

On visualization problems in a generalized computational experiment

A.E. Bondarev

Keldysh Institute of Applied Mathematics RAS

ORCID: 0000-0003-3681-5212, bond@keldysh.ru

Abstract

Modern development of computing systems and technologies allows to organize the construction of a generalized computational experiment in modeling problems of computational gas dynamics. The construction of such an experiment is based on numerical parametric studies and the solution of optimization analysis problems. Solving such problems implies a multiple solution to the direct problem of numerical simulation of a gas-dynamic process with different input data, where different sets of defining parameters are used as input data. The defining parameters of a class of problems, such as Mach number, Reynolds number, geometric parameters, etc., vary in certain ranges with a certain partitioning step. As a result, the resulting solution is a multidimensional volume of data. To analyze this volume, visualization is necessary. The paper attempts to systematize and briefly describe some types of visualization problems arising from processing the results of a generalized computational experiment. The aim of the work is to begin a broad discussion of the tasks of visualization and methods for their solution in a generalized computational experiment.

Keywords: generalized computational experiment, CFD, multidimensional data, visualization, visual analysis.

1. Introduction

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.

However, the discrete solution itself cannot provide an understanding of the results obtained. It requires a wide and creative use of the tools of scientific visualization [1,3] and visual analytics [8–12]. 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. On the one hand, the task becomes much more complicated, but on the other hand, in the future there is the possibility of obtaining a solution for a class of prob-

lems. Many articles have been devoted to the development of scientific visualization tools, including [1,3]. Various aspects of constructing a generalized computational experiment are considered in sufficient detail in [2, 4–6, 14]. The development of procedures for analyzing the results of a generalized computational experiment, presented in the form of a multidimensional data volume, is considered in [7, 13, 15]. This article is intended to systematize the tasks of visualization arising from the implementation of a generalized computational experiment, and begin a broad discussion of such problems and methods for their solution.

2. Generalized computational experiment

A formal description of a generalized computational experiment is given in sufficient detail in [2, 4–6, 14]. We give below a brief formal description, following [14]. According to [14], a generalized computational experiment involves the splitting of each of the determining parameters of the problem within a certain range. Thus, a grid partition is formed for a multidimensional parallelepiped composed of the determining parameters of the gas dynamics problem under consideration. For each point of this grid in the space of defining parameters, the problem is calculated. Formally, this can be written as follows.

Suppose that there is a reliable numerical method for solving two-dimensional and three-dimensional non-stationary problems of computational gas dynamics. Then we can for any point in the space of a countable region and at any time moment obtain a numerical solution $F(x, y, z, t, A_1, \dots, A_N)$, where x, y, z are spatial coordinates, t is time, A_1, \dots, A_N - defining parameters of the problem. As the defining parameters of the problem, we will keep in mind the characteristic numbers describing the properties of the flow in question, such as Mach number, Reynolds number, Prandtl number, Strouhal number, etc., and characteristic geometric parameters. Each of the characteristic parameters is limited in a certain range:

$$A_i^{min} \leq A_i \leq A_i^{max}, \quad i = 1, \dots, N$$

We divide each of the parameters A_i into $k-1$ parts, so we obtain for each parameter a partition consisting of k points. The volume of N - dimensional space formed by the set of defining parameters A_i is filled with a set of k^N points. Denoting a point from this set as (A_1^*, \dots, A_N^*) , we arrive at the fact that for each point of the set it is necessary to obtain a numerical solution of the gas-dynamic problem $F(x, y, z, t, A_1^*, \dots, A_N^*)$. This will require solving k^N gas-dynamic problems, which is impossible without the use of parallel computing in multitasking mode. Here we formulated the classical problem of parametric research. Parametric numerical studies allow one to obtain a solution not for one specific problem of mathematical modeling, but for a class of problems specified in a multidimensional space of defining parameters. Also, such a formal statement allows a numerical study of optimization analysis problems, when the inverse problem is solved at each point of the grid partition of the multidimensional space of defining parameters. Both types of similar problems are considered in the papers [2, 4-6, 14].

3. The problems of visualizing the results of a generalized computational experiment

So, as a result of a generalized computational experiment, we obtain a numerical solution of the gas-dynamic problem $F(x, y, z, t, A_1^*, \dots, A_N^*)$ for each point of space at any time and for each point of partition of the space of defining parameters (A_1, \dots, A_N) . Let's try to systematize the emerging tasks of visual presentation of this data. In the course of systematization, we will proceed from the types of data under consideration.

