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Study of radiation transfer using the computational educational manual on Monte Carlo methods*

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It is well-known that Monte Carlo methods are used for solving various urgent problems in mathematical physics [1, 2]. A lot of new numerical stochastic algorithms and models were elaborated in Institute of Computational Mathematics and Mathematical Geophysics (ICM and MG) SD RAS during last years. The Monte Carlo schemes can be effectively illustrated on computer and presented for students. On the other hand, the special instrumental environment based on hypertext technology is developed in ICM and MG. These computer tools can be used for elaboration of training mathematical courses.

Now the electronic manual "Foundations of Monte Carlo methods" is developed in ICM and MG for students of Novosibirsk State University [3, 4]. This manual is based on lectures of Prof. G.A. Mikhailov and Dr. A.V. Voytishek [1, 2]. The central themes of this course are:

- methods of realization of generators of standard random and pseudorandom numbers,
- methods of numerical modeling of discrete and continuous stochastic values (including standard and special algorithms for discrete values; the reverse distribution function method, randomization and rejection technique for continuous values),
- numerical realization of stochastic vectors,
- methods of modeling of stochastic processes and fields,
- methods of calculation of multiple integrals,
- numerical methods of solution of the integral equations of the second kind,
- numerical solution of equations of mathematical physics,
- applications of Monte Carlo methods (including problems of the radiation transform theory).

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The manual is divided in lessons containing many illustrations, diagrams, model tasks, exercises, questions, and comments. The model tasks are the effective means for study of mathematical courses. They satisfy a lot of requirements: simplicity of using, unified interface, multifunctionality on elements of training. In particular, the model programs provide the output of the formulas in usual mathematical form, window input of parameters, using of graphics for visualization of results, operative formulation of rules for dealing with programs.

Model tasks of the course "Foundations of Monte Carlo methods" can be divided in two classes:

- the tasks for study the basic concepts of Monte Carlo methods,
- the tasks for demonstration of the applications of Monte Carlo methods for modeling of processes and phenomena.

The model tasks of the first class provide the creation of diagrams, dynamic changing of their scales and coordinate systems, cleaning the fields of diagrams, setting their colours, creation of several diagrams on one field, comparative analysis of them, storage and reproduction of received graphic results. Some related tasks can be united to one complex task.

The model tasks of the second class provide the graphic illustration of structure and functioning of algorithms. The process of modelling is considered as a sequence of elementary random events. Individual realizations are repeated and the statistic data is collected. For study and demonstration of the algorithm it is possible to use step-by-step and series realizations.

For realization of model tasks of the electronic manual the Delphi system is used. It provides object-oriented visual discipline of programming. It is also convenient for development of the Windows applications. In the Delphi system the interface components are used as the structural units of visual programming. Every component is treated as an object, which has its own properties and methods for dealing with. The realization of a model task begins with the development of its project: the specifications and definitions of the requirements to the interface. The results of designing are defined then in terms of the Delphi objects. The Delphi system creates the program, which can be used outside of the system (in particular, it can be included in computer manual).

Consider the features of the computational educational manual on Monte Carlo methods using as an example the lesson "Investigation of problems of the radiation transform theory".

The typical mathematical model of the transfer process is as follows.

Let G be a convex domain (in the electronic manual it is possible to choose the geometry of G), which includes non-homogemeous substance, and in the point $\bar{r}_0 \in G$ the source of radiation (directed or stochastic) is located (Figure 1). The small particles of radiation (fotons, neutrons,

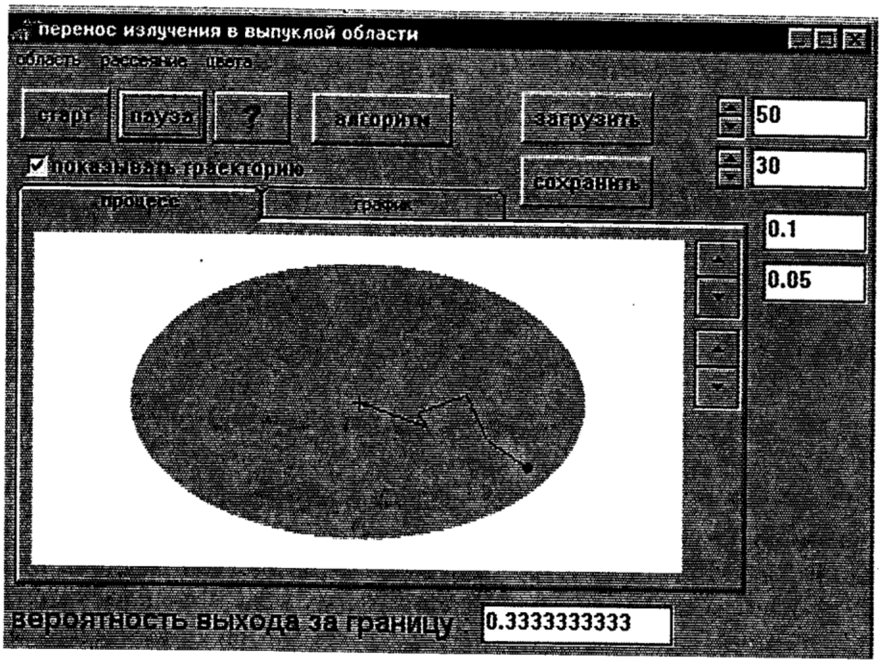

Figure 1. The main window for the lesson "Investigation of problems of the radiation transform theory"

