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IMPROVEMENT OF THE METHOD OF FUNCTIONAL REPRESENTATION OF THE SHAPE OF A THREE-DIMENSIONAL OBJECT

The object of research is the process of creating a three-dimensional computer model of an aerodynamic product.

The research is devoted to solving the problem of combining a Transformer class model and a method of representing figures through a Fourier series. Such a combination is possible provided that a universal method of representing multidimensional data of different types is used. The results of the combination can improve the solution of the problem of creating a 3D model that meets the specified environmental requirements with sufficiently high accuracy. However, the issues of applying a universal method of representing multidimensional data remain largely unexplored.

A universal method of representing mathematical descriptions of a 3D object and the physical environment that affects the characteristics of this object has been improved. A new method of calibrating the action orbit of the similarity group of figures by displacement has been developed. A method of applying the Fourier transform for figures that form multiple-valued functions after the second phase of the transformation has been improved. A quantitative quality assessment of the functional representation of a figure based on the Hausdorff distance has been developed. A method for eliminating the existing shortcomings of this distance has also been developed.

An experimental verification of the obtained research results has been carried out. It has been established that the use of the proposed improvements ensures the invariance of the functional representation with respect to spatial characteristics of 99.9%. The largest root mean square deviation is 0.000008 absolute units of the Hausdorff distance.

The obtained results provide a universal method for representing any three-dimensional objects. Unlike most existing methods, the improved method allows to operate on 3D models as points in the Hilbert functional space. This possibility allows to significantly simplify the use of modern machine learning models of the Transformer class for solving scientific and applied problems of mathematical physics.

Keywords: *3D modeling, functional representation, Transformer, Fourier transform, calibration of the action orbit of the similarity group, quality assessment of the functional representation.*

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1. Introduction

Among the various spheres of human activity, the sphere of production of goods with specific characteristics should be especially highlighted. A vivid example of this sphere is the production of aerodynamic products. In the business processes of this production, individual processes can be distinguished that require the involvement of a large number of specialists, and, accordingly, significant costs for paying for their labor. An example of such processes is the process of creating a three-dimensional computer model (3D model) of a future product. The quality of the computer model determines the subsequent costs for cycles of implementing corrections and improvements based on tests of the aerodynamic product in real conditions. The expected results of this process are based mainly on the expertise of a specialist. Such expertise is characterized by significant subjectivity and not very high accuracy. In addition, the process of creating a complex three-dimensional computer model of a product requires significant time costs. No less important for the production of aerodynamic products is the compliance of the 3D model of this product with certain physical characteristics. Existing software tools allow to determine these characteristics of the product only with a certain level of accuracy.

The objectivity and accuracy of the process of creating a three-dimensional computer model of an aerodynamic product can be significantly improved as a result of the use of artificial intelligence models, methods and technologies. The creation of specialized software complexes based on such technologies can significantly automate and accelerate the implementation of this process. Among the mentioned models and methods, Transformer class models should be especially highlighted. In the field of 3D modeling, the use of these models has proven to be quite promising. In particular, algorithms for generating three-dimensional shapes can significantly reduce the time for creating computer models.

However, there is currently no holistic technology that would allow combining the capabilities of a three-dimensional modeling tool using Transformer class models and a modeling tool used to determine the aerodynamic characteristics of the product. The combination of these tools would allow to quickly create 3D models that meet the specified requirements with sufficiently high accuracy. One of the approaches to solving the problem of such a combination of technologies is to create a universal method of formal representation of both the 3D model of the product and the physical environment. In [1], this approach is considered only at the level of a general concept. Therefore, conducting

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research in the field of developing new and improving existing models and methods within the framework of the specified approach is relevant from a theoretical and applied point of view.

The review research [2] provides a fairly comprehensive list of industries where Transformer class models are actively and successfully used. Among them: natural language processing, computer vision, multi-modal, audio and speech, signals. In each industry, Transformer class models can perform various tasks: both analytical (classification, clustering) and tasks of information synthesis and transformation (generation, translation, compression). However, in [2], a significant number of publications devoted to the use of Transformer class generative models for generating a product shape that would satisfy a set of specific physical (in particular, aerodynamic) properties were not considered. However, [2] lists many researches that demonstrate the high efficiency of this type of machine learning in the field of 3D modeling. [2] also provides references to several works devoted to the use of Transformer class models to replace classical methods of approximating solutions to mathematical physics problems (in particular, partial differential equations (PDEs)).

One of the earliest results of research into the integration of Transformer class models into the field of three-dimensional object generation is the PointGrow model presented in [3]. This model is capable of generating a sequence of points in space. However, the disadvantage of this approach is the difficulty of constructing a unique sequence of tokens for the same object. This stems from the unstructured nature of the point cloud as a way of representing a three-dimensional shape [3]. Another disadvantage of generating a point cloud is the lack of clear connectivity of points into a single structure, which creates the risks of "detached" artifacts. In addition, the model does not operate with topological and geometric information about the shape of the object's surface, which significantly limits the further development of this method in the direction of more complex generative conditions (for example, aerodynamic characteristics). The risks of forming "detached" artifacts can be mitigated to some extent by using a mesh as a method of representing a three-dimensional object. In researches [4, 5], the use of Transformer class models for generating a sequence of nodes and edges of a mesh was considered. It should be noted that the MeshGPT model proposed in [5] is more compact than the PolyGen model proposed in [4]. However, both models have common shortcomings, among which the structural ambiguity of the token sequence should be especially noted, as well as ignoring the general topology and geometry of the figure.

To overcome the structural ambiguity, in research [6], an approach to representing the figure in the form of a certain tree-like structure was proposed. The results of the research presented in [6] are quite encouraging. However, the shortcomings associated with ignoring the general topology and geometry remain relevant for this approach as well.

