*Materials of Conferences*

## ON SOME GEOMETRIC ASPECT OF INTERPRETING HOMOGENEOUS COORDINATES

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As known, synthetic geometry is a foundation of explorations in analytic geometry. It is proved by sayings of G. Kantor [1]: «…for a long time complications arose at the way of introducing complex values, before their geometric presentation with points and ranges on a plane has been found»; and F. Klein [2]: «…historical emergence of the idea of irrational values has its roots in geometric intuition», etc.

In his work, F. Klein specifies: «...two types of geometry are outlined: synthetic geometry…and… analytic geometry… A third type can be studied besides these two, ..it is a generalization of the first two types». It is known that one of synthetic geometries is called descriptive geometry that studies methods of displaying spatial forms onto a plane.

The display process includes:

– an original;

– display apparatus;

– a model (an image);

– model bearer.

Any spatial objects serve as an original, a point is the simplest one of them, it is explicitly defined by three coordinates with regularity $\infty^3$ (a point on a plane has regularity $\infty^2$, a point on a curve (straight) has regularity $\infty^1$) [4].

Curved (straight) lines or surfaces (planes) can serve as projecting apparatus.

A model (image) of a point will be represented by a point while projecting with a curved (straight) line or a curve (straight) while projecting with a surface (plane).

A surface (plane) or a curved (straight) line can serve as a bearer of the model.

To express the provided information, we will take a point as an original, in other words:

A point is the original

An original is a point

cluster ($S$) or clusters of straights are the display apparatus

a point or points are the model

a plane is the model bearer.

Besides, a necessary requirement while projecting a space point that has regularity  is that its model has the same regularity $\infty^3$.

Clusters of straights ($S_1$) and ($S_2$)are the projecting apparatus, and plane $P$ is the model bearer. Space point $A$ is projected form the center of $S_1$ to the point $A_1$ on the plane $P$ (Fig. 1) that has regularity $\infty^2$, and all points of the beam $SA_1$ are projected into the point $A_1$. In order to meet the projection requirement, we take another projection center $S_2$, and points $S_1$ and $S_2$ will define the straight in the space, and it will cross the plane $P$ in point $F_0$ that is constant for this projections apparatus and will discharge beam of straights ($F_0$) on the plane $P$. Then, $A_1$ will discharge the straight from the beam of straights ($F_0$), and onto it we will project the point $A$ from the center $S_2$ into the point $A_2$ with regularity $\infty^1$. As a result, we will have a model of point $A$ on the plane $P$ – a couple of points $A_1$ and $A_2$, in other words, the model regularity will equal $\left.\begin{matrix} A_1 - \infty^2 \\ A_2 - \infty^1 \end{matrix}\right\} = \infty^3$, and here we can see that regularities of the original and the received model are equal.

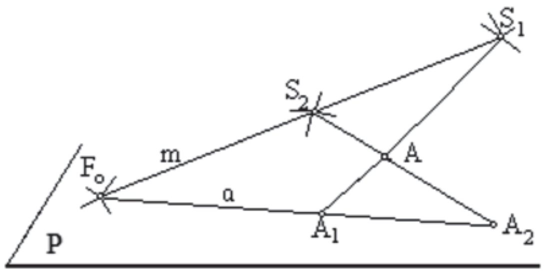


Fig. 1

If a body will serve as an original, it will separate into cut-offs as a beam ($m$). The cut-offs will model from projection centers ($S_1$) and ($S_2$) in the beam of straights ($F_0$) on the plane $P$.

Thus, descriptive geometry solves two problems: a direct problem – receiving a model of an original via projection apparatus according to the given original; and an indirect problem – receiving an original via projection apparatus according to a given model. The direct problem of descriptive geometry is called modeling, and the indirect problem is called constructing.

Let us explain the process of modeling and constructing, using Fig. 1.

We model point $A$ via projection apparatus with two beams of straights аппаратом ($S_1$) and ($S_2$) onto the surface $P$. Projection centers $S_1$ and $S_2$ will define the line $m$ in space, and it will cross the plane $P$ in point $F_0$ that defines the beam of straights ($F_0$) on the plane $P$. Modeling space point $A$ is carried out in the plane $\Delta(A, m)$. Point $A$ from the center $S_1$ is projected into the point $A_1$ that defines, for example, the straight $a$ from the beam of straights ($F_0$). On it we will project the point $A$ from the center $S_2$ into the point $A_2$. As a result, model of the point $A$ is represented by the couple of points $A_1$ and $A_2$.

