067864**	0.068658	0.118186	0.083747	0.081846

Table 11

M=4, norm L_2

β	rCF	pCF	sF	QGDF, 0.1	QGDF, 0.125
6	**0.023404**	0.024647	0.033670	0.030672	0.030168
10	**0.040436**	0.041336	0.064471	0.053262	0.052127
15	**0.062858**	0.063287	0.106589	0.079213	0.077403
20	0.080578	**0.079388**	0.145689	0.098895	0.096634

It should be noted that during the calculations the authors were interested in the high error that appeared at Mach number $M = 2$ and angle $\beta = 20°$ for the solvers rhoCentralFoam and pisoCentralFoam in norm L_1. A similar phenomenon was observed in the calculations at the same Mach number and angles β = 15°, 20° for the L_2 norm. When solving these solvers numerically, oscillations perpendicular to the shock wave front appear (Figure 1). The QGDFoam solver has a parameter that affects the numerical dissipation and, with the optimal values of the parameter used, the oscillations are not visually distinguishable (Figure 2). This is serious evidence of the advantages of the QGDFoam solver, which has the ability to limit undesirable oscillations due to the presence of controlled dissipative properties.

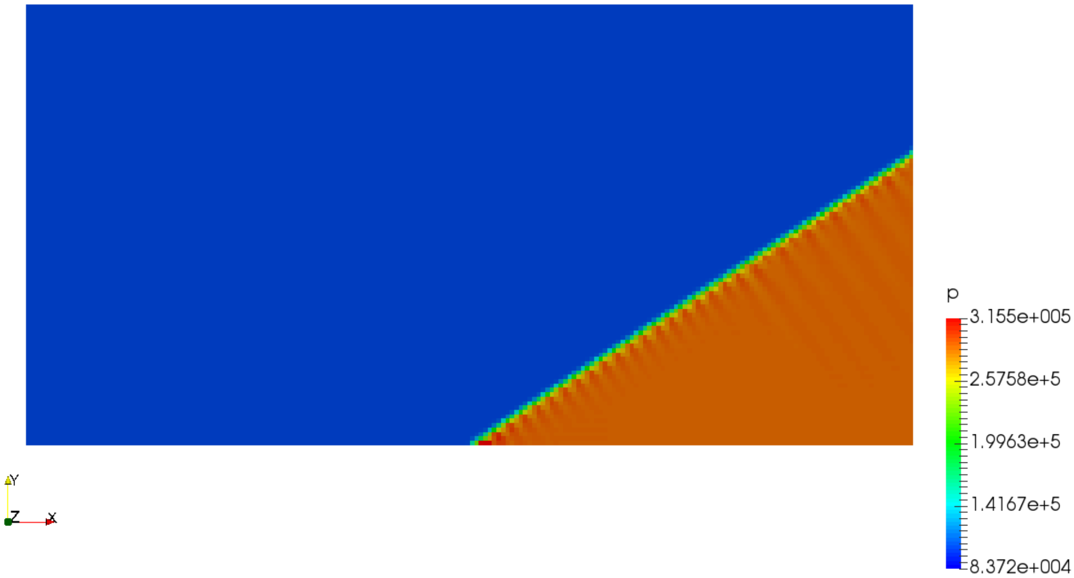

Figure 1: Pressure for pisoCentralFoam

Figure 2: Pressure for QGDFoam

5. Results of numerical experiments

During numerical experiments, the problem formulation fully corresponded to that described in [6, 7]. We considered a two-dimensional problem of oblique shock wave formation. A supersonic flow of inviscid gas falls on a half-plate at the angle of attack. An oblique shock wave is formed at the end of the plate. The problem was considered with a variation of the defining parameters, where the Mach number was varied from 2 to 4 in 0.5 step, and the angle of attack was varied from 6° to 20°. The deviation from the known exact solution in different norms, L_1 and L_2, was calculated. Based on the data obtained, error surfaces were plotted for all solvers involved in the calculations.

Figure 3 shows the error surfaces in the L_2 norm for all four solvers that took part in the comparison. The calculations for the QGDFoam solver were performed with a single chosen value of $\alpha = 0.1$.