Of the existing generators of three-dimensional objects based on Transformer class models, the most promising is the G3PT model [7]. In addition to overcoming the problem of the structuredness of the token sequence, the authors of [7] tried to implement the ability to encode the general topology and geometry of the surface through the latent space using the encoder neural network (which is a component of this model). The idea is to divide the 3D model into different abstract levels of detail, which are encoded by sets of tokens of different lengths. This allows generating deeply detailed surface shapes. As a drawback of the G3PT model proposed in [7], it should be recognized that this model relies too much on the trained encoder component. This drawback significantly complicates the synchronous training of the Transformer class model and the encoder neural network, which forms tokens for different levels of detail of the same figure. In the field of computational fluid dynamics (CFD), Transformer class models are currently not used as actively as, for example, Diffusion type models. However, in [8] it is proposed to use the Transformer class model to establish a correspondence between the figure and the vector field of the aerodynamic flow. The possibility of applying this type of machine learning to CFD problems taking into account the shape of the figure as boundary conditions is demonstrated. However, in [8] only one method of representing the shape of the surface is shown through parameterization using Non-uniform rational B-spline (NURBS), which covers a rather small group of smooth surfaces. How exactly the proposed model works with other methods of representing more complex figures is not described in [8]. Among the variety of methods of representing three-dimensional shapes of objects, methods that encode functions in a certain way deserve special attention. As a key advantage of such methods, it should be noted that a complete description of a figure in parametric space is much shorter than if this figure were described in a conventional coordinate space. That is, such methods of representation allow to operate with objects at a more abstract level, without wasting resources on a detailed coordinate-by-coordinate description of the figure.

Methods for representing shapes through functions can be divided into three main approaches:

– fourier series decomposition of the shape surface;
– PDE application (in particular, the heat conduction equation or the Schrödinger equation) to describe the shape through spectral space;
– description of the shape through the signed distance field (SDF).

The last of the above approaches has a significant drawback: it describes unnecessary information about the internal and external space around the shape surface. In addition, it is not invariant with respect to the spatial characteristics of the shape, which is also a drawback in this context. Therefore, the class of methods for representing shapes through functions, which is based on this approach, is not considered in this research.

To describe the shape through the spectral space, the so-called spectral descriptors are used, such as Heat Kernel Signature [9] or Wave Kernel Signature [10]. They are completely invariant with respect to the spatial characteristics of the figure, in particular to translation and rotation, although they are not invariant to scaling. Unlike Heat Kernel Signature [9], Wave Kernel Signature [10] showed greater sensitivity to small details and can describe detailed complex figures without "smearing". However, the biggest drawback of both of these descriptors (in the context of this research) is invariance to isometric deformations of the figure, which, in fact, is a transition to a completely different figure.

The most optimal in the field of this research is considered to be the method of representation through the expansion of the figure as a function in a Fourier series, that is, finding the coordinates of the figure in the orthogonal basis of Hilbert space. There are a number of researches on this topic, which offer different variants of the so-called Fourier Descriptor. One of the first methods was proposed to encode the figure through rays and planes [11]. However, the main disadvantage of this option is the rather complex calculations that arise due to the need to simultaneously perform one-dimensional and two-dimensional Fourier transforms. In addition, for this option, invariance is guaranteed only with respect to rotation.

In [12, 13], methods based on the three-dimensional Fourier transform are described. The advantage of both methods is complete invariance with respect to all spatial transformations of the figure. However, the method proposed in [12] is limited only to topological surfaces of the zeroth genus, which significantly narrows the possibilities of such a functional representation. In addition, both methods have significant computational costs due to the use of the three-dimensional Fourier transform, since it is difficult to perform tokenization acceptable for Transformer models from the obtained set of coefficients.

In [14], a method is described that uses only the two-dimensional Fourier transform. However, this method uses two-dimensional projections, which somewhat limits the possibilities of such a descriptor to encode complex non-convex figures.

Based on the results of the analysis of modern scientific research, the following conclusions can be drawn:

– the high efficiency of using Transformer class models for 3D modeling of various figures has been recognized;

– the possibility of using Transformer class models for CFD problems taking into account the shape of the figure as boundary conditions has been proven;

– for representing a 3D figure through functions, the most optimal methods in modern research are considered to be those based on the expansion of the figure description into a Fourier series;

– existing methods of representing figures through a Fourier series (one-dimensional, two-dimensional or three-dimensional transformation) have significant limitations and shortcomings that do not allow these methods to be effectively used in modeling figures that exist in a dynamic external environment.

Therefore, from a scientific and applied point of view, the problem of combining the Transformer class model and the method of representing figures through the Fourier series is relevant. Such a combination is possible provided that a universal method of representing multidimensional data of different types is used. The results of such research can significantly improve the solution of a number of scientific and applied problems and, in particular, the problem of creating a 3D model that meets the specified environmental requirements with sufficiently high accuracy.

The basis for the work is a previous research [1], in which the authors developed a method for universalizing data in generative machine learning models based on the functional representation of 3D objects. But this method had a number of significant limitations that narrowed the class of figures that can be transformed into their functional representations without distortion.

The object of research is the process of creating a three-dimensional computer model of an aerodynamic product.

The aim of research is to complete the proof of the hypothesis about the possibility of using a functional representation for any closed figure. This completion was decided to be achieved by improving the method described in [1]. The use of the improved method will allow to construct a full-fledged vector space of the forms of three-dimensional objects. Over this space, it is possible to construct and approximate relations with other spaces, in particular, with the space of solutions of partial differential equations. The use of these relations will allow to significantly simplify the solution of the problem of creating a 3D model that meets the given requirements of the environment with sufficiently high accuracy.

To achieve this aim, it is proposed to solve the following objectives:

1) to improve the method of calibrating the action orbit of the similarity group of figures;

2) to improve the method of applying the Fourier transform for figures that form multiple-valued functions;

3) to develop a quality assessment of the functional representation of a figure;

4) to conduct experimental researches of the obtained results.

2. Materials and Methods

The subject of research is a universal method for representing mathematical descriptions of a three-dimensional object and the physical environment that affects the corresponding characteristics of this object. These representations are such that they can be used by generative models of the Transformer class.

The main hypothesis of research is the hypothesis of the possibility of representing any three-dimensional closed figure in the form of a series of vectors that can be used in generative machine learning models of the Transformer class or GPT.

The theoretical basis for this research is the method proposed in [1]. This method can be briefly described as the transformation of an array of coordinates of points on the surface of a closed three-dimensional figure (this is the input data for the method) into a matrix of vectors (tokens, which are the output data for the method), which is a certain unique mapping (encoding) of the function that describes the shape of the curvature of the surface of the figure. This transformation can be divided into three phases:

a) *Phase 1:* calibration of the action orbit of the similarity group of the figure (finding a standard representative of the set of all "versions" of the figure with respect to the operations of translation, rotation and scaling);

b) *Phase 2:* transformation of the obtained surface of the figure into a periodic function of two arguments by transition to spherical coordinates;

c) *Phase 3:* search for the coordinates of the obtained periodic function in the trigonometric basis of the Hilbert space (expansion into a Fourier series) and construction of a matrix of vectors of the obtained coordinates.