Construction of the space point $A$ is carried out if the point model that is a couple of points $A_1$ and $A_2$ on the plane $P$ and projection apparatus, for example, couple of beams of straights ($S_1$) and ($S_2$) in space, is given. As earlier, projection centers $S_1$ and $S_2$ will define the straight $m$ in space, and it will cross the plane $P$ in the point $F_0$ that defines the beam of straight bearers of space points ($F_0$). The given points $A_1$ and $A_1$ lie on one of the straights of the beam of straights ($F_0$), they can lie on the straight $a$, for example. Crossing straights $a$ and $m$ define the plane $\Sigma(a, m)$ – the plane of constructing the point $A$. Beams of projecting the point $A_1$ from the projection center $S_1$ and the point $A_2$ from the center $S_1$ that lie in the plane $\Sigma(a, m)$ will cross in one point $A$. Therefore, we can see that the original can be constructed having two model projections.

On the plane $P$ projections of space points will come in to types that we will explain in Fig. 2, 2'.

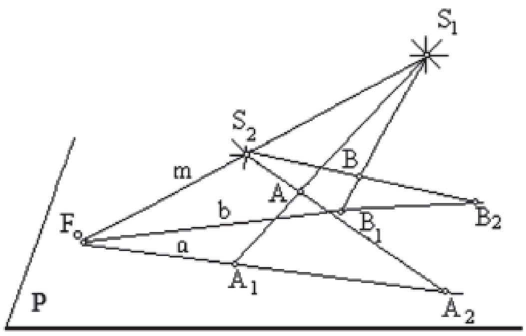


Fig. 2

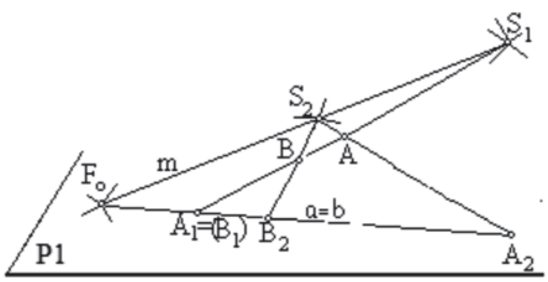


Fig. 2'

We model two points $A$ and $B$ from centers $S_1$ and $S_2$on the plane $P$. Points $A$ and $B$ will discharge two planes from the beam of planes ($m$), and these planes will cross the plane $P$ along straights $a$ and $b$ of the beam of straights ($F_0$) (Fig. 2). From the projection center points $A$ and $B$ are projected correspondingly by the pair of points $A_1$ and $A_2$ on the straight на $a$ and $B_1$ and $B_2$ on the straight $b$. A specific case of placing spatial points $A$ and $B$ is possible. These points can be located on one beam of straight cluster ($S_1$) or ($S_2$). In this case points $A$ and $B$ will belong to one plane of the beam of planes ($m$), and this plane will be by two crossing straights $m$ and $(AB)$(). This plane will cross place $P$ along the straight $a = b$ of the beam of straights ($F_0$) (Fig. 2). Points $A$ and $B$ from the projection center $S_1$ will project into the concurred projections $A_1 = (B_1)$, such point on a projection plane are called rival [5, 6]. Projections of points $A$ and $B$ from the projection center $S_2$ project onto the plane $P$ into two different points $A_2$ and $B_2$ of the straight line $a = b$.

**Emergence of a problem**

Let us study implementation of descriptive geometry methods in order to solve some problems of analytic geometry. To do it, let us examine affine coordinates on a plane.

The simplest coordinate system on a straight can be imagined, if we set a starting point on it, point $O$, a unit with coordinate 1, and positive or negative spacings $x$ from point O (Fig. 3).

On the plane or in space we will take two or three coordinate straights $x, y$ or $x, y, z$ with a mutual point O and random angles that are formed between these straights. Angles that are formed between axis equal 90°. Affine straight is unlimited in both directions, but we will never achieve any point that lies on the opposite direction on it.


Fig. 3

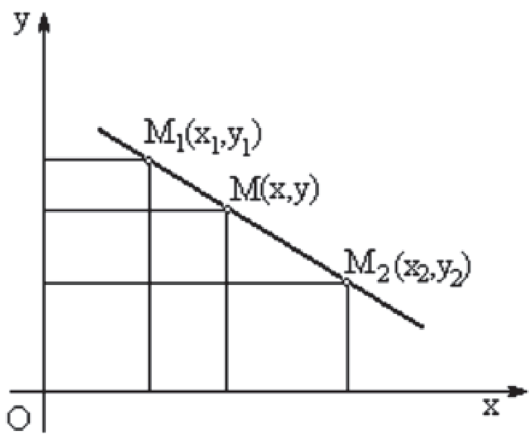


Fig. 4

The special feature of an affine plane is that parallel straights do not cross on it.