etc.) interact with larger particles of substance in the domain. They can be absorbed by large particles or dissipate under some stochastic law. The trajectories of small particles of radiation can be numerically realized and it is possible to calculate various characteristics of the radiation process. Consider, for example, the problem of calculating the probability P of the following stochastic event: the small particle of radiation is absorbed in the domain G (in other words we determine the quota of the absorbed radiation in G). There are a lot of applications of such models: protection of nuclear reactors, climatic problems, problems of laser sounding of atmosphere and ocean and many other (corresponding examples are presented in the lesson "Applications of Monte Carlo methods").

In the electronic manual it is possible to investigate the process of radiation transform using step-by-step realization of trajectories of radiation particles.

At first, for each particle the direction of movement from the point $\bar{r}_0$ is determined. In the three-dimensional case this direction is a two-dimensional (in spherical coordinates) stochastic vector $\bar{\omega} = (\omega_1, \omega_2)$. If the joint stochastic distribution density $p_{\bar{\omega}}(u_1, u_2)$ of this vector is given, then we construct the algorithm of its realization using the approaches from the lesson "Numerical realization of stochastic vectors". The joint density is presented as a product

$$p_{\bar{\omega}}(u_1, u_2) = p_{\omega_1}(u_1) p_{\omega_2}(u_2 \mid \omega_1 = u_1), \tag{1}$$

where

$$p_{\omega_1}(u_1) = \int p_{\bar{\omega}}(u_1, u_2)\, du_2, \qquad p_{\omega_2}(u_2 \mid \omega_1 = u_1) = \frac{p_{\bar{\omega}}(u_1, u_2)}{p_{\omega_1}(u_1)},$$

or

$$p_{\bar{\omega}}(u_1, u_2) = p_{\omega_2}(u_2)\, p_{\omega_1}(u_1 \mid \omega_1 = u_2), \tag{2}$$

where

$$p_{\omega_2}(u_2) = \int p_{\bar{\omega}}(u_1, u_2)\, du_1, \qquad p_{\omega_1}(u_1 \mid \omega_2 = u_2) = \frac{p_{\bar{\omega}}(u_1, u_2)}{p_{\omega_2}(u_2)}.$$

The choice of presentation (1) or (2) is a problem for investigation. Let, for example, formula (1) be chosen. Then the first coordinate ω_1 is realized with respect to the density $p_{\omega_1}(u_1)$, and the second coordinate is realized with respect to the conditional density $p_{\omega_2}(u_2 \mid \omega_1 = u_1)$, here u_1 is the result of modeling of ω_1. Algorithms for realization of stochastic values with respect to the given densities are studied in the lessons "The reverse distribution function method", "Randomization technique", and "Rejection technique". Corresponding model tests of these lessons allow to construct histograms and polygon of frequencies which interpolate the densities under realization.

After choosing the direction $\bar{\omega}$, the length of free run τ of the small particle (i.e., length of a piece of particle's way without collisions). The following assumption is used: the probability $\tilde{p}$ of a collision in an interval $(x, x + \delta x)$ (the axis x has the direction of particle's movement) is equal to

$$\tilde{p} = \Sigma(\bar{r})\, \delta x + o(\delta x). \tag{3}$$

The function $\Sigma(\bar{r})$ ($\bar{r}$ designates the coordinate of a particle in the "external" three-dimensional coordinate system) is supposed to be given, it is called *the complete interaction section of a particle with environment.* It is simple to obtain from (3) that the random length of free run of a radiation particle has the distribution function

$$F(x) = 1 - \exp\Big(-\int_0^x \Sigma(\bar{r} + \bar{\omega} s)\, ds\Big). \tag{4}$$

In the case when $\Sigma(\bar{r}) \equiv \text{const}$ (it means that the substance in G is homogeneous) the function F from (4) is the exponential distribution function, which is investigated in every detail in the lesson "The reverse distribution function method"; the modeling formula is $\tau = -\ln\alpha/\Sigma$. Here α is a standard stochastic number, i.e., a realization of the uniformly distributed on

$[0, 1)$ stochastic value; corresponding numerical algorithms are presented in the lesson "Methods of realization of generators of standard random and pseudo-random numbers".

For the non-constant Σ there exists a lot of algorithms for realization of τ in various situations (including the rejection technique). Students also have the possibility to realize and investigate their own numerical procedures for realization of τ. Many interesting problems are related with the case, when $\Sigma(\bar{r})$ is a stochastic function. There exists a wide class of algorithms for realization of trajectories of stochastic functions, some of them are presented in the lesson "Methods of modeling of stochastic processes and fields". For every trajectory of Σ its own series of trajectories of small particles is realized.