In [1], the unique inversion of such a transformation with the corresponding inverse operations of each phase was shown, which proved the possibility of using this method to perform the task. However, in [1] a number of limitations were not considered. Among these limitations, the most significant are the following.

First, the use of the implementation of Phase 1 proposed in [1] can potentially lead to the fact that the zero coordinates will be outside the boundaries of the figure. In this case, after Phase 2, a function with empty values may be formed. Such a function will receive significant distortions during interpolation, which will negatively affect the final functional representation.

Secondly, there are figures that, after Phase 2 of the transformation, formed functions in certain areas of which high values of the total variation were observed. The term "high" should be used to refer to values of the total variation that are much larger than the size of the area of the function itself. Such figures also undergo significant distortions during interpolation and subsequent transformations.

Thirdly, there is a separate class of figures (including topological surfaces of non-zero genus) that, after Phase 2 of the transformation, form set-valued functions (SVF). Such functions cannot be decomposed into a Fourier series by conventional methods.

In addition to the limited class of figures, the proposed implementations of each transformation phase can form solutions with a certain degree of ambiguity. This is especially clearly manifested during the implementation of Phase 1 of the method.

Thus, some improvements to the method [1] were developed, which will be described in the following sections. A number of experiments were conducted to substantiate the feasibility of these improvements.

For experimental researches, a dataset was generated based on the Thingi10K dataset [15], since it has a classification of figures by topological genus (genus) and the ability to filter models with incorrect meshes. The dataset thus generated [16] contains representations of three-dimensional figures of different topological genera (from 0 to 4) with various geometric shapes (10 for each topology). When selecting such figures, in addition to topological and geometric diversity, the following criteria were used:

– absence of intersections between triangles of the mesh;

– absence of triangles of zero area.

The experiment was designed so that the entire dataset was processed in one session, at the end of which the corresponding graphs with statistics were generated. Given the time consumption (about 2 hours) and the need for RAM, the experiment was conducted in the AWS cloud environment using a virtual EC2 server of type t3.2xlarge, which has 8 CPU cores and 32 GB of RAM and runs on the Ubuntu operating system. The software code that implements the proposed method, calculates all derived data from the dataset and generates statistical graphs is written in Python and is presented in [16].

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3. Results and Discussion

3.1. Results of improving the method of calibrating the action orbit of the similarity group of figures

The method of searching for the canonical representative of the similarity group of a figure consists of the following steps:

Step 1. Calculating the center of mass of all points of the surface of the figure and moving the coordinates to zero (calibration by displacement).

Step 2. Orienting all points of the figure so that the point closest to the center of mass lies on the straight line formed by the linear envelope of one of the vectors of the canonical orthogonal basis (calibration by rotation).

Step 3. Changing the size of the figure so that the distance between the center of mass and the closest point of the surface to it is equal to 1 (calibration by scaling).

Calibration by rotation and by scaling generally do not depend on the shape of the three-dimensional figure, since they do not affect the definiteness of the function after the second phase of the transformation. However, calibration by displacement can significantly affect the formation of a set of points in which the multi-valued function has empty values. Such an undesirable property of a figure can be formulated as follows

$$E=\{x\in X\,|\,F(x)=\varnothing\}, \quad (1)$$

where $F(x)$ – the value of a multivalued function (the result of the second phase of the transformation).

An example of a figure for which, as a result of Phase 2 of the transformation, there is a function in which the set E from definition (1) is non-empty is shown in Fig. 1.

Fig. 1 shows the calibrated figure on the left, and the transition to spherical coordinates on the right in Phase 2 of the transformation. The empty values that arise as a result of such a transition are explained by the fact that for non-convex sets the center of mass may lie outside the figure.

Therefore, it is proposed to improve the method for calibrating the action orbit of the similarity group on the figure. The main attention is proposed to be paid to the modification of Step 1 of the method for finding the canonical representative of the similarity group of the figure. At the same time, other steps of this method also undergo some adaptive changes.

The main criterion for calibration by displacement is proposed to be formulated as follows: the zero of the coordinates should always be inside the figure, regardless of its topological properties. Mathematically, this principle can be written as follows: let F be the set of all closed figures with nonzero volume, and $Sim(n)$ be the similarity group in n-dimensional space. Then

$$\forall F\in\mathcal{F},\ \exists g\in Sim(n): 0\in int(g(F)). \quad (2)$$

To determine a single candidate among all the interior points of a figure, an algorithm was chosen to search for the point furthest from the boundary of this figure. To describe such an algorithm, it is first necessary to define a closed figure in the paradigm of the theory of metric spaces, taking into account interior, boundary and exterior points. This definition is formulated as follows: a subset F of a metric space X with metric d (respectively, the definition of an open ball $B_r(x)$ with radius $r>0$ and center at x) is called a closed figure if

$$int(F)\neq\varnothing;\ \partial F\neq\varnothing;\ ext(F)\neq\varnothing, \quad (3)$$

where ∂F – the boundary of the figure. In other words, the boundary is the set of points $x\in X$, which are determined by the following condition

$$B_r(x)\cap F\neq\varnothing\wedge B_r(x)\cap(X\setminus F)\neq\varnothing. \quad (4)$$

The interiority $int(F)$ is determined by the non-fulfillment of the second element of this conjunction with the simultaneous fulfillment of the first element, and the exteriority $ext(F)$ is determined by the opposite.

