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RESEARCH OF MAJOR INFORMATION TASKS SOLVED BY THE MATHEMATICAL MODELING OF DIFFUSION PROCESSES

Muayad Omar Abdullah, Anatoly A. Berezovsky

Odessa National Polytechnic University,
1 Shevchenko Ave., Odessa, 65044, Ukraine; e-mail: omarukrain@yahoo.com

The multimedia information technology to implement tools of mathematical modeling in anomalous diffusion processes are considered. The basic information tasks are studied and the basic requirements for information technology, focused on solving the problems of mathematical modeling are analyzed.

Keywords: multimedia information technology, diffusion process, mathematical modeling, numerical experiment

Introduction

The main set of problems being solved in the mathematical modeling, comprises the development of mathematical models (MM) processes being studied and the development of computational and numerical methods of implementing these MM. In this case, as a rule , the conservation laws (of mass, energy, momentum, etc.) which derive the dynamic equations, initial and boundary conditions (the essence is MM) are studied; the analytical and numerical methods for solving the dynamic equations are developed ,as well as the qualitative properties received as a result of the solutions (the research of existence, uniqueness, convergence and accuracy of the solutions; the definition of computational costs of the solutions, carrying out testing of the proposed MM, etc.).

However, there should be also recognized the important issues related to the presentation obtained through the solutions of the mathematical modeling. First of all, this aspect relates to the use of information technology (IT) and is associated with the submission, analysis and implementation of the solutions obtained.

The aim of the work

The aim of this work is identification and analysis of the basic requirements for the information technology oriented to presenting the results of the mathematical modeling in the diffusion (including the so-called «anomalous») processes.

The main part

The problems arising (as noted above) in interpreting the results of the mathematical modeling consist in the following. In a number of important practical cases in the mathematical modeling the diffusion processes (DP) are considered as processes with distributed parameters. The spatial area of RP processes in the simulation is a finite grid nodes [1–3] or finite elements [4, 5], and the function of the state an array of values of the grid functions at these nodes (or functions in finite elements). Depending on the desired accuracy of the solution, obtained grid functions array (in finite elements) have considerable

dimensions ($10^2 - 10^5$ values). Considering such quantity of values the possibilities to interpret the solutions become of paramount importance (for example, the ordering of arrays of values and form of presentation, methods of storage and handling, conversion, etc.).

In addition, the results of mathematical modeling are often only an intermediate link in the solved application problem. For example, in solving problems of technological or natural processes control (technical objects) as a result of mathematical modeling receive function of the state of the object on which (taking into account the control law) control action is synthesized. Thus, usually, the control action synthesis must be manipulated in real (or even accelerated) time-scale in the case of solutions of optimization or multivariate tasks. Given the fact that the technological or natural processes (technical facilities), as noted earlier, primarily represent RP processes (RP-objects) (with their inherent features and complexities of mathematical modeling and above all – the considerable size of arrays that define the values of state function), the rational methods of data processing is a priority. In these circumstances, the IT oriented to development and application of methods and tools for processing the results of mathematical modeling are relevant scientific and applied technical problem.

Implementation of computer simulations in the practice of theoretical studies and a wide range of data processing technology has solved fundamentally new problems, and, in some cases, has led to the emergence of new domains, the existence of which was not possible before the appearance of modern computer technology (CT) and the development of IT. Formation of a broad class of modern theoretical and applied areas of research (such as those associated with the atmosphere, mining and other physically complex processes and facilities that are experiencing a certain kind of diffusion anomalies) was fully possible only thanks to the emergence of computer simulation. Examples of the most important areas of research in which mathematical (computer) modeling plays a major role, are, in particular, the problem of numerical weather prediction, climate change, and issues related to air pollution and other environmental components.

The need for the use of IT, in this case, is due to several reasons:

- the equations that describe the various processes that can not be solved analytically without using numerical methods, the implementation and interpretation of which are due to the use of IT tools;
- modeling of this class of processes related to the huge amount of computation, often requiring the use of the most powerful computational tools and advanced IT;
- the only experimental data on the state of the complex processes are the data of many observations (for example, for geological processes is well-drilling and measurement of reservoir pressure in them; for processes in the atmosphere is the definition of the characteristics of it condition by ground stations, weather balloons, aircraft, various systems remote sensing based on ground-based radars and satellites in orbit), and the assimilation of such an extensive set of data from different sources is not possible without the use of modern processing systems, data collection and transmission of information;
- conducting simulations (including mathematical) involves the manipulation of large size of intermediate data and analysis (for example, ordering the long-term prognosis, etc.) of the obtained results, the effective carrying out of which is not possible without the use of various IT;
- series of mathematical modeling (especially in the field of regional and global climate seismic surveying and geo-ecology; variational data assimilation of complex technological processes) is the need to maintain huge data archives, regular and effective access to which is to be provided by means of IT.

