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Generalized Computational Experiment State Analysis Using Three-Dimensional Visual Maps

A.A. Zakharova[1,A,B], D.A. Korostelyov[2,A, C], A.G. Podvesovskii[3,A, C], A.E. Bondarev[4,A], V.A. Galaktionov[5,A]

[A] Keldysh Institute of Applied Mathematics RAS
[B] Institute of Control Sciences RAS
[C] Bryansk State Technical University

[1] ORCID: 0000-0003-4221-7710, zaawmail@gmail.com
[2] ORCID: 0000-0002-0853-7940, nigm85@mail.ru
[3] ORCID: 0000-0002-1118-3266, apodv@tu-bryansk.ru
[4] ORCID: 0000-0003-3681-5212, bond@keldysh.ru
[5] ORCID: 0000-0001-6460-7539, vlgal@gin.keldysh.ru

Abstract

The paper continues a series of publications of the authors' research materials in the field of developing an approach to dynamic planning and control of a generalized computational experiment based on visualization methods and visual analytics. A generalized computational experiment involves multiple solution of a numerical simulation problem for different sets of values of model defining parameters, which makes it possible to obtain a solution immediately for a certain class of mathematical modeling problems specified in a multidimensional parameter space. The paper considers an extension of the existing authors' approach to analysis of a generalized computational experiment state using visual maps, based on visualization metaphors that can display not only individual images but also their relationships. A method is proposed for constructing visual maps of a generalized computational experiment focused on visualizing relationships between single computational experiments in three-dimensional space. The method is based on the mechanism of formalization of the relationships between single computational experiments, as well as the concept of a graph model visualization metaphor that defines a visual map prototype. A description is given of a software system for constructing and analyzing three-dimensional visual maps of a generalized computational experiment. The paper also considers examples of its application in estimating the accuracy of numerical models of the OpenFOAM software platform for a three-dimensional problem of inviscid flow around a cone.

Keywords: generalized computational experiment, generalized computational experiment state, generalized computational experiment control, visualization, visual map, visual map prototype, graph model, graph visualization, visualization metaphor, problem of flow around a cone, OpenFOAM.

1. Introduction

This paper continues a series of publications of the authors' research materials in the field of visualization and visual analytics in control of a generalized computational experiment (GCE). The GCE is understood as multiple solution of the direct or inverse problem of numerical simulation for different sets of values of model defining parameters [1]. Such an approach makes it possible to immediately obtain a solution for a certain class of mathematical modeling problems specified in a multidimensional space of defining parameters, which in turn makes it possible to simultaneously study the influence of several parameters on the model characteristics of interest, including their joint influence in various combinations of change ranges.

Carrying out a GCE with subsequent analysis and interpretation of its results is a very resource-intensive task, which is associated with the need to process large volumes of multidimensional data. Moreover, it is not possible to conduct an experiment with all possible combinations of models and simulation parameters. Therefore, it is necessary to resort to GCE planning, that is formation of a specific scenario for its implementation taking into account available computing resources and time.

In [2], a model for managing a GCE was proposed based on GCE planning with the possibility to dynamically adjust the plan during the experiment. The GCE plan is understood as a sequence of single computational experiments to be carried out for a given multidimensional array of simulation parameter values with selected methods for analyzing and interpreting the results of the experiment. The advantage of the dynamic GCE planning is the possibility of reducing the volume of insufficiently effective experiments and, on the contrary, providing a more detailed experimental study of those ranges of input data values and defining model parameters that require confirmation and refinement of the patterns found, or rechecking the experimental results if they do not correspond to expected patterns.

In accordance with [2], the general principle of constructing a dynamic GCE plan can be described as follows: based on a series of experiments for a certain set of values of input parameters and processing its results, together with the results of previous series of experiments, current GCE state is fixed. The generalized computational experiment state is determined by a set of computational experiments already carried out and is specified by a multidimensional array of experimental data obtained with the current partition of the space of defining parameters, by a set of generalized indicators obtained as a result of processing this array, as well as by a set of patterns identified on the basis of analysis and interpretation of these indicators. The GCE state is subjected to analysis in which indicators are evaluated that determine the effectiveness of the experiment, in the researcher's opinion. Based on the results of this analysis, the researcher adjusts the space partition of the defining parameters, refines and corrects other conditions if necessary, and proceeds to a new series of computational experiments.