Now it is necessary to define the scalar field formed by the figure. The exterior points for the given problem have no significance, so it is possible to limit ourselves to the definitions of interiority and boundary. The scalar field of the figure is the function $f_g: X\to\mathbb{R}$ (the subscript g is from the term "gauge") of the following form:

$$f_g=\begin{cases} f_{int}(x),\ x\in int(F),\\ 0,\ x\in\partial F.\end{cases} \quad (5)$$

The described scalar field is partially undetermined, that is, all values at the interior points are a set of unknowns, and the boundary points can be set to zero. A feature of the concept of "global distance" from the boundary is the direction of the gradient vectors of the scalar field in the direction of the interior points furthest from the boundary, the values of which are maximal. That is, there are points at which the gradient vectors "converge". This property can be formalized as the negative divergence of the scalar field at all interior points

$$\nabla\cdot\nabla f_{int}=C,\ C<0. \quad (6)$$

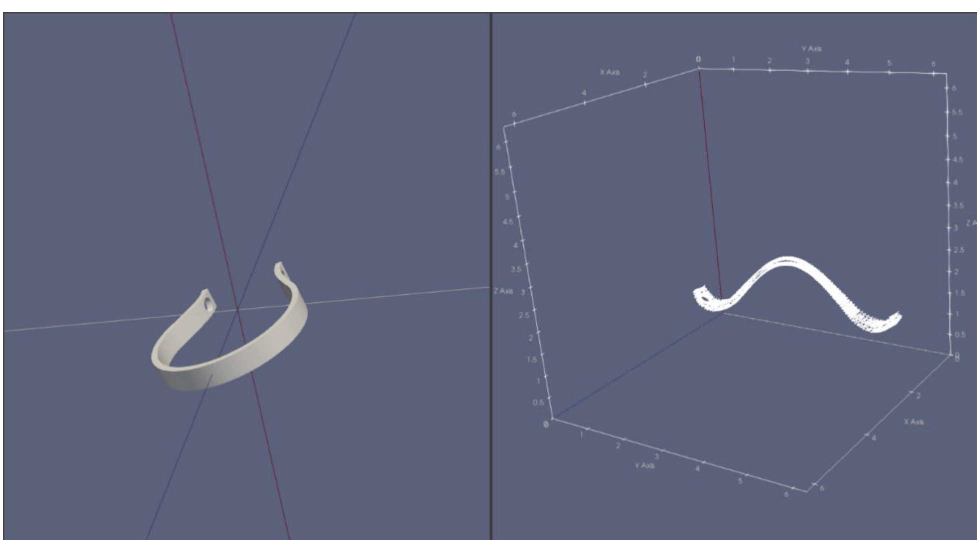

Fig. 1. The figure and the result of its transformation after Phase 2 into a function with empty values on the domain of definition $[0, 2\pi]$

Expression (6) is a Poisson equation with a negative constant C on the right-hand side of the equation. Solving this differential equation at each interior point will give the required scalar field, from which the most distant point (the largest field value) can be chosen as the basis for the first step of orbit calibration. This point is the reference point of the shift

$$x_{tr} = \arg\max_{x \in F} f_g(x). \quad (7)$$

It is convenient to solve such equations using the finite element method (FEM), which has a fairly efficient implementation in Python in the scikit-fem library. Therefore, during the experimental verification of the proposed results, it was decided to use this library.

The first calibration step is performed when an internal point for the shift is selected and the corresponding shift of the entire figure is performed so that the selected point is at zero coordinates. The uniqueness of the result of this step is not guaranteed and depends on the number of internal points furthest from the boundary. For completely symmetric figures, the selection of the point for the shift can be completely random, which will not affect the result of the transformation into a functional representation. However, for figures that are partially symmetric or completely asymmetric, the selection of the point for the shift will significantly affect the functional representation. This fact is a limitation of the method described in [1] regarding the uniqueness of the transformation. Overcoming this limitation may be a topic of future research.

For calibration by rotation, it is necessary to select two points in the space X (currently, the three-dimensional space R^3 is considered). Based on such points, it is possible to select a plane passing through the zero coordinate, to rotate the figure around the zero coordinate so that the selected two points are on two coordinate axes. For calibration by scaling, it is necessary to change the size of the figure so that the boundary points closest to the zero coordinate are at a unit distance from the origin. The most unambiguous and simplest is the scale calibration, because, having the internal point selected during Step 1, it is possible to uniquely determine at least one point closest to zero (i. e., to the support point for the shift, which according to the results of Step 1 is at zero). Therefore, its implementation is proposed to be left unchanged (except that the point closest to zero does not necessarily have to be on one of the coordinate axes).

Eliminating the need for the closest-to-zero boundary point to be located on one of the coordinate axes after Step 2 allows expanding the possibilities for the mechanism for selecting a reference point for rotation calibration. The uniqueness of the closest-to-zero boundary point that arose after Step 1 of the method is not guaranteed at all. Therefore, this method of selecting a reference point for rotation is not justified. The reference point can be any (it does not have to be a boundary point, the main condition is the complete uniqueness of this point for the figure). In addition, this point x_{rot} should not coincide with the reference point for the shift x_{tr}, because then it will be impossible to determine the rotation angle for calibrating this component of the similarity group. Mathematically, this can be formulated as follows

$$x_{tr} \neq x_{rot}. \quad (8)$$

The reference point of the shift according to the results of calculations according to the proposed changes to Step 1 of the calibration method will always be an internal point of the figure. Therefore, to fulfill condition (7), the most reliable option would be to choose an external point or a boundary point. Another condition for such a point is the complete dependence of the calculation of its coordinates on the set of coordinates of the boundary points. Moreover, during the action of the rotation group element on the figure, the same element of the rotation group must act on this point.

Therefore, the following requirements were formulated for the reference point of rotation:

– the point must not be internal $x_{rot} \notin \mathrm{int}(F)$;
– the definition of the point must depend only on the boundary points and on free non-random constants;
– during the action of the rotation group element on the figure, the reference point is subjected to the action of the same group element.

The fulfillment of the first condition for the center of mass of all boundary points is not guaranteed. However, the center of mass fully satisfies the second and third conditions. Thus, the center of mass can be taken as the basis. In this case, it is necessary to apply a deterministic algorithm to "remove" the center of mass beyond the boundaries of the figure. Simple coordinate translations will violate the third condition. Therefore, such coordinate translations are required that will completely depend on the boundary points.

As such an algorithm for "removing" the center of mass, it is recommended to choose a certain iterative algorithm that will gradually shift the point, and each such shift will depend on the boundary points. And the stop of this iterative algorithm will occur when the point is outside the boundaries of the minimum sphere described around the figure (i. e., further than all the boundary points furthest from zero).

The main conditions for choosing such a removal algorithm are:

– uniqueness of the initial point x_0 for any figure – the center of mass as the initial point;
– complete dependence of the direction of removal of the initial point on the coordinates of the boundary points of the figure at each step of the algorithm;
– moderation of the algorithm without sharp jumps;
– complete determinism of the algorithm without stochastic elements.

