
# Creation of an algorithm and software complex for solving parabolic type boundary value problems by statistical modeling method

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**ABSTRACT**

The constant and unrelenting interest in the application of statistical modeling (Monte Carlo methods) both for research purposes and for solving practical problems is due to many factors. First of all, Monte Carlo methods are used for computational experiments to determine the properties of such phenomena for which the probabilistic model is, on the one hand, the most adequate and, at the same time, quite effectively implemented.

**Keywords:** Monte Carlo method, Schwartz, Brownian movement, random point.

At the same time, the complexity of the problem being solved can increase by changing just one parameter. In particular, when solving systems of algebraic equations, there is such a threshold value of dimension, after which the application of the Monte Carlo method becomes obviously more efficient. A similar situation arises as a result of the complication of the geometry of the computational domain in computer graphics problems, as well as in problems of calculating the macroscopic properties of the medium and individual molecules.

In many cases, probabilistic models for describing a phenomenon are used in conjunction with various other models that differ from each other in scale, degree of detail, and, as a result, the applied mathematical apparatus. The coordination of these models, as well as the algorithms created to solve the problems posed within the framework of these models, is a natural requirement that ensures their validity and consistency. For natural phenomena, which are described at the macrolevel by differential equations in partial derivatives of elliptic and parabolic types, the matching conditions are that the macroparameter that satisfies the equation is represented as a functional of a random diffusion process.

The relevance of continuing research in this direction and creating new statistical modeling algorithms for estimating the parameters of natural phenomena described by parabolic and elliptic equations is explained, in particular, by the need to solve problems of determining the macroscopic properties of disordered media and bodies with complex geometry, such as, for example, macromolecules, immersed in a salt solution. Despite the rapid development of computer technology, computer simulation of solutions

to such problems, based on a detailed description of the molecular structure, is feasible only for the simplest cases. For this reason, various averaged models are used, leading to elliptic or parabolic equations.

The specificity of the mathematical formulation of these problems lies in the fact that at the boundary conditions are required not only for the solution of the differential equation itself, but also for the conditions that the flow must satisfy, that is, in fact, the limit value of the normal derivative of this solution. Accounting for such boundary conditions is a difficult algorithmic problem, due to the fact that the boundary surfaces have a very complex structure. Additional difficulties arise as a result of the need to solve the problem not in a limited area, but in the entire space.

The use of statistical modeling algorithms makes it possible to overcome many of the existing problems. A feature of the Monte Carlo methods applied to solving problems related to elliptic and parabolic equations is the ability to accurately take into account complex geometric details and the behavior of the solution at infinity.

Theorem 1.1. If the estimate ξ[uj](x) defined by equality (1) is an unbiased estimate of the solution of the Dirichlet problem in each of the subdomains Gj considered separately, then the estimate ζ[u](x) constructed in accordance with the formula ( 2) will be an unbiased estimate of the solution of the Deer problem to the left of the entire domain:

$$G = \bigcup_{j=1}^{M} Gj.$$

If estimate(1) has some bias:

$$E\xi[uj](x) = uj(x) + \delta j(x),$$

where $|\delta j(x)| \le \varepsilon Bj$, and $Bj = \sup|uj(x)|$, then the estimate ζ(x) of the solution of the Dirich left domain problem $x \in GjG$ is also biased and:

$$|E\zeta(x) - u(x)| \le \frac{\varepsilon}{1-(\varepsilon+q)} B,$$

where $q = \max_{i,k} qi,k$, $B = \sup_{x \in G} |u(x)|$. Here $qj,k<1$ is the lemma constant

Schwartz in application to the parapods of the Gj and Gk areas.