In paper [3], an approach to assessing the GCE state was proposed and studied based on visualization of experimental data specifying it, followed by analysis of the resulting set of visual images. Construction of a visual map of a generalized computational experiment was considered as a visualization method. The GCE visual map is understood as a set of interrelated visual images that characterize the GCE state and are arranged in accordance with certain rules. At the same time, in the mentioned paper, mainly two-dimensional visual images were considered, and proposed methods for constructing a visual map were limited to various ways of arranging visual images. This approach to a large extent limits visualization of relationships both between single computational experiments that make up the GCE, and between GCE states at different stages of its implementation. Nevertheless, it is these two types of visualization that are most conducive to identifying input data areas where model correction is required, as well as to detecting patterns that may require additional computational experiments with new sets of parameters to confirm and refine them.

This paper proposes an extension of the existing approach to building visual maps of a generalized computational experiment by using visualization metaphors that can display not only individual images but also their relationships. The problem of constructing GCE visual maps focused on visualizing relationships between single computational experiments in three-dimensional space, and analyzing the GCE state using this type of visual maps, is considered.

2. Method for constructing a three-dimensional visual map of a generalized computational experiment

In view of the foregoing, the extension of the approach to construction of visual maps of a generalized computational experiment is possible in the following directions:

1. Visualization of relationships between single computational experiments, each of which is carried out for a given model and some fixed set of values of its defining parameters. In this case, the relationship between single computational experiments can be considered as some relation between the values or groups of values of a set of defining parameters (or some of its subsets). The resulting visual map sets a visual image of the GCE state and can be used both to assess the effectiveness of the state as a whole and the impact of various combinations of defining parameters on the resulting GCE indicators.

2. Visualization of relationships between GCE states at different stages of its implementation. With this approach, the relationship can determine a certain transition from one variant of space partitioning of defining parameters to another, carried out by expanding or adjusting it. In particular, the relationship can set the rules for such a transition. This visualization problem is more complex, but the resulting visual map makes it possible to analyze dynamics of changes in GCE states, as well as to visualize various scenarios for its implementation.

In this paper, we will consider the first problem – construction of a GCE visual map with visualization of relationships between single experiments. At the same time, we note that its solution also creates the basis for solving the second problem, since the applied approaches and visualization methods can be further expanded and adapted to visualize links between GCE states.

2.1. Formalization of GCE structure and its state considering relationships between single computational experiments

Let us perform the necessary formalization of the concepts related to the GCE based on the formal representation of a GCE introduced earlier in [2], refining and concretizing it in the context of the visualization problem being solved.

Let $M = \{ m_1, m_2, \ldots, m_{Nm} \}$ be a set of models on which the GCE is carried out, where N_m is the number of models; $P = \{ p_1, p_2, \ldots, p_{Np} \}$ is a set of model defining parameters (we assume that this set is the same for all models from the set M), where N_p is the number of defining parameters.

Each single computational experiment within the GCE framework is carried out for a given model and a fixed combination of values of the defining parameters belonging to the set P. Accordingly, for each parameter p_k ($k = 1, \ldots, Np$) an ordered set of values $V_k = (p_{k,1}, p_{k,2}, \ldots, p_{k,nk})$ is specified, for which computational experiments are carried out. Here $p_{k,j}$ are specific chosen values of the parameter p_k, $j = 1, \ldots, n_k$, where n_k is the number of such values for the parameter p_k. In the simplest case, for the numerical parameter p_k, the set V_k can be a set of equidistant points within the selected range of parameter values.

In this case, situations are possible when, for individual combinations of values of the defining parameters, computational experiments are not carried out or are not carried out on all models. Thus, each model $m_i \in M$ is associated with a space partition of the defining parameters:

$$V(m_i) = (V_1 \times V_2 \times \ldots V_{Np}) \cap Q_i,$$

where Q_i is restrictions on admissibility of combinations of values of the defining parameters imposed by the model m_i ($i = 1, \ldots, N_m$).

