



## **METHODS OF MODELING BIOLOGICAL PROCESSES AND SYSTEMS**

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<b>Received:</b> 20 <sup>th</sup> December 2022 <b>Accepted:</b> 24 <sup>th</sup> January 2023 <b>Published:</b> 26 <sup>th</sup> February 2023	This article provides information on the diversity of modern research in the field of medical biological processes in biology and the very rapid development of the fields of mathematical modeling in biological research, the theory of biosystems, the activity of biological systems, phenomena in organs and organisms, and dynamic systems.
<b>Keywords:</b> mathematical modeling, activity of biological systems, computer modeling, biosystem theory, phenomena in organs and organisms, dynamic system.	

Due to the diversity of modern research in the field of mathematical biology and the rapid expansion of the fields of application of mathematical modeling in biological research, this article does not intend to fully cover all existing areas of mathematical biology. Its task is to introduce the reader to a number of typical biological processes (substance transport, chemical kinetics, types of interactions in biological systems, etc.) consists of Models using complex biological systems modeling methods and analysis methods; discuss the use of various calculation schemes for model calculations; introduce classical models in biology and demonstrate the importance of mathematical and computer modeling to understand the nature of biological processes and the functioning of biological systems; to introduce the current situation in the field of mathematical modeling of living systems of biology; consists of discussing new directions of research in the field of mathematical biology and bioinformatics, bioengineering, integrative biology, systems biology.

The selection and presentation of the material in this article included the materials of the authors' training courses and A. B. Rubin, G. Yu. Familiarity with the monographs of Rznichenko and A. A. Antonov had an impact. Many references in the text of this article. J.D. Murray's *Mathematical Biology*, as well as J.P. Keener and J. Sneyd's monographs on "Mathematical Physiology" are also important and useful, and contain extensive material on the subject of support.

In recent decades, significant progress has been made in the quantitative (mathematical) description of the functions of various biosystems at different levels of life organization: molecular, cellular, organ, organism, population, biogeocenological (ecosystem). Life is determined by the many different characteristics of these biosystems and processes that occur at the appropriate levels of system organization and are integrated into a single whole during the functioning of the system. Models based on important postulates about the principles of system operation, describing and explaining a wide range of phenomena, and expressing knowledge in a compact, formalized form can be called biosystem theory.

The construction of mathematical models (theories) of biological systems became possible thanks to the intense analytical work of experimenters: morphologists, biochemists, physiologists, molecular biology specialists, etc. creates an interaction.

The second very important situation that facilitates the involvement of the mathematical apparatus in biology is the careful experimental determination of the rate constants of many intracellular reactions that determine the functions of the cell and the corresponding biosystem. Without knowledge of such constants, a formal mathematical description of intracellular processes is impossible.

Finally, the third condition determining the success of mathematical modeling in biology was the development of powerful computing tools in the form of personal computers, supercomputers, and information technology. This is due to the fact that there are usually many processes that control one or another function of cells or organs, which are covered by forward and feedback chains and therefore are described by complex nonlinear equation systems with

a large number of unknowns. Such equations cannot be solved analytically, but can be solved numerically using a computer.

Numerical experiments on models capable of reproducing a wide class of phenomena in cells, organs and organisms allow to assess the correctness of the assumptions made in the construction of the models. Note that although experimental facts are used as model postulates, the need for some assumptions and assumptions is an important theoretical component of modeling. These assumptions and conjectures are hypotheses that can be subjected to experimental verification. Thus, models become sources of hypotheses, which, moreover, are experimentally verified. An experiment aimed at testing this hypothesis can reject or confirm it and thus contribute to the improvement of the model. This interaction between modeling and experiment is constantly occurring, leading to a deeper and more accurate understanding of the phenomenon: the experiment defines the model, the new model suggests new hypotheses, the experiment defines the new model, and so on.

Currently, the field of mathematical modeling of living systems combines a number of different and already established traditional and more modern disciplines, the names of which sound very general, so it is difficult to strictly delimit specific areas of their use. This is biophysics or mathematical biophysics, which studies the physical basis of biological systems using a mathematical description of physical processes; mathematical biology or theoretical biology, which covers any area of life modeling, traditionally includes population dynamics, ecosystem modeling, climate; systems biology, traditionally referring to models of complex intracellular systems, including proteomics (the science of proteins), metabolomics (the science of metabolic processes); computational biology, which also refers to mathematical models of complex biological processes and systems implemented in computer experiments; bioinformatics, traditionally associated with modeling in genomics.