Let $S = \{a_1, a_2, ..., a_n\}$ be the set of points of the figure boundary. Then, to calculate the direction of the center of mass displacement, the formula

$$G(x) = \sum_{i=1}^{n} \frac{x - a_i}{\|x - a_i\|^p}. \quad (9)$$

The vector $G(x)$ obtained on the basis of (9) depends exclusively on the set of points of the figure boundary; therefore, it provides the second criterion. The parameters p were chosen empirically ($p = 1$) according to the criterion of the greater curvature of the path of the center of mass displacement. The greater curvature will allow to uniquely construct an orthogonal vector based on the vector obtained as a result of executing this algorithm, which, together with the zero coordinates, will form the reference plane of rotation of the figure.

Now, based on the direction vector $G(x)$, it is possible to construct a gradual path to the displaced point outside the boundaries of the sphere described around the figure. At each step, the direction vector will be corrected, which will allow to move more smoothly and accurately in the direction of the gradient. The iterative formula for determining this path has the form

$$x_{k+1} = x_k + \eta \frac{G(x_k)}{\|G(x_k)\|}, k = 0,1,2,\ldots \quad (10)$$

The parameter $\eta > 0$ regulates the speed of the center of mass removal. For experimental tests in the research, $\eta = 0.1$ was chosen.

The condition for stopping the algorithm and final fixation of the first removed center of mass v_1 can be formulated as follows:

$$R = \alpha \max_{i \in \{1,2,\ldots,n\}} \|a_i\|, \alpha = 1 + \varepsilon,$$
$$0 < \varepsilon \ll 1, \|x_k\| > R. \quad (11)$$

For experimental verification, the value $\alpha = 1.005$ was taken.

The second point of removal v_2 is determined by the same iterative algorithm, but the direction vector is a normalized projection of the original vector $G(x)$ onto a plane orthogonal to the vector v_1. To calculate the projector matrix P_u, it is necessary to first normalize the vector v_1 (u – the normalized v_1). This matrix is calculated by the following formula

$$P_u = I - uu^T, \quad (12)$$

where I – the identity matrix.

Thus, it is possible to obtain two orthogonal vectors, or three points (together with zero coordinates), the linear envelope of which forms a subspace that is the reference plane of rotation of the figure. Now this result can be used to uniquely rotate the figure so that the vector v_1 is on the coordinate eye Ox in the positive direction (i. e., the values of the coordinates y and z will be zero, and the coordinate x will have a positive value), and v_2 is on the positive direction of the axis Oy.

Another change to the basic method of calibrating the orbit of the action of the figure similarity group is aimed at optimizing the calculations. It is proposed to perform scale calibration at Step 2, which will allow immediately stabilizing all components of the orbit before calibration by rotation, for the algorithm of "removing" the center of mass of which stability by scale is required. If to do the opposite, then after the scale calibration it would be necessary to actually perform the algorithm of "removing" the center of mass again, because the number of iterations depends on the distance between the zero of the coordinates and the most distant point of the boundary.

3.2. Results of improving the method of applying the Fourier transform for figures that form multiple-valued functions

The second phase of transforming a figure into a functional representation is described only taking into account the boundary of the figure as a surface (so in the future the term "surface" will be used instead of "boundary"). Therefore, in this phase, the construction of a periodic function of the radius from two angular arguments is provided through the parameterization of the surface of the figure and the transition to spherical coordinates. Mathematically, this construction can be represented as follows:

$$f(\theta,\varphi)=\begin{cases} r(\theta,\varphi)\sin\theta\cos\dfrac{\varphi}{2}, \\ r(\theta,\varphi)\sin\theta\sin\dfrac{\varphi}{2}, \\ r(\theta,\varphi)\cos\theta, \end{cases} \theta\in[0,2\pi], \varphi\in[0,2\pi], \quad (13)$$

where $r(\theta, \varphi)$ – the desired periodic function of two arguments.

Among the limitations of such a transformation is the possibility of forming a multiple-valued function for some figures (one combination of angles has a finite set of radius values). To overcome this limitation, it is proposed to divide this function into "layers" taking into account the following principles:

Principle 1. All sets must be sorted in ascending order for each pair of values of the angle arguments.

Principle 2. The number of layers is equal to the maximum number of radius values of the function among all sets.

Principle 3. For all combinations of angle arguments that do not have a radius value on the layer, a zero value is set.

Thus, a two-dimensional Fourier transform (the third phase of transformation into a functional representation) can be applied to each layer. All the resulting matrices of complex coefficients of the Fourier series are transformed into a matrix of four-dimensional vectors (since in the two-dimensional Fourier transform each pair of frequencies has four real degrees of freedom). Next, all the vector matrices are combined into a common matrix with longer vectors in a sequence that corresponds to the first principle of dividing the function $r(\theta, \varphi)$ into layers.

The lengths of each vector of the resulting matrix of the functional representation are the same and equal to $4 \times n_L$ (where n_L – the number of layers). However, the number of layers for different figures can be different. Each such vector in itself can be considered as a token for models of the Transformer class. From such a token, it is possible to form an embedding, by analogy with the formation of embeddings for image pixels (which are also vectors, albeit only three-dimensional) in the GPT from pixels model [17].

During the inverse Fourier transform, in order to restore the shape of the figure, it is proposed to discard the zero values of the function $r(\theta, \varphi)$. Such an operation will not affect the quality of the inverse transform, because as a result of the first phase of transformation into a functional representation, the distance (and in terms of the second phase, the radius-value of the function $r(\theta, \varphi)$) from the zero of the coordinates to the points of the surface of the figure is not less than one. The range of values of this function is as follows:

$$\mathcal{P}([1,\infty)) = \{B | B \subset [1,\infty)\},$$
$$Im\, r(\theta,\varphi) \subset \mathcal{P}([1,\infty)). \quad (14)$$

Such a range of values allows to reject any values less than one. However, due to the nature of the Fourier transform, there may be minor outliers less than one. Therefore, during the experimental verification of the algorithm for transforming into a functional representation, the rejection of values lower than 0.7 was used.