A) Here F is a vector of gas-dynamic functions, such as pressure, density, temperature, velocity components. For each point of the partitioning of the spatial countable domain (x, y, z) at the moment of time t we have a whole set of solutions corresponding to each point of the partition of the space of defining parameters. From a practical point of view, the usefulness of such data is small, but such information can be very useful in assessing the contribution of the determining parameter A_i to the total variance at each point of the computational domain and at any time moment. Here, for visualization at each point, it is advisable to use a classic spider diagram with normalization to the range of change of the determining parameter.

B) For each split point of the space of defining parameters (A_1^*, \dots, A_N^*) we have a calculated flow pattern in the selected region of space (the calculated region). This makes it possible to apply the entire rich set of scientific visualization methods and software [1, 3], developed earlier for gas dynamics problems. Possible types of informative visual representations include:

- visualization of scalar and vector fields in parallel sections of the computational domain and cross-sections;
- animation of scalar and vector fields in the constructed sections;
- construction of combined visual representations.

Figure 1 shows an example of a visual presentation using cross-sections of the process of propagation of a low-velocity air jet in the computational domain [1]. Figure 2 shows an example of a combined presentation - a combination of temperature distribution in parallel sections with surfaces “stretched” on the velocity vectors [1].

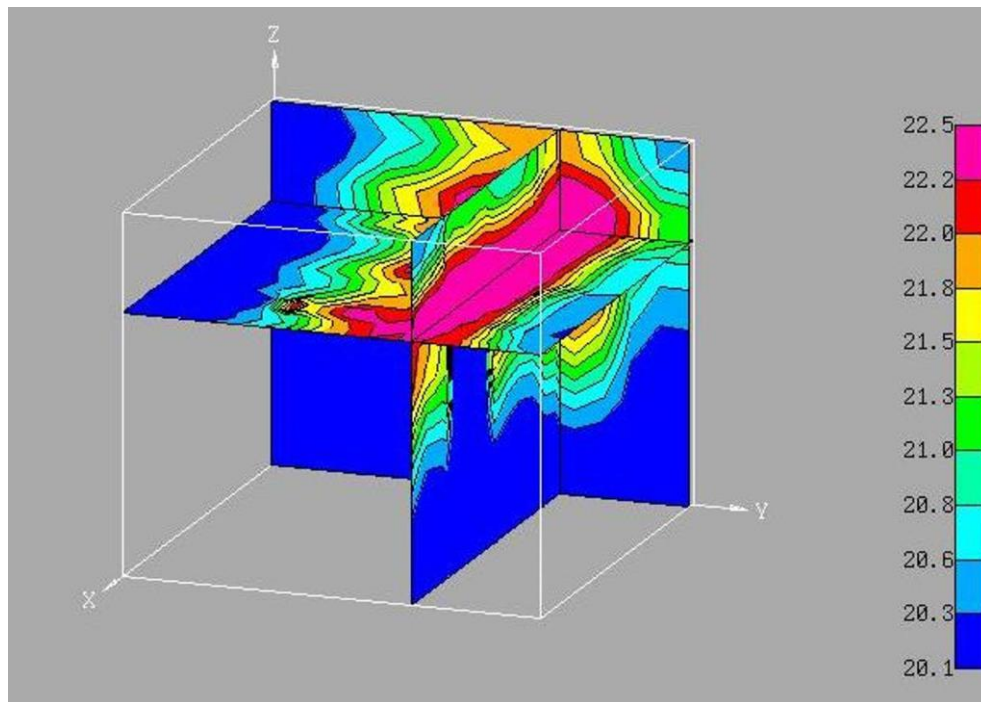


Fig. 1. An example of the use of cross-sections [1].