If we consider the mathematical modeling in conjunction with implementing its IT, then, in this case, it is permissible to speak of information and mathematical modeling (MI-simulation) [4, 6]. The process of MI-simulation includes: gathering the necessary information (in accordance with the intended purpose), component (determining) the

information model of the process (object) processing of the data (their organization or structuring) and the algorithm to convert the data (encapsulation), the formation of MM process (object); geometrization of the model or the results of its numerical implementation (computer visualization using computer graphics – perform geometric constructions).

Thus, we can conclude that for solving mathematical modeling problems the IT provide the preparation (and if necessary, collection, such as in the case of atmospheric modeling) source data and interpret the results of the solution in a convenient form or, more generally, act as an IT tool implementation methods and mathematical modeling, accounting, in conjunction with the latter, the basis of MI-simulation in which IT resources and mathematical modeling of the most effective complement each other in the course of solving applied problems.

Typical information technology structure, focused on solving the problems of mathematical modeling. The most important factor in determining the effectiveness of IT is its structure (i.e., the elements that make up the IT and topological relationships between them).

Academician A. Samarskiy proposed IT [6, 7], the structure of which (Fig. 1) best meets the objectives of mathematical modeling solutions. The structure of the IT presented in the form of a triad «Model — Algorithm — Program» is uniquely defined plan of action using the methods of mathematical modeling:

- select (or construct) «equivalent» object reflecting in mathematical form, its most important properties - laws to which it is subject, communications inherent in its constituent parts, etc. (In other words, the essence MM);
- selection (or development) of the algorithm for implementation of the model on the computer;
- the creation of programs, «transforming» the MM algorithm and an available computer language.

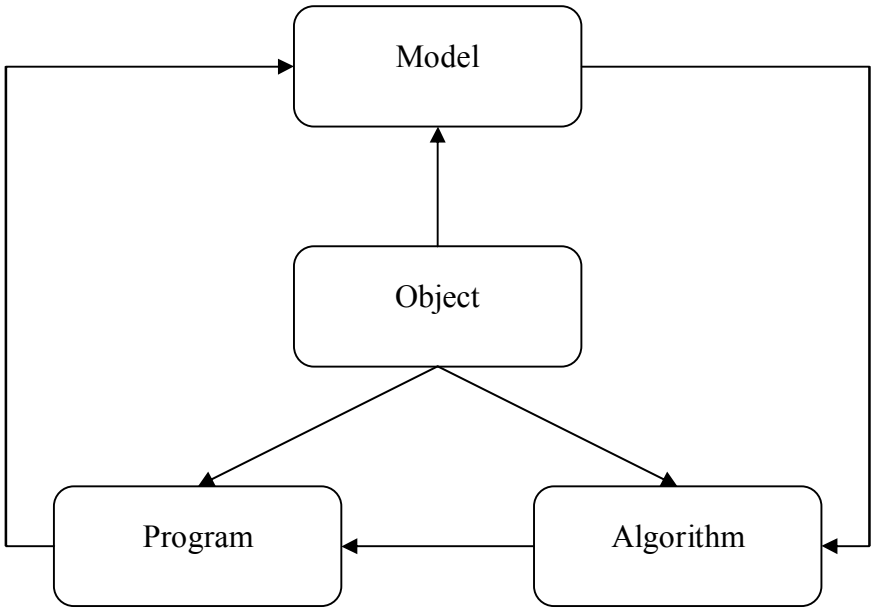

Fig. 1. The structure of IT oriented to solve mathematical modeling problems (typical structure)

About the properties of this structure is necessary to note the following. MM as the most important element of the triad should be adequate to the object under study (the process). This should be confirmed by an experiment of some kind (i.e., the «behavior» of the real object (process) and MM under the same conditions should be the same). After

establishing the adequacy of the triad of the original object with MM held a variety of «experiments»: computational experiments that provide all of the required quality and quantity of the properties and characteristics of the object (process). Computational experiment is designed to study, forecasting, optimization of complex (including multi-parameter and nonlinear objects (processes)), which theoretical and experimental research with traditional methods is difficult.

Computational experiment, in contrast to the experiments on full-scale objects (processes) can accumulate the results obtained in the study of a variety of problems, and then quickly and flexibly to apply them to solve problems in completely different areas. This property has a «universal» MM formalizing the majority of PD. For example, the nonlinear heat equation is suitable for describing not only the thermal processes, but also the diffusion of matter, the movement of ground water, gas filtration in porous media. Changes only the physical meaning of the quantities in this equation. The modeling process is accompanied by the improvement and refinement, as appropriate, all parts of the triad.

It should be noted that the current state of CT and modern numerical methods performs simulations of objects that describe the behavior of highly complex mathematical relations, such as non-linear systems of differential or integral equations. But the complex computational algorithms have their own internal properties, which are not always similar, even up to the error of approximation, the properties of the original MM. This may give rise to effects that are purely computational nature. Therefore, an important problem in the theory of numerical methods is (in relation to the structure under consideration IT) development of computational algorithms that exclude or minimize the occurrence of such situations. The problem of developing adequate MM to describe the various DP, as well as methods of implementing, remains relevant. An important role in this triad play programs realizing computational algorithms. They need to ensure the effectiveness of the solution of a mathematical problem with a minimum of computational effort.