Any point belonging to this partition specifies a certain combination of values of the defining parameters for which the computational experiment is carried out: $(v^i)_t = (p_{1,t1}, p_{2,t2}, \ldots, p_{Np,tNp})$, $p_{k,tk} \in V_k$, provided that $(p_{1,t1}, p_{2,t2}, \ldots, p_{Np,tNp}) \in Q_i$.

The total number of such combinations for the model m_i will be denoted by T_i.

Further, let $C = \{ c_1, c_2, ..., c_{Nc} \}$ be a set of output parameters of the experiment, which can be generalized indicators that are the results of processing primary experimental data [4, 6], N_c is the number of output parameters.

Thus, the single computational experiment conducted for the model m_i and a fixed combination of values of the defining parameters $(v^i)_t$ is given by the set:

$$E = < m_i, (v^i)_t, C(m_i, (v^i)_t) >, \quad (1)$$

where $C(m_i, (v^i)_t) = (c_l(m_i, (v^i)_t) \mid l = 1, ..., Nc)$ is an ordered set (vector) of values of the output parameters obtained as a result of the experiment for the given model and combination of values of the defining parameters.

Accordingly, the state of the GCE can be specified by combining sets (1) for all possible models and combinations of values of the defining parameters:

$$E^{GEN} = \{ < m_i, (v^i)_t, C(m_i, (v^i)_t) > \mid i = 1, ..., Nm; t = 1, ..., T_i \}. \quad (2)$$

As an example, let us consider the GCE, which was carried out to assess the accuracy of OpenFOAM platform solvers when modeling a three-dimensional problem of inviscid flow around a cone [4] (in the terminology of OpenFOAM, solvers are software modules that implement various numerical models of mechanics of continua [5]). Solvers rhoCentralFoam, pisoCentralFoam, sonicFoam were used as models. The defining parameters of the models (set P) are: the Mach number (Ma, a dimensionless quantity), the cone half-angle (Betta, in degrees) and the angle of attack (Angle, in degrees). The output parameters of computational experiments (set C) are the results of calculating the norms L1 and L2 of deviation of the numerical solution from the analytical one.

The following ordered sets of values of the defining parameters were chosen as V_k: $V_1 = (3, 5, 7)$; $V_2 = (10, 15, 20)$; $V_3 = (0, 5, 10)$. At the same time, for the combination of the half-angle equal to 10° and the angle of attack equal to 10°, no computational experiments were carried out. Accordingly, for all models, the sets V of possible combinations v_t coincide and contain 24 ordered triples of elements belonging to sets V_k: $v_1 = (3, 10, 0)$; $v_2 = (3, 10, 5)$; ...; $v_{24} = (3, 20, 10)$.

The generalized representation of the GCE state in the form (2) for this example takes the following form:

$$\{ m_i, v_t, \text{L1}(m_i, v_t), \text{L2}(m_i, v_t) \mid m_i \in M; t = 1, ..., 24 \},$$

where M = { rhoCentralFoam, pisoCentralFoam, sonicFoam }.

Let us say that two single computational experiments are interconnected if there is some relationship between the combinations of the values of the defining parameters $(v^i)_t$ for some fixed model m_i, or between the combinations "model – values of the defining parameters". The possible structure of this relationship, as well as its interpretation, is largely determined by the structure of a specific GCE and the content of the tasks of analyzing its results that the researcher faces. However, we can consider general relationships that can be used to describe and analyze a wide class of computational experiments [7–10]. The following two situations can serve as examples of such relationships:

1) experiments are carried out with different models for the same values of the defining parameters;

2) experiments are carried out for one model, while the values of all defining parameters coincide, except for one, the values of which are adjacent in an ordered set. Combinations of values of the defining parameters that satisfy this condition will be called adjacent in what follows.