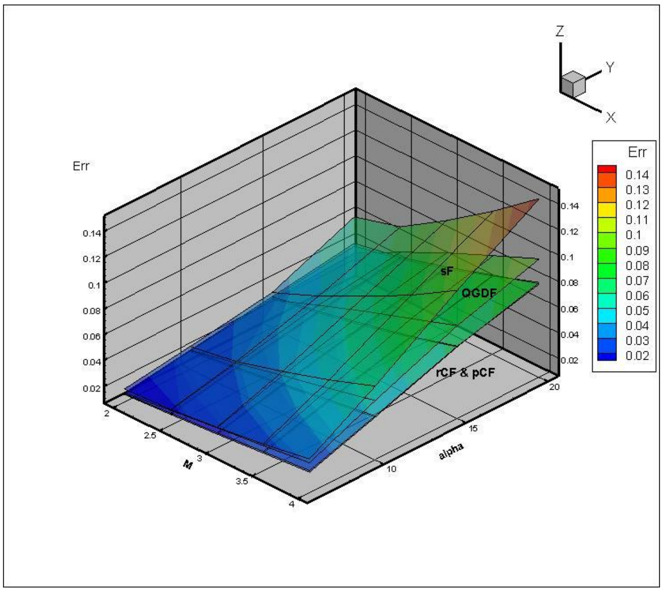

Figure 3: Error surfaces for the four solvers [7]

The Figure 4 shows the results for the same solvers in the L_1 norm, but added surface, denoted as QGDF*, calculated at α = 0.125. It can be seen that the variation of the parameter α reduced the error. The surface QGDF* lies substantially below the surface QGDF.

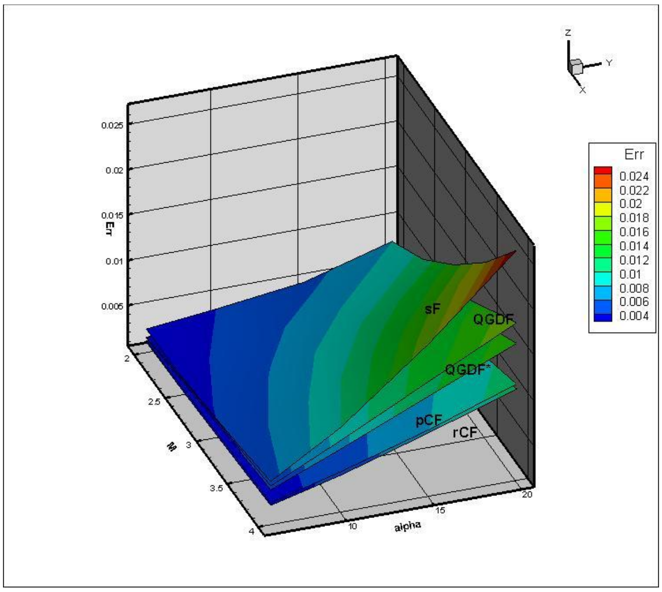

Figure 4: Error surfaces for the four solvers and the error surface for the solver QGDFoam at α = 0.1075 (QGDF*) in the L_2 norm

The following Figure 5 presents in the L_1 surface norm for the solver QGDFoam when choosing α = 0.1 (QGDF) and α = 0.125 (QGDF*).

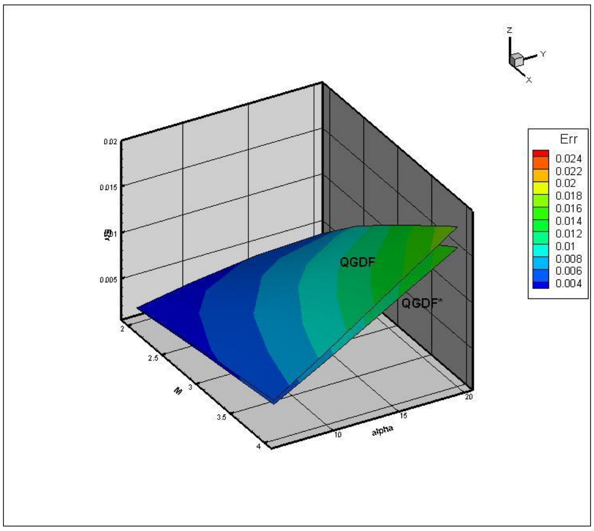

Figure 5: Error surfaces in the L1 norm for the QGDFoam solver when choosing α = 0.1 (QGDF) and α = 0.125 (QGDF*)

The figure shows a significant reduction in the error when the previously found value of the parameter α = 0.125 is chosen. The maximum error reduction is 12.6% with respect to the values obtained by choosing α = 0.1.