Special fields of application of mathematical modeling of living systems - mathematical physiology, mathematical immunology and mathematical epidemiology - are currently developing rapidly, aimed at developing mathematical theories and computer models of relevant systems and processes.

Undoubtedly, these interdisciplinary researches are the priority direction of world and local science, combining the efforts of specialists from different fields of knowledge - mathematicians, biologists, physicists, chemists and computer scientists.

Like any scientific discipline, mathematical (theoretical) biology has its own subject, research methods, methods and procedures. The subject of research is mathematical (computer) models of biological processes, which are simultaneously an object of study and a tool for studying biological objects. In connection with such dual nature of biomathematical models, they imply the use of existing methods and the development of new methods for analyzing mathematical systems (theories and methods of relevant branches of mathematics) to study the specific properties of the model. a mathematical object, as well as the use of a model to reproduce and analyze experimental data obtained in biological experiments.

The main way to study and use complex models of biological systems is computational computer experience, which requires the use of appropriate mathematical systems, computational algorithms, technologies for developing and implementing computer programs, and appropriate computing methods for computer storage and processing. simulation results. These requirements imply the development of general and special theories, methods, algorithms, and computer modeling technologies within various branches of mathematical biology, which is itself a component of this scientific discipline.

### **THE MODEL AS A DYNAMIC SYSTEM.**

When creating a quantitative model of any system or object, it is necessary to propose a method for determining the state of the object and describing the change in this state over time.

The state of an object is a set of the most important quantitative signs and variables describing the existence, behavior and evolution of an object or system.

Various measurable quantities can play the role of important variables in biological systems: concentration of substances in biochemistry; in microbiology, the number of microorganisms or their biomass; abundance of species in ecology; membrane potential in the biophysics of membrane processes, etc.

The change of the state of the system over time is the process of transition from one stable state (for example, stationary, i.e., time-invariant, or periodic, i.e., cyclically repeated in a certain time interval) to another stable state. includes. Such transitions, as a rule, occur as a result of an influence on the system that changes the parameters of the system or a jump that changes the state of the system itself. System parameters are constant (at least for a sufficiently long time) quantitative characteristics of process conditions in the system. For example, external parameters that determine the existence of a cell can be temperature and the ionic composition of the extracellular environment. The internal parameters of the dynamics of substances in the cell can be the properties of the molecular mechanisms that ensure their movement or change, for example, the electrical conductivity of the membrane, the density of ion pumps in the membrane, the maximum speed of the ion. exchangers, etc.

A dynamic system describes the change in the state of an object over time, that is, the processes accompanying the change of state. Traditionally, the term "dynamic system" has been applied to mechanical systems whose motion is described by differential equations and whose specific trajectory is determined by initial conditions (positions, velocities, etc.). Currently, the concept and theory of dynamical systems is widely used in various practical

fields, in particular, in the description of biological systems that may not have mechanical variables, and the rate of movement is replaced by the rate of change of state.

In the theory of dynamical systems, the state of the system is associated with a phase point or phase vector  $X$ , whose components are variables  $\{x_k, k=1,2,3,\dots,n\}$  describing the state of the system at a certain moment (Greek from phase - appearance, a certain moment in any process). The dynamic system describes the time change of the state  $X(t)$  in the phase space, that is, in the space of all allowed values of the elements of the phase vector. These representations work particularly well in a 2D dynamical system (two variables describing the state), when the phase space is a phase plane, or in the 3D case, when the phase space can be viewed as a familiar 3D coordinate system. The process of changing the state in time can be represented as the movement of a phase point along a phase trajectory corresponding to the given initial conditions  $X_0 = X(0)$  at the initial time  $t = 0$ .

The law of the relationship between the variables and parameters of the system is written as a system of equations, where there must be a time  $t$  that indicates possible changes in the state of the system. In this case, time can be continuous  $t \in [0, \infty]$  or discrete  $t \in \{0, t_1, t_2, \dots\}$ . In the discrete case, the phase trajectory becomes a set of points in the phase space  $\{X_0, X_1, X_2, \dots\}$  and is often called an orbit.