On the affine straight let us study the division of the section $M_1M_2$ by the straight point $M$ in this relation of $m/n$, where and are random numbers (Fig. 4). Coordinates of the point $M(x, y)$accordinging to the coordinates of points $M(x_1, y_1)$ and $M(x_2, y_3)$are produced in textbooks on analytic geometry [7, 8, 9], where $x = \frac{nx_1 + mx_2}{m+n}$; $y = \frac{ny_1 + my_2}{m+n}$ for the point $M$ that lies inside the section and $(m/n) > 0$, if point $M$ will lie outside of the section, $(m/n) < 0$. If $m/n = 1$, point $M$ with coordinates $x = \frac{x_1 + x_2}{2}$ and $y = \frac{y_1 + y_2}{2}$ will divide the section $M_1M_2$ in halves. If $m/n = -1$, coordinates of the point $M'$ will be $x = \infty$ and $y = \infty$, such points are called unlimitedly remote, and are not studied in affine geometry. These unlimitedly remote points have been introduced into geometry as nonintrinsic elements.

Thus, a nonintrinsic point is produced on a straight, and nonintrinsic is produced on a plane, and nonintrinsic is produced in space. Therefore, each straight obtains a nonintrinsic point that is represented on a closed line (Fig. 5). Now parallel straights have obtained a mutual nonintrinsic point. Producing nonintrinsic points on a straight allowed us to simplify many suggestions, for example, two straights cross on a plane now. Therefore, it is claimed that, while moving in any direction, along a straight we can return to an initial point through the unlimited one. Such straight has been called projective straight, and plane – projective plane, and space – projective space. Studying the problem of dividing the section of the straight $M_1M_2$ in relation to $m/n$ on the projective straight, point $M_\infty(\infty)$ in now legalized, and we can suggest that it divides the section $M_1M_\infty M_2$ in relation $m/n = -1$.

Besides, nonintrinsic geometric images cannot be set with affine coordinates. Therefore, a new definition of coordinates is introduced. It is set for the straight so that each point on the straight has not one, but two corresponding coordinates $x_1$ and $x_2$, we have a redundancy of coordinates for a straight [3]. Moreover, a multiplicity of value systems will be set in correspondence to a single point on a straight, they will be represented as $(\rho x, \rho y)$, for example, point $x - 1$. I in the Fig. 6 where $\rho$ is random but not equal to zero number, $x_1$, $x_2$ obtain any values except for their simultaneous equality to zero. In this case we receive a specific single point on a straight, and in case $x_2 = 0$ and $x_1 = \lambda$ we receive a nonintrinsic or unlimited point. Thus produces coordinates are called **homogeneous coordinates**.

**Rival points**

Let us study the coordinate $x = \frac{x_1}{x_2}$, on axis $Ox$ more carefully, where $x_1$ and $x_2$ alter from 0 to $\infty$ and, it is necessary to consider that while $x_1$ grows and $x_2$ remains constant, $x$ grows, and if $x_1$ remains constant, and $x_2$ grows, $x$ decreases. Let us place variables $x$, $x_1$, $x_2$ on straights, $x$ – on a horizontal straight, and variables $x_1$ and $x_2$ on parallel straights with an inverse count from the center of axis.

