Processing and visualization of the results of parametric numerical calculations

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Abstract. In modern problems of mathematical modeling in computational gas dynamics, it is increasingly necessary to implement parametric studies. In these cases, the key factors of the problem under consideration vary with the chosen step within the given ranges. Calculations of this kind can be effectively carried out by constructing 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 a generalized computational experiment are multidimensional arrays, where the dimension of the arrays corresponds to the number of key factors. Processing and visual presentation of such arrays requires solving a number of separate tasks. The processing and visual presentation of the results are carried out for target functionals represented as a function of many variables. The report presents examples of solving specific processing and visualization problems based on the implemented generalized computational experiment for 3D cone in supersonic flow.

1. Introduction

Processing, visualization and analysis of multidimensional data is currently one of the most relevant areas of research. The need to analyze multidimensional data arises in almost all areas of human activity. It was to ensure the analysis of multidimensional data in the early 2000s that such a multidisciplinary direction of research as visual analytics emerged. The main ideas, approaches and methods of visual analytics are presented in the works [1–3]. Visual analytics combines a variety of methods and approaches that allow the processing, visualization and analysis of data regardless of their nature of origin. Visual analytics methods allow solving problems of classification and clustering of multidimensional data, highlighting key parameters, finding hidden dependencies between key parameters, etc.

Visual analytics techniques were commonly used as post-processing tools. However, now more and more often these methods are used as components of a unified computational technology. An example of such use is the construction of a generalized computational experiment in problems of mathematical modeling, namely, in the field of computational gas dynamics [4–7, 11–14]. The possibility of constructing a generalized computational experiment has appeared due to the development of parallel technologies and visual analytics tools.
2. Generalized numerical experiment and visualization problems

The theory, approaches and methods of constructing a generalized computational experiment are described in sufficient detail in the author's works [4–7, 12]. A generalized computational experiment is a computational technology for carrying out parametric numerical solutions to problems of mathematical physics using parallel technologies, obtaining results in the form of multidimensional data volumes together with the analysis and visualization of these volumes. In this case, the object of analysis can be not only the data obtained in the calculations, but also the target functionals calculated from these data.

Let us briefly consider the construction of a generalized computational experiment for problems of computational gas dynamics. Suppose we have a unified formulation of the problem, which includes a system of equations and a set of boundary conditions, and an algorithm for the numerical solution of this problem. This setting allows us to formulate the parametric problem as follows. Let's highlight a number of defining parameters. In gas dynamics, such parameters can be characteristic numbers arising when the system of equations is reduced to a dimensionless form, such as the Mach number, Reynolds number, Prandtl number, Froude number, etc. Also, the defining parameters can be the geometric characteristics of the problem chosen by the researcher. Let each of these parameters be varied within a certain range. Let us carry out a grid partition for each of these parameters and obtain a grid partition for a multidimensional volume in the parameter space, where the dimension of the volume corresponds to the number of defining parameters. At each node of the resulting mesh, it is necessary to carry out a numerical solution of the problem. Of course, from a computational point of view, this is very expensive. For example, considering a problem with six defining parameters and dividing the range of variation of each of them using 10 points, we come to the need to numerically solve one million problems. It's not easy, but this is where parallel computing comes in. Since we are solving the same problem with different input data, this solution can be carried out simultaneously using such parallel technologies as MPI [8] or DVMH [9, 10]. As a result of calculations, we obtain multidimensional data volumes that represent a numerical solution for a class of problems, where the class of problems is specified by a set of defining parameters and ranges of their variation. These volumes of data need to be visualized and analyzed. As a rule, the ultimate goal of analysis is to construct objective functionals as functions of many variables in an analytical form, similar to how it is done in physical experiments.

The visualization tasks arising in this case are described and classified in [12]. Let us dwell on the visualization of target functionals as functions of several variables, where the number of variables corresponds to the number of defining parameters. The most desirable for us is to reduce visualization to classic scientific visualization tools designed to visually represent two-dimensional and three-dimensional scalar and vector fields. Parallel or cross-section sets can be used to visualize a three-variable function. In the case of more than three variables, it is common to estimate the contribution to variance for each variable and cut off measurements with the smallest contribution. In any case, visualization is necessary for the subsequent construction of an approximating dependence for the target functional. For the case of using three variables, the use of parallel sections and cross sections often does not allow getting a full picture of the type of function. In these situations, it is more expedient to select the variable with the least contribution to the variance and implement the visualization as a group of two-dimensional surfaces.

An example of constructing a generalized computational experiment and visual presentation of the results for the problem of supersonic flow around a cone at an angle of attack is presented in the next section.

3. The example of solving a problem of flow around a cone and visualizing the results

To construct a generalized computational experiment, a three-dimensional problem of a supersonic inviscid gas flow around a cone at an angle of attack was chosen. The defining parameters here were the angle of attack \( \alpha \), the Mach number \( M \), and the half-angle \( \beta \) of the cone. The angle of attack varied from 0° to 10° with a step of 5°, the Mach number varied in the range from \( M = 3 \) to \( M = 7 \) with a step
of 1, and the half-opening angle of the cone varied in the range $\beta = 15^\circ - 30^\circ$ with a step of $5^\circ$. The flow scheme is shown in figure 1. The conditions of the incoming flow at the inlet are indicated by the subscript “$\infty$”. For the calculation, a system of Euler equations was used, supplemented by the equation of state for an ideal gas.

![Flow scheme](image)

**Figure 1.** Flow scheme.

The main goal of the generalized computational experiment was to carry out a comparative assessment of the accuracy of three solvers of the OpenFOAM open source software package. This problem has a reference solution presented in tabular form [19]. It was necessary to construct the error as a function of the determining parameters for each of the three solvers participating in the comparison.