Next chapter is devoted to the application of the constructed methods of statistical modeling to solving model and applied problems. The first section presents the results of calculations obtained based on the use of algorithms developed in the dissertation and Monte Carlo to determine the diffusion-conditioned constant you are the reactions. A macromolecule is considered as a compact set $G \subset R\ 3$ , bounded by a simply connected piecewise Lyapunov surface ∂G. The reaction constant of a macromolecule G with Brownian particles is determined by is expressed as the integral flux of these particles on the surface of the molecule. The problem of calculating the diffusion-conditioned reaction constant K reduces in the stationary case to solving an external boundary value problem for Laplace equations:

$$\Delta u(x) = 0\,,\ x \in G_1 = \mathbb{R}^3 \setminus \overline{G}\,,$$
$$\kappa_s(y)u(y) - D\frac{\partial u}{\partial n}(y) = \kappa_s(y),\ y \in \partial G\,,$$
$$\lim_{|x|\to\infty} u(x) = 0\,.$$

Here u = 1 − ρ. ρ(x) is the particle concentration, D is the differential coefficient fusion. The calculations are based on the formula K = 4πRD u(R), where u(r) = ∫

$$\int d\Omega\ \frac{1}{4\pi} u(r, \Omega),$$

and R is such that G ⊂ B(x, R) for some x. Randomize the use use of this formula leads to the following Monte Carlo estimate:

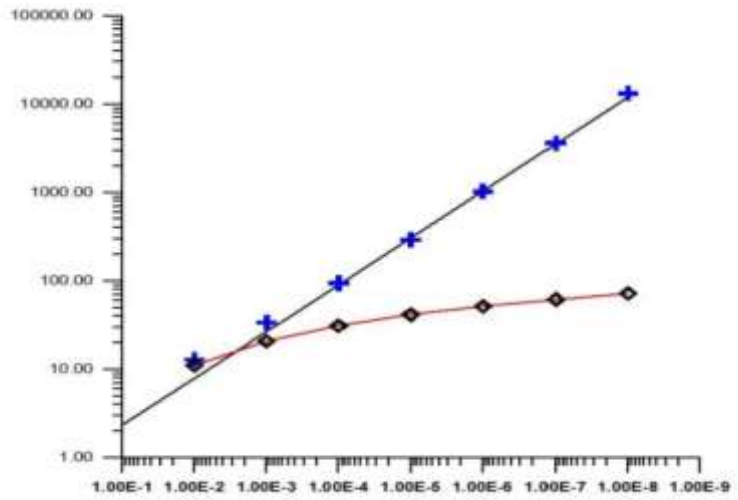
K = 4πRD E ξ(x0)

Here the random point x0 is uniformly distributed on S(x, R), and ξ is not an estimate of the solution of problem (35) that depends on it. This estimate is based on the vectors of random walk over spheres with direct simulation of drift to infinity (A.S. Sipin's method).

At the first hit in ε- neighborhood of the boundary, the randomization of the finite-difference approximation to the boundary

condition of the third kind. For a particular case, mix boundary value problem (Solc-Stockmayer model) or the Neumann problem using uses an algorithm based on the randomization of the mean formula, built in the first chapter. The results of test calculations show the effect the effectiveness of the proposed algorithms in comparison with those used earlier estimates based on direct modeling of the Brownian movement.

The second paragraph presents the results of numerical experiments for solving problems with boundary conditions that include the normal derivative of the solution. The properties of the constructed methods are clarified. On the example of a mixed problem for a cube in which the Neumann condition is satisfied on one of the faces, and the solution is equal to zero on all the others, the efficiency of the algorithm constructed in the first chapter is shown (see Fig.1).




Rice. 1: Dependence on ε (width of the border strip, in log-log scale) of the average number of transitions in a sphere walk, in which the reflection from the boundary with the Neumann conditions was carried out in accordance with with the spherical mean relation (7) (diamonds). Calculation results are approximated by the dependence EN = −4.419 ln ε−9.505, i.e., EN has the same order as in solving the Dirichlet problem. For comparison, we show the dependence of the average number of transitions when using the finite difference approximation to the normal derivative (crosses). The calculation results are approximated by the power dependence EN = 0.691 h −1.059. Here h = ε −1/2 is the approximation step.

The supplement describes the results of research on the development of algorithms and numerical experiments for solving equations that are neither elliptic nor parabolic. The results of calculations for solving the equations by Monte Carlo methods are presented. Euler (ideal gas dynamics) in integral form.

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