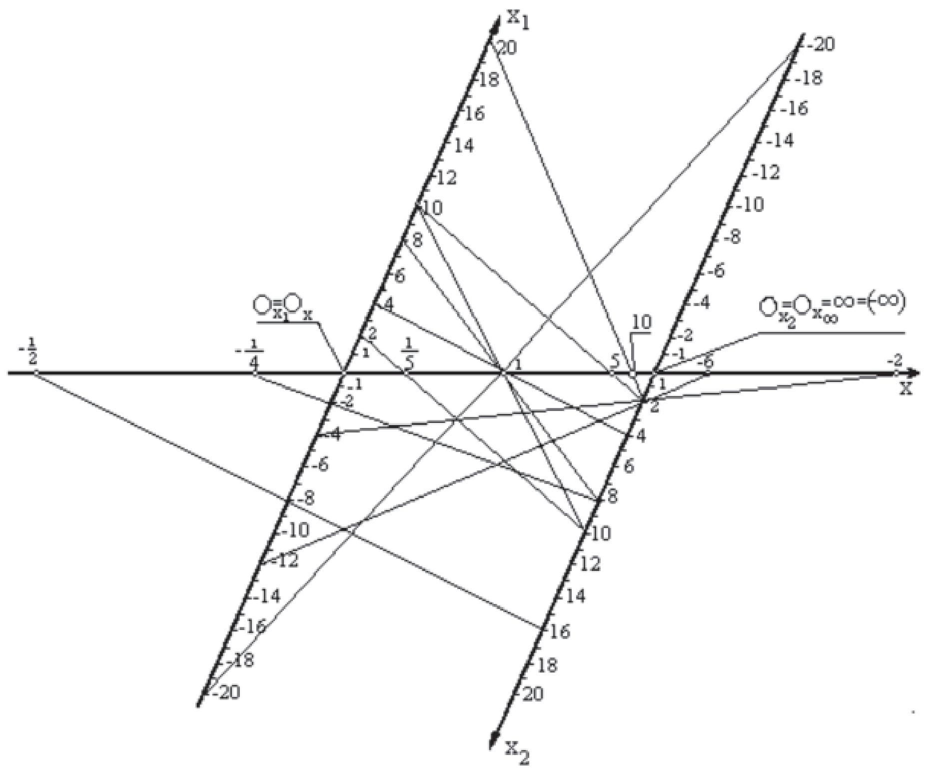


Fig. 5

Let us place the point on infinity within the limits of our sight, it will be the point of crossing between axis $Ox_2$ and $Ox$, then we will examine the behavior $x$ in this case.

Therefore, we can add a theorem to the claim by G. Kantor on that the point ∞ is the only one on a projective straight [3]: **Two point of space ∞ and –∞ project into rival point on a projective straight.**

Let us study alterations of on the axis (Fig. 5), it decreases from ∞ to 0, and further to –∞. Therefore, the highest valuedecreases down to the smallest value ∞ on a digital axis. However, –∞ cannot transfer toand backwards. In the Fig. 6 we can see that ∞ closes with the point $O_{x_2} = O_x$ on the right, and point –∞ – on its left, and these points coincide with the point $O_{x_2} = O_x$. In other words, projection of points ∞ and –∞on a projective straight are **rival points** (it can be observed in Fig. 2' with points $A_1 = (B_1)$. Therefore, an original of the projective straight will be represented as a broken spatial curve.

If now values of $x$ increase from $x = 0$ to ∞ in point $O_{x_2} = O_x$, values of will decrease to the left of zero in point $O_{x_1}$ down to –∞ in point $O_{x_2} = O_x$.

In case straights (2, –2), (–3, 3), (10, –10) etc. are parallel to the axis and are straight of beam of straights $M_\infty(-1)$ point $x = -1$ will be located in the infinity.

Thus, it is obvious that there is no point $x = \frac{0}{0}$ on axis O$x$.

According to the provided information, we can see that, in order to construct pint on a projective straight, one has to escape to a plane. Two planes are required to construct points on a plane where two axis – $Ox$ and $Oy$ operate, in other words, $x = \frac{x_1}{x_3}$ and $y = \frac{x_2}{x_3}$ require two planes, and their crossing line will care O$x_3$ and axis $Ox$ and $Oy$ will be parallel to it.

Since the studied projective straight is a model of a spatial object, we cannot construct it, as a projective straight has only one projection. Each point of an original of a projective straight projects into one point on the model, and only two points –∞ and –∞ project into rival points. There are several spatial lines, and one projection of them represents a closed line with two rival points, for example, a wind of a helical cylindrical line, if ∞ and –∞have been placed at the end and the beginning of the wind while projecting it by a beam of straights with their center in a nonintrinsic point (Fig. 6), or a wind of cone helical line that is projected by a beam of straights from point $S$ that coincides with the cone vertex (Fig. 7). A wind of a helical line that is placed on an unilocular hyperboloid will have a similar projection.