In the finish point of the free path of small particle, two situations may occur: the small particle leaves the domain G (for this case the trajectory of the particle stops), or the collision when the large particle takes place. For every collision, we draw the event of absorption or dissipation. This procedure is equal to the realization of the Bernoulli stochastic value, corresponding algorithms are studied in the lesson "Methods of numerical modeling of discrete stochastic values". The section function $\Sigma(\bar{r})$ is presented as a sum of non-negative functions $\Sigma(\bar{r}) = \Sigma_a(\bar{r}) + \Sigma_d(\bar{r})$ and $p_a(\bar{r}) = \Sigma_a(\bar{r})/\Sigma(\bar{r})$ is treated as a probability of absorption in the point $\bar{r}$; the probability of dissipation is equal to $p_d(\bar{r}) = 1 - p_a(\bar{r}) = \Sigma_d(\bar{r})/\Sigma(\bar{r})$. It is also possible to draw in the same way some other events: the splitting of the small particle, the changing of the type or energy of a particle and so on.

If the absorption occurs, then the trajectory stops, otherwise, a new direction of free path is realized with respect to conditional density $g(\bar{\omega} \mid \bar{\omega}')$ (which is called *the indicatrix of dissipation*), where $\bar{\omega}'$ is the direction before the collision. Then, a new free path τ is realized, absorption or dissipation is drawn, and so on till a leaving from G or a collision with absorption occurs. The probability P is approximately equal to $P(N) = N_a/N$, where N is the number of realized trajectories and N_a is a number of absorbed small particles. In the computional manual, it is possible to obtain the graph of the dependence $P(N)$, see Figure 2.

Note that the process of radiation transfer can be defined in terms of integral equations of the second kind. Thus, the weighted algorithms can be used in the case, when the given distributions are not handy for numerical realization. These algorithms are investigated in the lesson "Numerical methods of the solution of the integral equations of the second kind".

So the lesson "Investigation of problems of the radiation transform theory" gives students the opportunity to study many important applications of Monte Carlo methods and also to consolidate knowledge about fundamental facts of the theory of stochastic modeling. They can also test new numerical methods in this field.

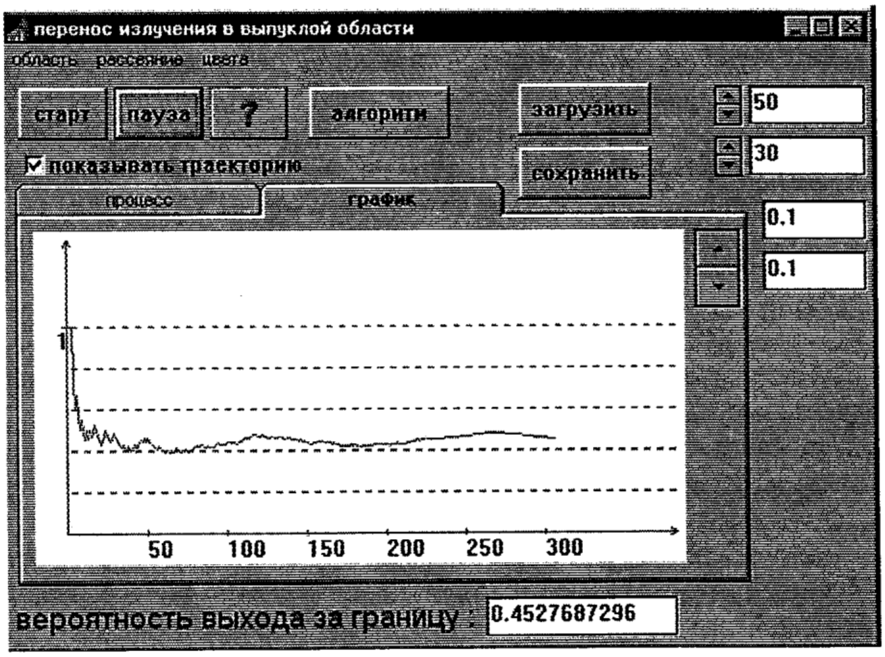

Figure 2. The window for the graph of the dependence $P(N)$

References

[1] Ermakov S.M., Mikhailov G.A. Statistical Modelling. – Moscow: Nauka, 1982 (in Russian).

[2] Voytishek A.V. Foundations of the Monte Carlo Methods in Algorithms and Problems. Parts 1–5. – Novosibirsk State University, 1997–1999 (in Russian).

[3] Bezanova M.M., Voytishek A.V., Kvashnin G.A., Moskvina L.A. Principles of arrangement for the computational supply "Foundations of the Monte Carlo Methods" // Proceedings of International Sceintific Methodological Conference "New Information Technologies in University Education". – Novosibirsk, 1996. – P. 36–37 (in Russian).

[4] Bezanova M.M., Voytishek A.V., Kvashnin G.A., Moskvina L.A. Architecture and functioning of mathematical educational course // Proceedings of International Sceintific Methodological Conference "New Information Technologies in University Education". – Novosibirsk, 1997. – P. 22–23 (in Russian).