In the considered GCE for assessing the accuracy of solvers, examples of adjacent combinations of values of the defining parameters are combinations (3, 10, 0) and (3, 10, 5) or combinations (7, 15, 5) and (7, 15, 10).

Binary relations can be used to formalize relationships between single computational experiments. These relations can be both symmetric (for example, in cases where the fact of adjacency of two combinations of values of the defining parameters is simply established) and antisymmetric (if, for example, in addition to this, adjacent values are compared).

In addition to establishing the presence or absence of a relationship between single experiments, one can also evaluate the degree of its intensity, that is strength. Conceptual interpretation of the relationship strength, as well as the relationship itself, largely depends on the tasks facing the researcher and the methods used to analyze and interpret the GCE results. In the example with the GCE for assessing solver accuracy, one of the possible options for interpreting the strength of the relationship between single experiments is the degree of closeness of the relationship between the values of the error magnitudes L1 and L2 obtained for different solvers with adjacent combinations of values of the defining parameters. This indicator can be estimated using a correlation coefficient, and it can be considered as a kind of measure of sensitivity of numerical calculation result deviations from the analytical solution with small changes in the defining parameters. Low values of this indicator for adjacent combinations of parameters may indicate both errors in experiments and the need for a more detailed study of the corresponding range of values of the defining parameters.

2.2. GCE state representation in the form of a graph that defines a visual map prototype

Based on the foregoing, the GCE state taking into account the relationships between single experiments can be represented in the form of a graph model. In this case, the construction of a visual map of the GCE is reduced to the visualization of the corresponding graph on a plane or in space.

The weighted graph corresponding to the GCE state taking into account the relationships between single experiments allows the following formal representation, which we will call *the GCE visual map prototype*:

$$\mathbf{G} = \langle \mathbf{E}, \mathbf{W} \rangle. \tag{3}$$

Here $\mathbf{E} = \{E_1, E_2, ..., E_T\}$ is a set of vertices, each of which corresponds to a single computational experiment specified in the form (1). The cardinality T of this set, that is the total number of single experiments carried out within the framework of the GCE, corresponds to the total number of allowable combinations of values of the defining parameters for all models, that is

$$T = \sum_{i=1}^{Nm} T_i .$$

Here $\mathbf{W}$ is a set of edges, each of which is determined by the relationship strength between the corresponding vertices, that is

$$\mathbf{W} = \{w_{st} \mid s, t = 1, ..., T\}.$$

In general, the range of values for w_{st} depends on the method of their calculation and the way of interpretation, while the value $w_{st} = 0$ corresponds to the absence of a relationship. To adjust the visual display of the graph, it is also possible to normalize these values in order to bring them to a certain range of values.

A visual analysis of the GCE state is often carried out under some additional visualization conditions that set restrictions on the models under consideration, as well as ranges of values of the defining parameters and sets of values of the output parameters. Examples of such conditions are:

1) to build a GCE visual map for some fixed model m_i;

2) to build a GCE visual map for some subset of the defining parameters $P^{VIS} \subset P$ with fixed values or ranges of values of the remaining defining parameters;

3) to build a GCE visual map for some subset of the output parameters $C^{VIS} \subset C$ (other output parameters are not involved in the visualization).

Various combinations of the above conditions are also possible.

The fulfillment of conditions 1 and 2 is ensured by adjusting the visual map prototype (3) by selecting from the set of vertices **E** of a subset corresponding to the selected model and/or fixed values of the defining parameters that do not belong to the P^{VIS} subset. The fulfillment of condition 3 is ensured by reducing the set (1) by excluding from it the values of the output parameters that do not belong to the C^{VIS} set, and by correspondingly adjusting the set **E** in the visual map prototype (3).

2.3. Construction of a three-dimensional visual map of GCE based on the prototype visualization metaphor

Let a graph be given that corresponds to the GCE visual map prototype (3), for which adjustments are made taking into account the specified additional visualization conditions. To build a visual image of this graph in three-dimensional space, we use an approach based on the concept of a visualization metaphor. This approach was proposed in [11] and developed in the context of graph model visualization in [12]. In general, the visualization metaphor is a set of principles for transferring characteristics of the object under study into the visual model space. It includes two components: a *spatial metaphor* that determines the characteristics of the visualization space and the principles for placing visual model elements in this space, and a *representation metaphor* that determines characteristics of the visual model in order to visualize certain properties of the object under study, the most significant at the current stage of its analysis.