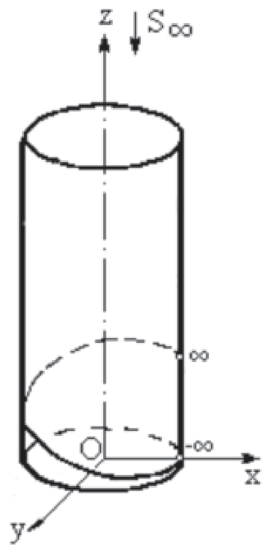

Fig. 6

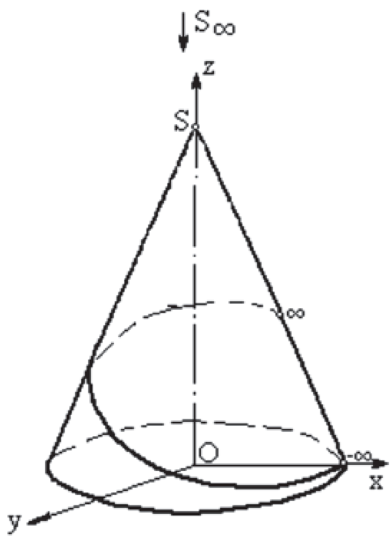

Fig. 7

**Resume**

Thus, we have geometrically proved that:

1) projections of spatial points ∞ and –∞are rival point on a projective line;

2) $x_1$ and $x_2$cannot equal zero simultaneously, as there is no such point on axis O$x$;

3) There is no point $x = \frac{x_1}{x_2}$ on an affine straight in homogeneous if $x_1 = -x_2$ or $-x_1 = x_2$.This point exists on a projective straight in point $M_\infty(-1)$.

Therefore, using methods of descriptive geometry, one can describe an original of a projective straight:

a) An original of a projective straight can be located on: a cone surface with its vertex in point $S_1$ and a directing projective straight, if a projective apparatus will consist of two beams of straights with intrinsic centers $S_1$ and $S_2$. Each point of an original will lie on one forming line of a conic surface, points ∞ and –∞ will lie on the same forming line of a conic surface.

b) An original of a projective straight can lie on a cylindrical surface with a directing projective straight and projection apparatus that consists of two beams of straights with centers $S_1^\infty$ and $S_2^\infty$ in nonintrinsic points.

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## THE DISTRIBUTED CALCULATORS MODEL FOR MOLECULAR-DYNAMIC SIMULATION OF STRONG INTERACTION SYSTEMS

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The model of distributed calculators makes it possible a parallel calculation of the correlated N-particle system with a complex multi-particle interaction (long-range ionic and short-range repulsive, two- and three-particle covalent interactions) with MPI and CUDA technologies. The computational model is based on the mathematical model of heterogeneous descriptors developed by the authors, that allows shift the focus from the describing the physical interactions in the system to the description of data flow between the descriptors. The results of computer experiments, which compare the time of the simulation on the cluster of 16 calculators and GPU NVIDIA are given. The model of distributed calculators was being tested with the software package of RIS «MD-SLAG-MELT»[1].

Nowadays, computer modeling (CM) is widely used in various fields of modern science. In particular, in physical chemistry we can study the properties and structure of materials and their relationships.

Molecular-dynamic (MD), Monte-Carlo and quantum-chemical methods are applied there and allow to define different sets of properties. The molecular-dynamics method allows to define the whole complex of properties (structural, thermodynamic, transport) and to investigate the interrelations of nanostructure and physical-chemical properties [1–5].

The size of the simulated system for MD modeling is extremely important. A significant increase in the size of the system provides the practical relevance of the results. The calculation of the systems with $10^5$–$10^7$ particles requires a large amount of time and computer resources and it makes impossible carrying out CM without high-performance computing [6, 7]. To solve this problem, the authors have developed a model of distributed calculators based on distributed computing methods for correlated N-particle system [8–10].

Physical phenomena that are adequately described by the classical and quasiclassical theory can be simulated (using *models of particles)* by molecular dynamics method. The term «*model of particles*» is the general one for a class of computing models in which the discrete description of the physical phenomena includes cooperating particles. Each modeling particle has a set of constant and variable attributes.

In this case molecular-dynamic simulation represents the numerical solution of the Cauchy's boundary task, which means that the initial system state in a bounded region of space (calculation area) is specified at the time $t = 0$ and the boundary conditions are reserved on it. Modeling is tracking the time evolution of this configuration. The main part of calculation is the cycle on a time step in which the state of physical system changes on time for a small step $\Delta t$.

The current condition of the physical system is defined by the attributes of the final ensemble of particles, and the evolution of the system is defined by the interaction laws of these particles. The most of the molecular-dynamics systems relates to the class of long-range potentials, or considering only short-range covalent interactions.

The subject of this work is an investigation of the polymerizing systems with multi-particle interactions which means uniting some types of interactions – two-particle contribution (long-range ionic and short-range repulsive) and multi-particle ones (two and three-particle covalent interactions). The description of this class of models is given in Table 1 [10].

The ionic model is a part of ionic-covalent model though for modeling ionic connections it can be used only independently. In the ionic model (IM) potential functions are built for the ion system. The