For the software implementation of the method described in [1], it is necessary to perform a uniform interpolation of the function $r(\theta, \varphi)$. Such interpolation is necessary because for the fast Fourier transform, the input set of function values must be distributed over the nodes of a two-dimensional grid of angular arguments. One of the features of the Fourier transform method for multi-valued functions described in this article is the use of zero as a "placeholder" for empty values in the layers (Principle 3 of the function layering). This feature limits the choice of the interpolation method. To ensure the correct operation of the third phase of the transformation into a functional representation and to avoid the appearance of unwanted artifacts when restoring the figure (which were observed in the previous version of the functional representation method described in [1]), it is proposed to use only the "nearest" method at the stage of interpolation of the function $r(\theta, \varphi)$. However, this method does not provide smoothness of the surface. Therefore, to improve the quality of the transformation, the method of filling the triangles of the figure mesh with additional points is used even before Phase 2 of the transformation into a functional representation (when the figure has its initial appearance, but is already calibrated). The number of points added to the triangle depends on the length of its longest edge. Then, it is possible to set the maximum length of all edges of the mesh and divide all triangles that do not meet the edge length restriction into such a number that will allow it to be fulfilled. Using this method allows to avoid dividing triangles that are already small enough, which is an element of algorithm optimization. It should be recognized that there are other methods of preliminary mesh compaction before interpolation. For example, one can focus not on the length of the longest edge, but on the area of the triangle. The proposed option with partitioning based on the edge was chosen due to the simplicity of implementing such an algorithm.

3.3. Results of the development of the quality assessment of the functional representation of the figure

The functional representation must be inverted. This means that the shape of the figure, which is restored from this representation using the inverse algorithm of the third and second phases of the transformation, must coincide or be as close as possible to the initial shape of this figure. For the tasks of generating 3D models of objects with certain physical properties, only the geometric and topological aspects of the shape of the surface of the figure are important. In the context of modeling aerodynamic products, spatial aspects (shift, rotation and scaling) are not important for the mechanisms of generating three-dimensional figures. Spatial information was specifically extracted from the mathematical model of the figure using the calibration algorithm in the first phase of transformation into a functional representation. This extraction allowed to narrow the mathematical model of the figure exclusively to the geometry and topology of the surface, which are invariant with respect to the global spatial parameters of the figure.

The term "Quality of functional representation" is proposed to denote a set of quantitative characteristics of the results (intermediate or final) of the transformation of a figure into a functional representation. These quantitative characteristics should be representative of each key aspect of the transformation. Based on the features of the functional representation method considered in the previous subsections, it was proposed to distinguish two key characteristics of this method:

a) the degree of uniqueness of the result of the first phase of the transformation (calibration of the action orbit of the figure similarity group);

b) the accuracy of the approximation of the shape of the figure through the functional representation.

Characteristic b) cannot take a value of 100%, since this representation, by its mathematical essence, is an expansion of a certain element of the Hilbert space by an orthogonal basis (in this case, the functional space). Hilbert spaces are infinite-dimensional, as a result of which it is impossible to implement this expansion with absolute accuracy in practice. Therefore, it is an approximating representation of the shape of the surface of a three-dimensional figure.

To calculate the values of both characteristics, this research proposes to use comparative methods. To estimate characteristic a), the figures obtained as a result of the transformation from the input figures of the same shape, but in different positions in space, different orientations and different sizes, should be compared. Next, the mean square deviation of pairwise comparative estimates within the set of spatial states for one figure should be calculated.

To calculate characteristic b), it is necessary to compare the calibrated figure with the corresponding figure restored from the functional representation matrix. Such an estimate will be used for a set of figures of different topologies and with different geometric features.

To perform these calculations, it is recommended to consider the figure as a finite set of surface points. In the theory of metric spaces, there are various mechanisms for calculating the difference (distance) between sets. For the task at hand, the sensitivity of the value of this difference to the deviations of individual points from the expected figure is important. Therefore, formulas for the distance between sets that contain averaging operations are not representative and can "hide" small distortions (especially if there are compensating elements).

In addition, it is more correct to determine the proposed characteristics through error terms, because the larger the values of the distances between sets, the worse the value of the corresponding characteristic. Therefore, in the results of experiments, these characteristics are presented precisely as quantitative indicators of calibration errors and figure approximation errors.

Taking into account the above, it was proposed to use the Hausdorff distance [18] as a mechanism for estimating the distance between figure descriptions. Mathematically, this distance is defined as

$$d_H\left(A,B\right)=\max\left\{\max_{a\in A}\min_{b\in B}a-b,\max_{b\in B}\min_{a\in A}a-b\right\}. \quad (15)$$

The disadvantages of such an estimate are sensitivity to the difference in the density of the point cloud and to the difference in the uniformity of the distribution of points in space. These shortcomings were taken into account for characteristic b), therefore, during the experiments, the normalization of the Hausdorff distance by the 99th percentile of nearest neighbor distances was applied. In assessing the degree of uniqueness of the calibration, these shortcomings had no effect, since the figure according to the results of the first phase of transformation does not undergo a change in the density and distribution of surface points. Therefore, for characteristic a), the normalization of the Hausdorff distance was not applied.

3.4. Conducting experimental researches of the obtained results

To conduct an experimental verification of the obtained results of improving the method of data universalization in generative machine learning models based on the functional representation of 3D objects, the generated dataset [16] was used.

During the experimental verification, 10 different initial spatial states were generated for each figure in the set (different positions in space, different angles of inclination and different sizes). Based on the results of such generation, the calibration error value of the similarity group action orbit was calculated for each figure. The distribution graph of these values is presented in Fig. 2.

The division into topological genera in this case is irrelevant, since calibration does not involve deformation or distortion of the shape of the figure.

As can be seen in Fig. 2, the calibration error distribution showed that for most figures the proposed algorithm provides complete invariance of the functional representation with respect to spatial characteristics. The largest root mean square deviation is only 0.000008 absolute (unnormalized) units of the Hausdorff distance. Fig. 1–9, which had some level of symmetry, as expected, showed the highest value of the calibration error in this experiment.

Next, the value of the estimate of the error of approximation of the shape of the figure through the functional representation was calculated. The results of these calculations are shown in Fig. 3.