With regard to the prototype graph under consideration, the spatial metaphor specifies location of the vertices and edges of the graph in a three-dimensional space, and its basis is various methods of spatial tiling of graphs. Considering the graph structure (3), it can be seen that in the case of a fixed model and the number of variable defining parameters (that is the cardinality of the subset P^{VIS}) equal to 3, the spatial tiling is reduced to constructing a rectangular grid in the three-dimensional space, the nodes of which correspond to the values of the variable defining parameters belonging to the associated sets V_k. With a larger number of variable defining parameters, application of more complex tiling algorithms is required [13, 14].

The result of applying the spatial metaphor is a spatial arrangement of the graph (this term was proposed in [15]). Further, the representation metaphor is applied to the spatial arrangement, which forms visual images of both individual vertices and edges of the graph (that is single computational experiments and relationships between them), and the graph as a whole (that is the GCE state taking into account additional visualization conditions). If within the framework of the spatial metaphor, combinations of values of the defining parameters and the relationships between them are mainly taken into account (this is the information that is used when forming the graph tiling), then within the framework of the representation metaphor, the main role belongs to the values of the output parameters of the experiment, since they create a visual image.

In accordance with the representation metaphor, the visual image of a single computational experiment, that is graph vertices, is determined by the following components:

– coordinates (x, y, z) obtained as a result of applying a spatial metaphor;

– a set of visual features, among which let us highlight the main ones: *Shape*; *Size*; *Color*, as well as additional ones, such as color saturation, orientation, texture, gradient, and others.

To build a visual image of a single experiment, it is necessary to prepare data, which consists in transition from the structure of the form (1) to the dependence of the following form:

$$F(x, y, z) = < Shape, Size, Color, \ldots >, \quad (4)$$

where each visual feature specifies the value of its associated output parameter belonging to the subset C^{VIS}. In this case, if the number of output parameters involved in the visualization (that is the cardinality of the subset C^{VIS}) exceeds 3, then additional visual features are involved (in formula (4), this corresponds to the ellipsis). If their number is less than 3, then some subset is selected from the set of visual features, and the features included in it vary, while the rest receive fixed values.

Visual image of the relationship between single experiments, that is edges of the graph, is determined by the following components:

– geometric characteristics of visual images of vertices connected by an edge – coordinates, size, orientation, and others;

– its own set of visual features, which, just as in the case of vertices, include shape, size, and color, but in this case, the shape is usually fixed, the size (thickness) can correspond to the relationship strength, and the color – to its sign.

3. Software system for constructing and analyzing three-dimensional visual maps of GCE

A tool in the form of an interactive software system has been created to construct and analyze three-dimensional visual maps of the GCE. The developed system allows loading pre-prepared data that specify information about the GCE state and, on their basis, builds a three-dimensional visual map of the GCE in accordance with the considered visualization metaphor. At the same time, navigation on the constructed visual map in an interactive mode is supported. The system was developed using the Microsoft .Net platform, the C# programming language, and the SharpGL library. The software system interface is shown in Figure 1.