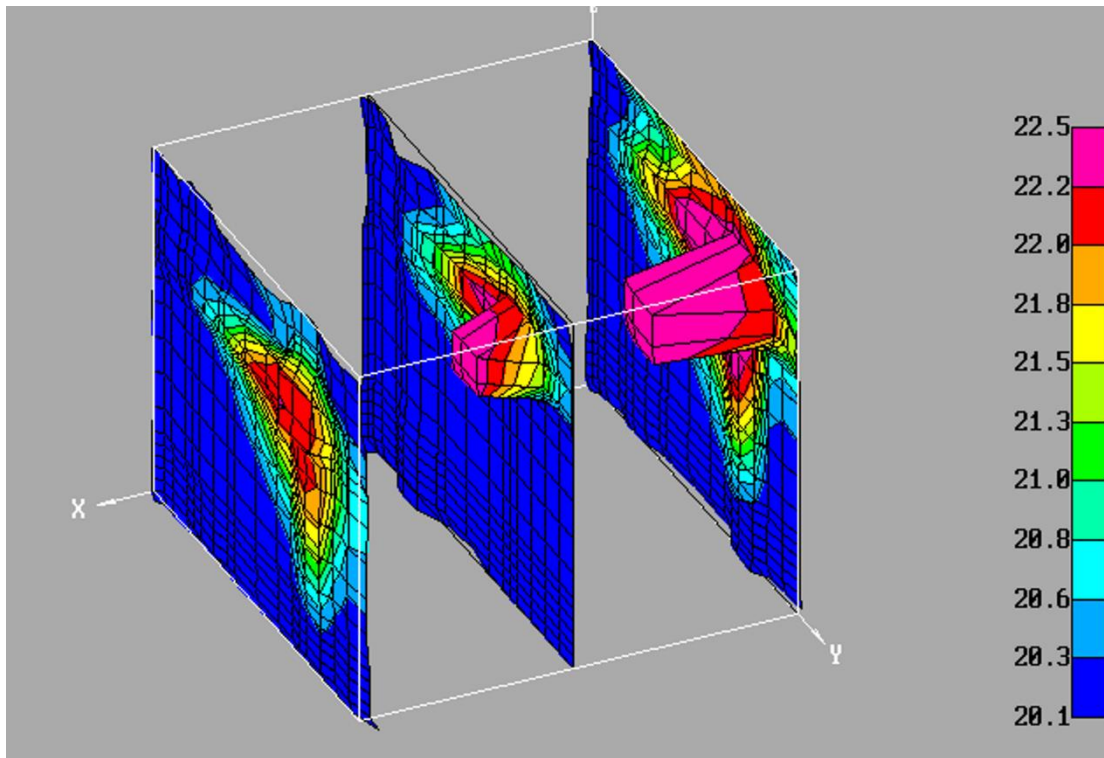


Fig. 2. Combined representation - a combination of temperature distribution in parallel sections with surfaces “stretched” on the velocity vectors [1].

We can create similar representations in the most diverse combinations for each fixed point of a partition of the space of defining parameters (A_1^*, \dots, A_N^*) .

Here we have a new opportunity to construct the boundaries of change of the defining parameters of interest from A_i^{min} to A_i^{max} for each A_i . This can be useful, for example, in the visualization of separation zones, where it is possible to single out the limits of the change in the position of the separation zones, depending on the choice of the determining parameter. It should be noted that such visual presentations for a particular class of problems can be created on the basis of already existing methods and algorithms implemented in many software systems, such as ParaView, VizIt, TecPlot.

C) From a practical point of view, when solving problems of computational gas dynamics, the primary interest to the user, as a rule, are valuable functionals calculated using the already computed gas-dynamic functions in the computational domain. The role of such a functional can be played by the total drag coefficient of a body in the flow or the friction drag coefficient for viscous problems. When analyzing the conditions for the emergence and decay of space-time structures in a flow field, such a functional can be the characteristic time of the structure's existence.

Here we come to the classical tasks of visual analytics [8-12], where the goal is to obtain maximum information about the multidimensional data array $\Phi(A_1, \dots, A_N) = \Phi(F(x, y, z, t, A_1, \dots, A_N))$ and hidden relationships between its defining parameters. For these purposes, a sufficient number of approaches have been developed [8-10]. One of the possible approaches presented in [6,13-15] is dimension reducing of the studied space of defining parameters to three, the visual representation of dependence obtained for $\Phi(A_1, \dots, A_N)$ and approximation of this dependence using a set of geometric primitives. The purpose of this approach is to represent the dependence of $\Phi(A_1, \dots, A_N)$ in an analytical form. If successful, this makes it possible to construct the obtained results of mathematical model-

ing in the form of a physical law for the class of problems in question. This area of research involves the development of a large number of approaches and software tools.