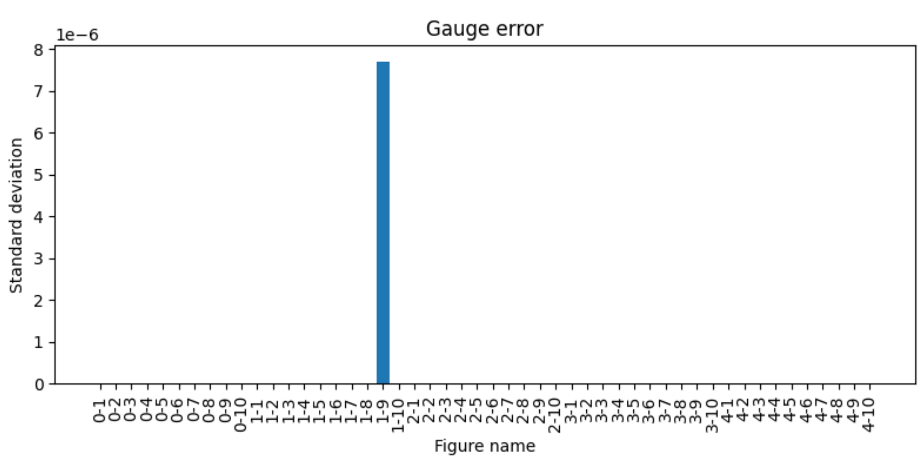

Fig. 2. Calibration error distribution graph

Here there is a statistical visualization of the distribution of approximation errors within the group of figures of each topological genus. As is seen, for all topological genera from 0 to 4 the distribution of approximation errors (according to the normalized Hausdorff distance) does not exceed 15 units. At the same time, there is no tendency for errors to increase with increasing topological genus. Point outliers are also observed in the sets of figures genus 0, genus 2 and genus 4 – the probable reason may be in the more complex shape of the figure. Adjusting the accuracy by increasing the depth of the functional representation can reduce the level of approximation error. Another potential factor may be the function interpolation mechanism (described in more detail in section 3.2).

Fig. 4 shows the distribution of the so-called depth of the functional representation – this is the number of layers into which the function $r(\theta, \varphi)$ is divided, and, accordingly, the number of Fourier transforms per figure.

As is seen in Fig. 4, the figure with the number 2–7 has the greatest depth value (this is the same non-convex shape as shown in Fig. 1). Other figures with a large value of the depth of the functional representation are also mostly non-convex. From this it is possible to conclude that the most difficult from the point of view of calculations while ensuring a low level of approximation error are non-convex figures. In general, reducing this indicator of the depth of the functional representation can become the basis for further improvements of the method.

For a visual comparative demonstration of the original and restored from the matrix of the functional representation of figures, one example was selected for each topological genus. These examples are shown in Fig. 5 (on the left is the original set of surface points; on the right is the one reconstructed from the matrix of functional representation vectors).

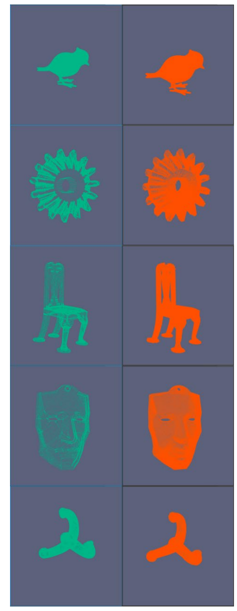

Fig. 5. Comparative demonstration of examples from each topological genus

From the visual comparison it is clear that after restoring the shape of the figure from the functional representation into the cloud of surface points, the density of these points increased. The reason for this phenomenon is the intermediate interpolation of the function that reflects the shape of the figure.

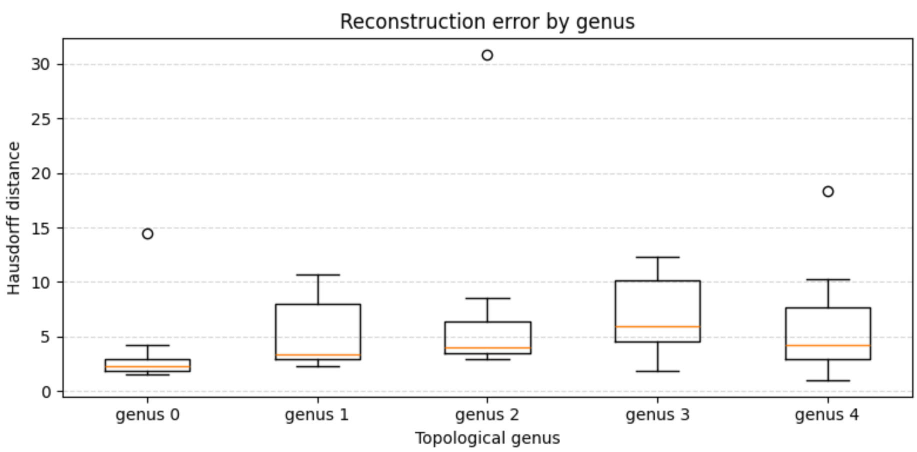

Fig. 3. Distribution of estimates of approximation errors of the shape of a figure

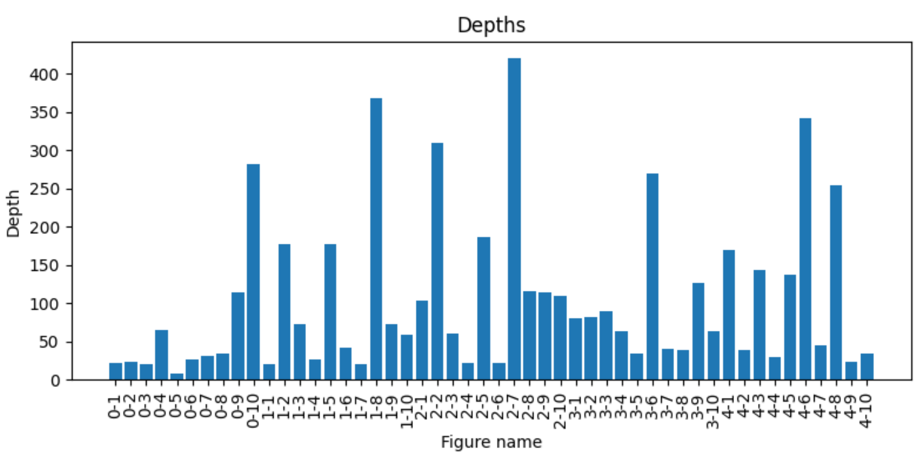

Fig. 4. Distribution of depths of the functional representation

3.5. Discussion of the research results

The research completed the proof of the hypothesis about the possibility of using a functional representation for any closed figure. This proof was carried out by improving the method of data universalization in generative machine learning models based on the functional representation of 3D objects described in [1]. In particular, the method of calibrating the action orbit of the similarity group of figures was improved. As a result of this improvement, a new version of the method of calibrating the action orbit of the similarity group of a figure was developed, which provides the maximum degree of invariance of the functional representation with respect to the spatial characteristics of the figure.