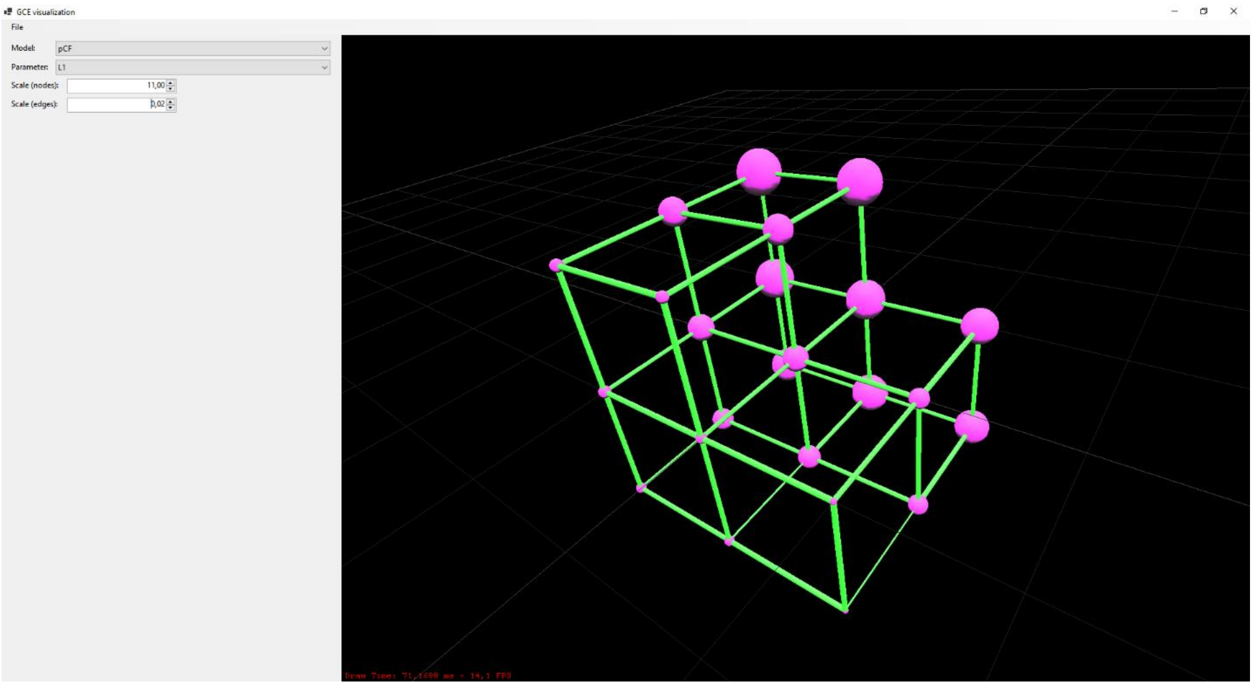


Figure 1 – Interface of the software system for constructing and analyzing three-dimensional visual maps of GCE

The software system implements a mechanism for selecting additional visualization conditions described in Section 2.2. In particular, it is possible to select a model and a subset of output parameters for which a visual map is built. Additionally, dynamical adjustability of parameters of visual features, such as the size of vertices and edges, is supported.

A full-fledged three-dimensional navigation capability on the GCE visual map allows changing the viewing angle for a more thorough study of its individual fragments.

4. Construction and analysis of visual maps of a generalized computational experiment for assessing the accuracy of OpenFOAM platform solvers

Let us return to the GCE described in Section 2.1 for assessing the accuracy of OpenFOAM platform solvers and consider building a visual map for it.

As a visual image of a single experiment, let us use a ball, the radius of which is determined by the value of the output parameter selected for visualization (the deviation norm L1 or L2), and the coordinates of the ball center are determined based on the corresponding values of the defining parameters.