4. Conclusion

Modern development of computing systems and technologies allows to organize the construction of a generalized computational experiment in modeling problems of computational gas dynamics. The construction of such an experiment is based on numerical parametric studies and the solution of optimization analysis problems. Solving such problems implies a multiple solution to the direct problem of numerical modeling of a gas-dynamic process with various input data. The defining parameters of a class of problems, such as the characteristic Mach number, Reynolds number, geometric parameters, etc., vary in certain ranges with a certain partitioning step. As a result, the resulting solution is a multidimensional amount of data. To analyze this volume, visualization is necessary. The paper attempts to systematize and briefly describe some types of problems arising from processing the results of a generalized computational experiment. The aim of the work is to begin a broad discussion of the tasks of visualization in a generalized computational experiment and methods for their solution.

5. References

- [1] Bondarev A. E. and Bondarev E. N. Visualization Functions in Computational Fluid Dynamics / *Obshcheros. NauchnoTekhn. Zh. Polet (Mashinostr, Moscow, 2000)*, No. 10, pp. 53–60 [in Russian].
- [2] Bondarev A. E. Optimization of hybrid difference scheme taking into account the influence of viscosity and turbulence based on the solution of inverse problems // Conference proceedings « High performance computing in problems of mechanics and physics», Moscow, 2009. p. 39-44.
- [3] Bondarev A.E., Galaktionov V.A., Chechetkin V. M. Analysis of the Development Concepts and Methods of Visual Data Representation in Computational Physics / *Computational Mathematics and Mathematical Physics*, 2011, Vol. 51, No. 4, pp. 624–636.
- [4] Bondarev A.E. Analysis of unsteady space-time structures using the optimization problem solution and visualization methods // Conference proceedings of 22-th International Conference on Computer Graphics and Vision, Lomonosov Moscow State University, October 01-05, 2012, p.184-188.
- [5] Bondarev A.E., Galaktionov V.A. Analysis of Space-Time Structures Appearance for Non-Stationary CFD Problems / *Proceedings of 15-th International Conference On Computational Science ICCS 2015 Rejkjavik, Iceland, June 01-03 2015, Procedia Computer Science*. Vol. 51. P. 1801–1810.
- [6] Bondarev A.E., Galaktionov V.A. Multidimensional data analysis and visualization for time-dependent CFD problems / *Programming and Computer Software*. 2015. Vol. 41. №. 5. P. 247–252. DOI: 10.1134/S0361768815050023
- [7] Bondarev A.E., Galaktionov V.A., Shapiro L.Z. Processing and visual analysis of multidimensional data / *Scientific Visualization*. V.9, № 5, c.86-104, 2017, DOI: <http://doi.org/10.26583/sv.9.5.08>
- [8] Thomas J. and Cook K. *Illuminating the Path: Research and Development Agenda for Visual Analytics*. IEEE-Press, 2005.
- [9] Kielman, J. and Thomas, J. (Guest Eds.) (2009). Special Issue: Foundations and Frontiers of Visual Analytics / *Information Visualization*, Volume 8, Number 4, p. 239-314.
- [10] Keim D., Kohlhammer J., Ellis G. and Mansmann F. (Eds.) *Mastering the Information Age – Solving Problems with Visual Analytics*, Eurographics Association, 2010.
- [11] Gorban A., Kegl B., Wunsch D., Zinovyev A. (Eds.), *Principal Manifolds for Data Visualization and Dimension Reduction*, LNCSE 58, Springer, Berlin – Heidelberg – New York, 2007.

- [12] Gorban A.N., Zinovyev A. Principal manifolds and graphs in practice: from molecular biology to dynamical systems / *International Journal of Neural Systems*. 2010. Vol. 20. №. 3. P. 219–232. DOI: 10.1142/S0129065710002383
- [13] Bondarev A.E., Galaktionov V.A. and Shapiro L.Z. Processing and visual analysis of multidimensional data / *Scientific Visualization*, 9(5) 2017, p 86-104.
- [14] Bondarev A.E. On the Construction of the Generalized Numerical Experiment in Fluid Dynamics // *Mathematica Montisnigri*, Vol. XLII, 2018, p. 52-64.
- [15] A.E. Bondarev, A.V. Bondarenko, V.A. Galaktionov (2018) Visual analysis procedures for multidimensional data. *Scientific Visualization* 10.4: 109 - 122, DOI: 10.26583/sv.10.4.09