A traditional object of the theory of dynamical systems in the continuum state is ordinary differential equations (ODE), which formalize the laws of the relationship between the rate of change of state ( $dX/dt$ ) and the current state  $X$ :

$$dX/dt=F(t,X). \tag{1}$$

The right-hand side of the dynamic system (1) takes into account the interaction between the components of the phase vector and the operating conditions of this system, that is, the equations include system parameters  $Q=\{f_1, f_2, f_3, f_m\}$ . As a rule, the right-hand side of the system (1) is clearly independent of  $t$  (so the phase trajectories do not depend on the initial moment of time and are determined only by the starting point of the phase space). Such systems are called autonomous systems and are written as such.

$$dX/dt=F(X) \tag{2}$$

In the discrete case, the dynamic system is described by difference equations and expresses the law of connection between the state at the next moment of time and the state at previous moments, for example:

$$X_{n+1}=F(X_n) \tag{3}$$

Note that in the description of systems (1)-(3) above, the term "space" appeared only in connection with phase space, referring to the set of properties that describe the state of the system. In this case, the real physical space in which this system exists (for example, the volume 3-dimensional space we are familiar with) is not considered, as if all the processes under consideration take place in some physical point or area of points. In fact, where the values of the phase properties under consideration are the same in any part of this region. Such a simplification is often quite reasonable (we will discuss the possibilities of such assumptions later). Corresponding systems are called point or aggregate. This assumption does not work when the distribution of observed quantities in space (for example, concentrations of substances or other quantitative descriptions of processes) is not substantially uniform. The reason for this can be, for example, very slow (compared to the characteristic times of the size change over time) transport of substances or slow propagation of the signal between different spatial regions of the considered volume. Such systems are called distributed. In this case, the state of the system depends on its spatial coordinate, that is, it is characterized by the quantity  $X(t, r)$ , where  $r$  is the spatial position vector of  $X$ .

For example, in 3-dimensional space  $X(t,r)=\{X_i(t), X_j(t), X_k(t)\}$  where  $X_{(i)}(t)$  is the projection of the phase vector onto the corresponding coordinate. Mathematical description and subsequent analysis of distributed systems is more complicated than that of integrated systems. Here, ODE are replaced by systems of partial differential equations, which, in addition to the time derivative (the rate of change of state with time), have derivatives with respect to spatial coordinates (the rate of change of state in space) appears. An example of a diffusion model is given in Section 6 on diffusion modeling. The complexity of biological systems consists of:

- 1) *open systems* - continuously interact with the external environment in the form of energy, matter, information exchange;
- 2) *non-equilibrium systems* - they operate far from thermodynamic equilibrium and therefore require energy expenditure to maintain their existence;
- 3) *multi-scale systems* (multi-scale system) - combine processes of different physical nature (electricity, mechanics, magnetism, chemistry, optics, etc.) with an unprecedented characteristic spatial size scale and time scale of processes. the existence of a system for inanimate nature.

For example, processes occurring at different levels of system organization are combined in the human body: molecular nanolevel with characteristic times of the order of femto- ( $10^{-15}$ ) s and spatial dimensions of the order of nano- ( $10^{-9}$ ) m, cellular micro- or meso- (micro- ( $10^{-6}$ ) m and micro- or milli- ( $10^3$ ) s, tissue and organ macro levels (spatial dimensions range from millimeters to meters and from milliseconds to days time characteristics -  $10^5$  s and decades -  $10^8$ ).

Therefore, a universal model of a biological system cannot be imagined. Such a hypothetical model corresponds to the words of the founder of cybernetics, Norbert Wiener: "The best model of a cat is another cat, preferably the same cat". It doesn't get any easier to learn than the original object. Therefore, the construction of the model should answer the specific questions of the researcher, and the mathematical tools of modeling should depend on the specific problem being solved.

Naturally, given the complexity of biological systems and the corresponding mathematical models, the main tool for their analysis is computational experience. In this course, we will look at classical models of mathematical biology, which are mainly small-scale concentrated systems. An important step in the analysis for these models is the qualitative analysis of the dynamical system, which is discussed in later sections of this section.

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