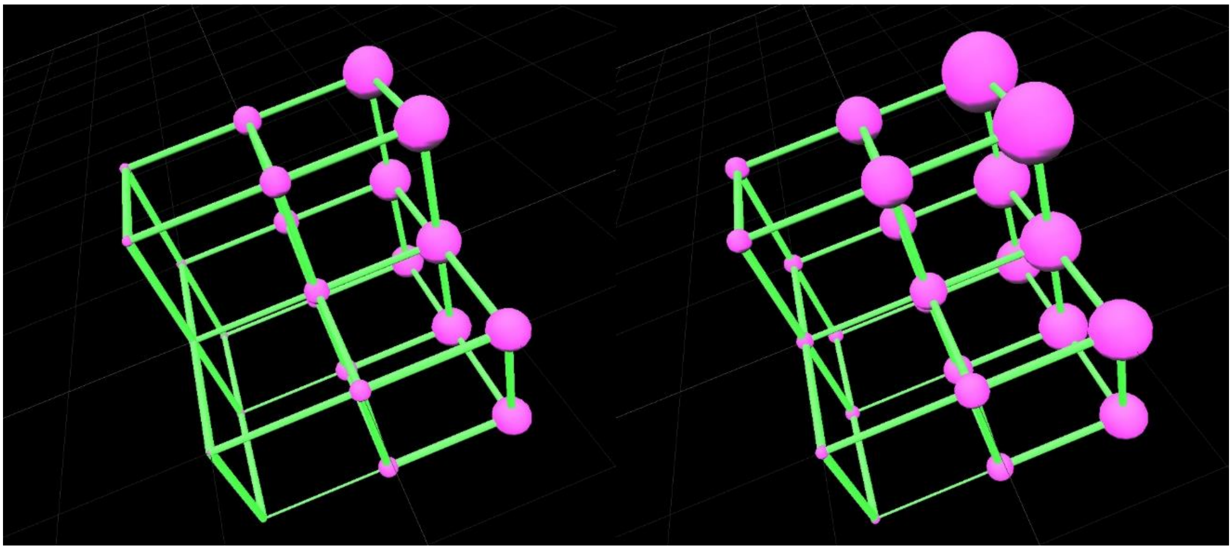
The structure of relationships between graph vertices was determined on the basis of the previously considered adjacency relation between combinations of values of the defining parameters. Since the number of such parameters in the example under consideration is 3, then for any fixed model (solver), the spatial arrangement of the graph can be represented as a three-dimensional grid, the node coordinates of which can be obtained by normalizing the values of the defining parameters to the intervals [–1; 1] so that the minimum value is converted to –1, the average to 0, and the maximum to 1. For example, the set of values (3; 20; 0) after normalization is converted to the set of values (–1; 1; –1), and (7; 10; 10) to (1; –1; 1). At the same time, since only one selected output parameter is rendered within each visual map, the color of the ball is fixed, and additional visual features are not used. Thus, function (4) takes the form:

$$F\,(Ma^*, Betta^*, Angle^*) = < \mathrm{Ball}, R, \mathrm{Magenta} >,$$

where *Ma*, Betta*, Angle** are the normalized values of the defining parameters (Mach number, half-angle and angle of attack, respectively), *R* is the ball radius. Variable values are in italics, and constants are in roman type. The following formulas are used to determine the ball radius: R = L1 / 10 for the L1 norm and R = L2 / 10 for the L2 norm.

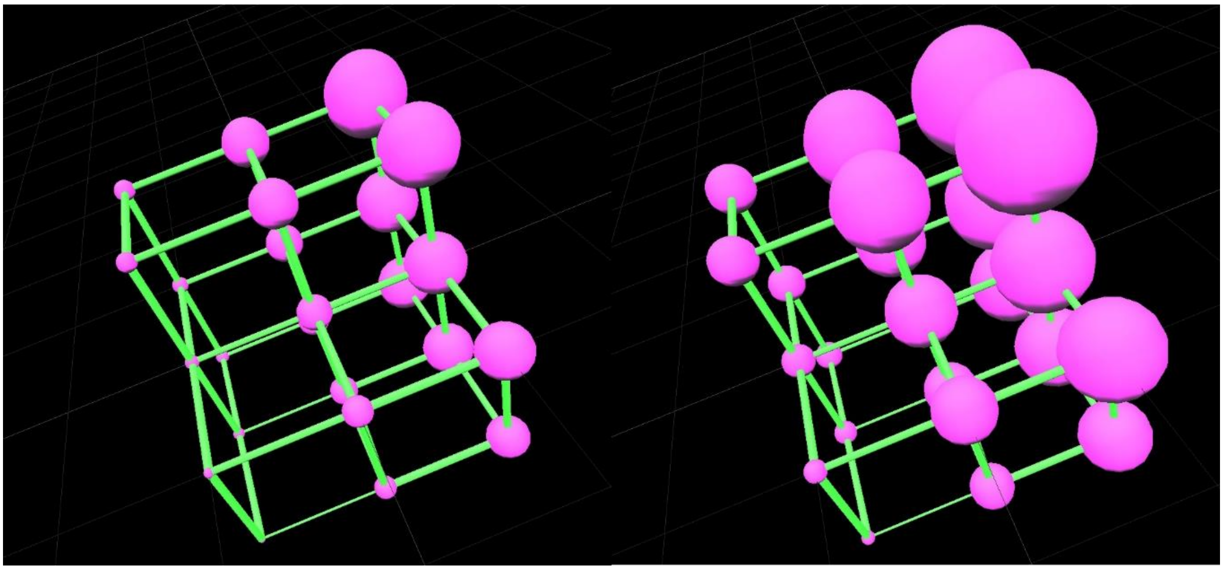
As an indicator of strength of relationship between single experiments, the degree of closeness of the relationship between the values of the error values L1 and L2 obtained for different solvers with adjacent combinations of values of the defining parameters was used. To evaluate this indicator, calculation of the correlation coefficient between the corresponding rows was performed, where each row contains the values of the output parameters L1 and L2 obtained using all solvers for a given combination of values of the defining parameters (each row, therefore, contains 6 values). The results of calculating these indicators were used to build visual images of relationships, which are cylinders with a diameter proportional to the relationship strength.