Further, to improve the third phase of the method, a new method of Fourier transformation for multiple-valued functions was proposed. This method is based on the principle of interpolated function stratification.

Further, it was proposed to use the Hausdorff distance for quantitative quality assessment of the functional representation of the figure. At the same time, possible shortcomings of such an assessment were taken into account for characterizing the accuracy of the approximation of the shape of the figure using the functional representation. These shortcomings had no effect on assessing the characteristic of the degree of uniqueness of the calibration.

After conducting experimental researches of the results obtained, it was established that the distribution of errors in the approximation of the shape of the figure showed a sufficiently high accuracy of the improved method. The largest value of the Hausdorff distance normalized to the minimum distance between the points of the surface of the original figure does not exceed 15 points of the normalized scale. In this experiment, one point of this scale corresponds to an increase of 0.1 in the values of the fixed metric (the metric is fixed with a scaling factor of 1). Thus, the accuracy of the approximation of the figure can be considered sufficiently high.

Among the factors that influenced the values of the characteristics, the following were identified in the course of experimental researches:

– the resolution of the grid for the Fourier transform (the factor influenced the accuracy of the approximation of the shape of the figure);
– the density of the initial grid of the figure;
– the symmetry of the figure (the factor influenced the invariance of the calibration);
– the number of layers of the function $r(\theta, \varphi)$ (the factor influenced the accuracy of the approximation and could depend on the algorithm for calibrating the action orbit of the similarity group of the figure).

To normalize the integrity of the initial grid of the figure (since each figure has a different uneven density of the grid), the method of dividing the edges to a length that did not exceed 0.1 was used. This allowed minimizing the influence of this factor on the accuracy of the approximation.

The obtained research results provide a universal way of representing any three-dimensional objects. Unlike most existing methods of representation, the improved method allows to operate on 3D models as points in the Hilbert function space. In well-known researches [11–14], there have already been attempts to factorize three-dimensional shapes as points in the function space. However, the disadvantages of these methods were weak invariance with respect to the spatial characteristics of objects, limitations in terms of topological properties of figures, etc. The method improved in the research overcomes most of the shortcomings of previous developments in this area. In addition, such a representation of figures with the possibility of tokenization opens the way to implementing this method in generative models of the Transformer class. In existing researches on this topic, such an opportunity was not in the focus of the authors, therefore some aspects (for example, representation in the form of a matrix of vectors) were not taken into account.

Implementation of the results of this research in the field of generative machine learning models is one of the main practical aspects of applying the obtained results. Another aspect is the possibility of combining the developed method with specialized models dedicated to solving mathematical physics problems. Such a combination becomes possible due to the derivation of three-dimensional figures into the function space, in which the PDE solutions are also located. This is precisely the versatility of this method, because it provides the opportunity to represent both a 3D object and an entire dynamic physical process in the same way. This will allow constructing models, in particular Transformer class models, for solving mathematical physics problems. However, the issues of constructing such models require further research.

The obtained research results have application limitations in terms of variability of detailing of the three-dimensional form, judging by the distribution of the depth of the functional representation (i. e., the number of layers of the function $r(\theta, \varphi)$). According to this indicator, it can be concluded that figures with a more elongated geometry require a greater depth of functional representation to ensure high approximation accuracy.

Such an increase in depth leads to an increase in computational costs, namely, RAM. Therefore, when collecting the dataset for experimental researches, some figures were replaced with "easier" ones for calculation. This is a disadvantage of the improved functional representation method, the elimination of which requires further research.

The second disadvantage of the developed update of the functional representation method is the lack of a mechanism for normalizing the length of vectors (tokens) in the matrix of this representation. This may also partly depend on the method of stratification of the function $r(\theta, \varphi)$. Therefore, this element of the transformation algorithm also requires further research.

In order to more deeply empirically prove the hypothesis about the possibility of full-fledged application of the improved method in generative models of the Transformer class, it is necessary to conduct additional research and experiments with the selection of the most optimal architecture and model training algorithm. In addition, future researches devoted to optimizing the method of transforming the coordinate representation of a figure into its functional representation should investigate aspects of this transformation in more detail.

4. Conclusions

1. The method of calibrating the action orbit of the similarity group of figures has been improved. In contrast to the existing method of searching for the canonical representative of the group, a new calibration method by displacement has been developed. Improvements to other steps of the existing functional representation method have also been proposed. The solutions obtained have significantly reduced the probability of the occurrence of empty values of a multi-valued function that arise as a result of Phase 2 of the transformation into a functional representation.

2. The method of applying the Fourier transform to figures that form multi-valued functions after the second phase of the transformation has been improved. Unlike the method used in the previous version of the functional representation method, the improved method allows for the effective application of the two-dimensional Fourier transform for multi-valued functions. It has also been proposed to use the method of filling the triangles of the figure grid with additional points before the second phase of the transformation into a functional representation, which improves the accuracy of this transformation.

3. A quantitative quality assessment of the functional representation of a figure has been developed. For this purpose, it has been proposed to highlight two key characteristics of the quality of the functional representation and use the Hausdorff distance $d_h(A, B)$ for their quantitative assessment. A method has been also developed to eliminate the existing shortcomings of this distance during the quantitative assessment of the accuracy of the approximation of the shape of the figure using the functional representation.

4. An experimental research of the obtained results has been carried out. It has been established that the use of the proposed improvements ensures the invariance of the functional representation with respect to spatial characteristics of 99.9%. The largest root mean square deviation is only 0.000008 absolute (non-normalized) units of the Hausdorff distance.

Conflict of interest

The authors declare that they have no conflict of interest regarding this research, including financial, personal, authorship or other nature, which could affect the research and its results presented in this article.

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Data availability

The manuscript has associated data in a data repository.

Use of artificial intelligence

The authors used artificial intelligence technologies within the permissible framework to provide their own verified data, which is described in the research methodology section.

Authors' contributions

Yevhenii Ruksov: Software, Validation, Formal analysis, Resources, Data curation, Writing – original draft; ***Borys Moroz***: Conceptualization, Methodology, Writing – original draft, Supervision, Project administration; ***Maksym Ievlanov***: Methodology, Investigation, Resources, Writing – review and editing; ***Dmytro Moroz***: Investigation, Validation, Writing – original draft, Funding acquisition.

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