Next, we consider similar results for the norm L_2. Here, to plot the surface corresponding to the error for the QGDFoam solver, the parameter α = 0.1075 was chosen according to Table 1. Figure 6 shows the results for the solvers rhoCentralFoam, pisoCentralFoam, sonicFoam, and QGDFoam when α = 0.1 (QGDF) and α = 0.125 (QGDF*) were chosen.

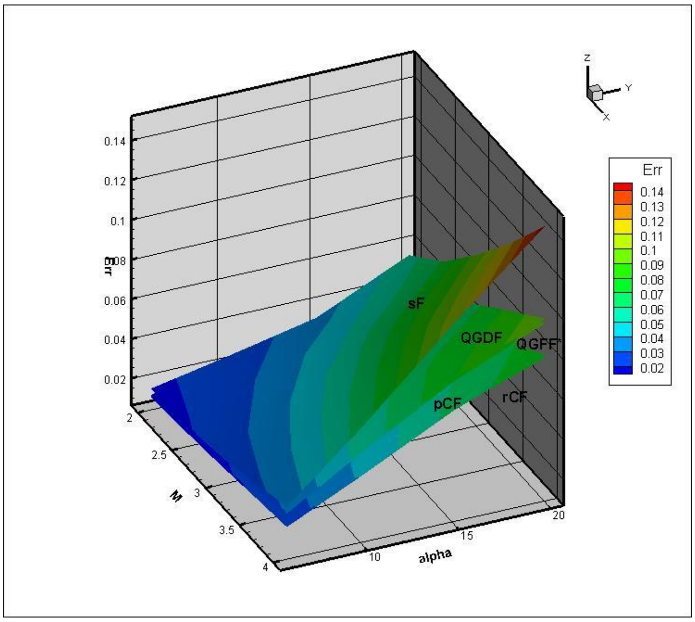

Figure 6: Error surfaces for the four solvers and the error surface for the solver QGDFoam at α = 0.1075 (QGDF*) in the L_2 norm

The overall picture is about the same as in Figure 4. However, for the norm L_2 the error reduction is significantly smaller. The maximum error reduction here is 2.3% with respect to the values obtained by choosing α = 0.1. The following Figure 7 presents in the L_2 norm a close-up of the error surface for the QGDFoam solver when α = 0.1 (QGDF) and α = 0.1075 (QGDF*) are chosen.

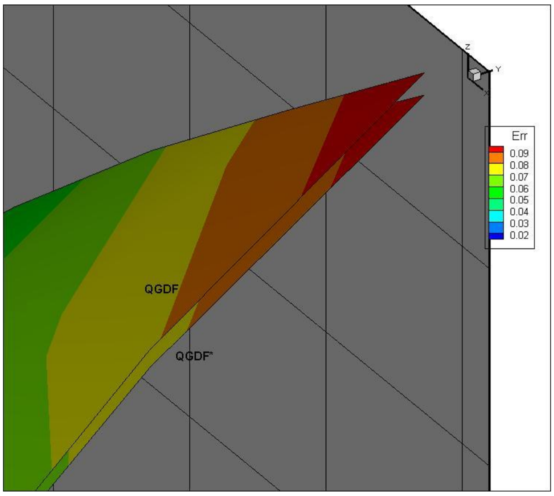

Figure 7: Error surfaces in the L_2 norm for the QGDFoam solver when choosing $\alpha = 0.1$ (QGDF) and $\alpha = 0.1075$ (QGDF*)

Thus, the implemented generalized computational experiment allows us to assert that variations of the parameter regulating the dissipative properties of the QGDFoam solver can significantly reduce the error in comparison with the reference solution and increase the accuracy of calculations. This should be considered as a clear advantage of this solver and a great potential in its use for solving practical problems of mathematical modeling.

6. Conclusions

In this paper, we studied the effect of variation in controllable dissipative properties on the accuracy of the QGDFoam solver and a visual representation of this effect. This work continues a series of studies on the comparative evaluation of various numerical methods accuracy and solvers built on their basis. The study is based on the construction of a generalized computational experiment for a comparative analysis of the accuracy of numerical methods and solvers based on them. The realization of the generalized computational experiment has shown that variations of the parameter regulating dissipative properties of the solver QGDFoam can significantly reduce the error in comparison with the reference solution and increase the accuracy of calculations.

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