Figures 2 and 3 represent some of the results of constructing visual maps of the considered GCE.



A) B)

Figure 2 – GCE visual maps for fixed pisoCentralFOAM solver and output parameters L1 (A) and L2 (B)



A) B)

Figure 3 – GCE visual maps for rhoCentralFOAM (A) and sonicFOAM (B) solvers and fixed output parameter L2

5. Results and discussion

As a result of the analysis of the GCE visual maps built for various solvers using the proposed approach, it can be seen that for all solvers, with an increase in the Mach number, the sizes of the graph vertices increase significantly, which indicates an increase in the values of the deviation norms L1 and L2. At the same time, at a fixed value of the Mach number and different values of half-angle and angle of attack, the difference in vertex sizes is no longer so significant. These facts may indicate a significant influence, first of all, of the parameter set by the Mach number on the accuracy of solvers.

In addition, the use of the proposed method for visualizing relationships between single experiments allows assessing visually the degree of relationship between the results of experiments with adjacent combinations of values of the defining parameters, since it remains the same for different solvers. And this, in turn, allows determining visually “strong” and “weak” relationships. As noted earlier, “weak” relationships (which correspond to edges of smaller thickness) may indicate both experimental errors and the need for a more detailed study of the corresponding range of values of the defining parameters.

6. Conclusion

Construction of a three-dimensional visual map of a GCE with support for visualizing relationships between its constituent single computational experiments expands the possibilities of using visualization methods and visual analytics to assess the GCE state in models of dynamic planning and management of its implementation. The paper proposes a method for constructing such a visual map based on the representation of the GCE state in the form of a graph model and its visualization using an approach based on the concept of a visualization metaphor. The proposed method makes it possible to build three-dimensional visual maps for a GCE with many defining parameters, providing their reduction to a three-dimensional visual image with the possibility of analysis in various sections by fixing the values of various defining parameters and selecting the resulting indicators.

Use of the proposed visualization method and the developed software tool that supports this method contributes to an increase in the level of interactivity of the researcher’s interaction with GCE visual maps, which in turn has a positive effect on the efficiency of their analysis.

Development of the functionality of the software system for constructing and analyzing three-dimensional visual maps of a GCE is possible in the following areas:

1) building visual GCE maps for several models on a single three-dimensional scene;

2) support for various methods of assessing relationship strength between single experiments;

3) automation of predicting the results of planned experiments;

4) support for three-dimensional text annotation of GCE visual maps.

An important direction for further research is the solution of the mentioned problem of visualizing the relationships between GCE states at different stages of its implementation. This will make it possible to provide adaptive planning of a GCE based on analysis of the dynamics of changes in its state. Also, an urgent task is to develop mechanisms for integrating software tools for constructing visual maps with a GCE repository, the structure and principles of which are described in [16].

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