Thus, IT, supporting computational experiment in the structure include: methods of construction of the MM information support to the implementation of recent search and selection algorithms and software for the numerical solution of problems, methods and control of accuracy and correctness of calculations made of the applicable programs.

Given the above, the structure IT, shown in Fig. 1, can be taken as a typical model (generalized), which is focused on solving the problems of mathematical modeling, as it covers all the main aspects of the solution of this class of problems. On the basis of the typical structure of IT the IT structure are formed, intended for applications of mathematical modeling.

Analysis of the basic requirements for information technology, focused on solving the problems of mathematical modeling of diffusion processes

Obviously, the IT solution providing a particular class of mathematical modeling (in particular, simulation of diffusion processes) must meet certain requirements. These requirements reflect the connection between the main (basic) properties studied in the mathematical modeling of objects, processes and phenomena with the means used by IT and, ultimately, determine the effectiveness of the latter.

Let’s perform the analysis of the basic requirements for solving an IT-oriented problems of mathematical modeling of diffusion processes. Considering the mathematical modeling of diffusion processes, include the following requirements to the basic ones:

- the ability to handle the significant volume of arrays of numeric information, which is the field values of the unknown functions for the DP state. Moreover, this manipulation is to provide both a multi-dimensional array operations (mainly two-and three-dimensional) and the ability to obtain results in real (or even accelerated) time scale, taking into account the subsequent decision of multivariate optimization and control tasks;

- the ability to adequately reflect the qualitative dynamic behavior of DP at the stage of visualizing the solutions for mathematical modeling, taking into account mainly the distributed nature of the processes under study. In other words, when rendering the solutions received (or displayed) by this or that IT the former should adequately, i.e. up to the full-scale experiments on the real object (process) reflect its dynamic behavior considering the effect on of external disturbances and control on the object (process);
- the establishment of the effective (in terms of the computational cost) numerical methods for implementing the mathematical modeling of the DP in IM modeling procedures. The complexity of formalizing the problems of mathematical modeling in the DP imposes higher demands on the computational costs for the machine implementation of the methods applied in the use of IT for numerical study of DP, due to, in particular, the ultimate non-representability of the MM in DP, non-trivial character of spatial modeling and boundary conditions. Eventually, the computational costs for implementing the mathematical modeling methods determine the effects of these techniques (as part of the MI-simulation technology) under the specified criteria;
- the ability to automate the process of mathematical modeling in DP. That is, IT must ensure that the «liberation» of the man-researcher from unproductive labor-intensive operations of the computing process (for example, the task of geometry and spatial sampling areas, the definition of the parameters of discrete spatial regions, counting these parameters while solving the time-dependent and non-linear problems, task, counting and entering the initial and boundary conditions, etc.), leaving the man-researcher if necessary the function analysis and decision making based on the results of mathematical modeling.

Conclusion

The basic requirements to an IT oriented to problem solving of mathematical modeling in diffusion processes are presented. Possible ways of improving the effectiveness of IT in the applied research are described, as well as, the possibility of interpreting the structure of a typical IT to solve scientific and engineering problems is analyzed.

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ДОСЛІДЖЕННЯ ОСНОВНИХ ІНФОРМАЦІЙНИХ ЗАДАЧ, ЯКІ ВИРІШУЮТЬСЯ ПРИ МАТЕМАТИЧНОМУ МОДЕЛЮВАННІ ДИФУЗІЙНИХ ПРОЦЕСІВ

Омар Муааяд Абдуллах, А.А. Березовський

Одеський національний політехнічний університет,
просп. Шевченка, 1, Одеса, 65044, Україна; e-mail: omarukrain@yahoo.com

Розглядається мультимедійна інформаційна технологія реалізації засобів математичного моделювання аномальних дифузійних процесів. Досліджено основні інформаційні задачі та виконано аналіз базових вимог щодо інформаційних технологій, які орієнтовано на розв'язання задач математичного моделювання.
Ключові слова: мультимедійна інформаційна технологія, дифузійний процес, математичне моделювання, обчислювальний експеримент

ИССЛЕДОВАНИЕ ОСНОВНЫХ ИНФОРМАЦИОННЫХ ЗАДАЧ, РЕШАЕМЫХ ПРИ МАТЕМАТИЧЕСКОМ МОДЕЛИРОВАНИИ ДИФФУЗИОННЫХ ПРОЦЕССОВ

Омар Муааяд Абдуллах, А.А. Березовский

Одесский национальный политехнический университет,
просп. Шевченко, 1, Одесса, 65044, Украина; e-mail: omarukrain@yahoo.com

Рассматривается мультимедийная информационная технология реализации средств математического моделирования аномальных диффузионных процессов. Исследованы основные информационные задачи и выполнен анализ базовых требований к информационным технологиям, ориентированных на решение задач математического моделирования.
Ключевые слова: мультимедийная информационная технология, диффузионный процесс, математическое моделирование, вычислительный эксперимент