For a comparative assessment of the accuracy, three solvers were selected from the OpenFOAM software package:

- **rhoCentralFoam (rCF)** – based on the central-upstream scheme, which is a combination of the central-difference and upstream schemes [15]. The original Kurganov-Tadmor scheme [16] is a central difference scheme based on the Lax-Friedrichs scheme. A characteristic feature of Godunov-type schemes is that calculating the flow through the lateral faces of a cell requires solving the Riemann problem on the decay of an arbitrary discontinuity. The schemes with a central difference calculate the required values at the next time step without solving the Riemann problem; they integrate according to the Riemann fan. Consequently, there is no need to search for the Riemann integral and expansion of the solution in terms of characteristics, thus methods of this type are less expensive from a computational point of view. However, the OpenFOAM software package uses the Kurganov-Noel-Petrov scheme [17], a central upstream scheme. The scheme is central, since it does not require the solution of the Riemann problem, and upstream, since the information taken against the flow rate is used to estimate the width of the Riemann fan. This more accurate estimate makes the schemes less dissipative than the original Kurganov-Tadmor scheme.

- **sonicFoam (sF)** – based on the PISO (Pressure Implicit with Splitting of Operator) algorithm [18]. The essence of splitting methods is to separate the influence of various terms on the change in momentum in the computational cell. Usually, the contribution of the pressure gradient is separated from the contribution of spatial transport and viscous terms.
• pisoCentralFoam – a hybrid method, is a combination of a central-upstream scheme with the PISO algorithm. This solver is not included in the standard set of solvers in the OpenFOAM software package. It was created by an independent team of developers at the Ivannikov Institute for System Programming RAS.

Each solver was used to solve the entire set of problems formed by the grid partitioning of each of the varied parameters. 60 problems were solved for each solver. Considering the change of the solver as an additional determining parameter, it can be argued that, in total, 180 problems were solved for this generalized computational experiment. Thus, a set of numerical solutions was obtained. The exact solution was obtained by interpolating the tabular solution from [19]. Then, for each solver, the solution error was found in the $L_1$ and $L_2$ norms.

The boundary conditions are presented in table 1. The initial conditions correspond to the boundary conditions at the inlet boundary. Pressures are presented in pascals. Temperatures are presented in degrees Kelvin.

| Boundary | P    | T    | U              |
|----------|------|------|----------------|
| inlet    | 101325 | 300  | 3–7 Mach       |
| outlet   | zeroGradient | zeroGradient | zeroGradient |
| top      | zeroGradient | zeroGradient | zeroGradient |
| bottom   | zeroGradient | zeroGradient | zeroGradient |
| cone     | zeroGradient | zeroGradient | slip          |
| front    | zeroGradient | zeroGradient | zeroGradient |
| back     | zeroGradient | zeroGradient | zeroGradient |

In order to get an idea of the behavior of the error $\text{Err}$ as a function of the angle of attack $\alpha$, the half-opening angle $\beta$, and the Mach number $M$, we first estimate the contribution of three variables to the variance. At fixed values of the half-opening angle $\beta$ and the Mach number $M$, the smallest spread is provided by the variation in the angle of attack $\alpha$. Let us represent the function $\text{Err}$ in the form $\text{Err}(\alpha, \beta, M)$ at a fixed angle of attack $\alpha = 0^\circ$. Thus, we get an idea of the form of the surface $\text{Err}(0^\circ, \beta, M)$. Figure 2 shows the surface representing the dependence of the error on $M$ and $\beta$ at $\alpha = 0^\circ$ for the rhoCentralFoam solver.

Now let us present in a similar form the results of calculations for the rhoCentralFoam solver in the form of a group of surfaces, that is, in the form of three surfaces with the values of the angle of attack $\alpha = 0^\circ$, $5^\circ$, $10^\circ$. Figure 3 allows you to see three similar surfaces lying close to each other. As the angle $\alpha$ increases, the error increases.

Similar groups of surfaces are shown in figures 4 and 5 for the pisoCentralFoam and sonicFoam solvers, respectively, at the values of the angle of attack $\alpha = 0^\circ$, $5^\circ$, $10^\circ$. As for the rhoCentralFoam solver, the error increases with increasing angle $\alpha$. Figures 3, 4, 5 give a complete picture of the behavior of the error with the variation of the determining parameters for all solvers participating in the comparative assessment of the accuracy.

For greater clarity, we present one more figure. Figure 6 shows the dependencies of the error on $M$ and $\beta$ for the rhoCentralFoam, pisoCentralFoam, sonicFoam solvers at a fixed value of $\alpha = 10^\circ$. It can be seen that the error surfaces for the rhoCentralFoam and pisoCentralFoam solvers practically coincide. This is expected, since the pisoCentralFoam solver is a modification of the rhoCentralFoam solver. The sonicFoam solver provides the worst accuracy in the considered class of problems.
Summing up, it can be argued that the construction of a generalized computational experiment made it possible to obtain a full understanding of the comparative accuracy of three solvers of the OpenFOAM software package using the example of the problem of supersonic flow around a cone at an angle of attack. The problem was considered with the variation of three defining parameters - the angle of attack, the cone half-opening angle, and the Mach number.

It should be noted that for the results obtained, presented in the form of groups of surfaces, it is possible to construct sufficiently accurate analytical approximating formulas in the form of second-order polynomials. However, such a construction is a separate task.
4. Conclusions

The paper discusses the processing and analysis of multidimensional data that are the results of the implementation 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. A visual representation of the target functional is considered for an example of solving the problem of comparative assessment of the accuracy of three solvers of the OpenFOAM software package. The basic problem for the comparative assessment of accuracy is the problem of supersonic flow around a cone at an angle of attack, which was considered by varying three defining parameters - the angle of attack, the angle of half-opening of the cone, and the Mach number.

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