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CREATION OF NEW NUMERICAL SIMULATION ALGORITHMS FOR SOLVING INITIAL-BOUNDARY-VALUE PROBLEMS FOR DIFFUSION EQUATIONS

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Abstract. This article uses the Monte Carlo method to solve initial-boundary value problems in the diffusion equation. A Markov chain with absorption on the trajectory of this chain is constructed, an unbiased estimate for solving problems is constructed. Examples of estimates of solution functionals are given and the behavior of their variances is discussed. The resulting integral equation is solved using branched Markov chains with absorption.

Keywords: monte Carlo method, statistical modeling, diffusion equation, set-boundary problem, Markov chain, absorbing Markov chain, branching Markov chain, integral equation, dynamic solution generation, variance estimation, Brownian motion, transition function, parabolic equation, ultraparabolic equation, mathematical modeling, numerical mechanisms, e. conductivity, mathematics, investment portfolio, risk management, biological models, ecological processes, process algorithms, critical processes, boundary problems, diffusion processes, statistical control, computer modeling.

Аннотация. В данной статье для решения начально-краевых задач уравнения диффузии используется метод Монте-Карло. Построена цепь Маркова с поглощением на траектории этой цепи, получена несмещенная оценка для решения задач. Приведены примеры оценок функционалов решений и обсуждено поведение их дисперсий. Полученное интегральное уравнение решается с использованием разветвленных цепей Маркова с поглощением.

Ключевые слова: метод Монте-Карло, статистическое моделирование, уравнение диффузии, граничная задача, цепь Маркова, поглощающая цепь Маркова, разветвляющаяся цепь Маркова, интегральное уравнение, динамическое генерирование решений, оценка дисперсии, броуновское движение, функция перехода, параболическое уравнение, ультрапараболическое уравнение, математическое моделирование, численные механизмы, например, проводимость, математика, инвестиционный портфель, управление рисками, биологические модели, экологические процессы, алгоритмы процессов, критические процессы,

краевые задачи, диффузионные процессы, статистический контроль, компьютерное моделирование.

Annotatsiya. Ushbu maqola diffuziya tenglamasi uchun boshlang'ich-chegaraviy masalalarni yechish uchun Monte-Karlo usulidan foydalanadi. Markov zanjiri uning traektoriyasi bo'ylab yutilishi bilan tuziladi va muammolarni hal qilish uchun xolis baho olinadi. Yechim funktsiyalari uchun baholarga misollar keltirilgan va ularning dispersiyalarining xatti-harakati muhokama qilinadi. Olingan integral tenglama yutilishli tarvaqaylab ketgan Markov zanjirlari yordamida yechiladi.

Kalit so‘zlar: monte-Karlo usuli, statistik modellashtirish, diffuziya tenglamasi, chegaraviy masala, Markov zanjiri, yutuvchi Markov zanjiri, tarmoqlanuvchi Markov zanjiri, integral tenglama, dinamik yechim hosil qilish, dispersiyani baholash, Broun harakati, o‘tish funksiyasi, parabolik tenglama, ultraparabolik o‘tkazuvchanlik mexanizmi, nufuzli parabolik o‘tkazuvchanlik tenglamasi, mana shunday. matematika, investitsiya portfeli, risklarni boshqarish, biologik modellar, ekologik jarayonlar, jarayon algoritmlari, muhim jarayonlar, chegaraviy muammolar, diffuziya jarayonlari, statistik nazorat, kompyuter modellashtirish.

INTRODUCTION.

Diffusion equations (parabolic and ultraparabolic) are the object of research in such areas as mathematical physics, theory of dynamical systems, biology, ecology, economics, finance, management and mathematical modeling. Diffusion equations are the basis for solving a wide range of problems: thermal conductivity, nuclear physics, dynamic systems, gas dynamics, biological population dynamics and genetics, dynamics of changes in the securities market, management of investment and financial portfolios, financial risk management and analysis of environmental processes. Therefore, the study of mathematical models and the solution of diffusion equations remains an important task in the areas of applied mathematics, finance and management [1–5].

A.N. Kolmogorov [6] showed in 1931 that the transition function $P(x,t,\Gamma)$ is the probability that a Brownian particle leaving the point x, after time t, entering the set Γ, satisfies a certain diffusion parabolic differential equation. In the course of its development, the apparatus of the theory of probability began to be successfully applied in the study of boundary value problems. Therefore, the study of mathematical models and the solution of diffusion equations remains an important task in the areas of applied mathematics, finance and management, etc. Many scientific and applied research carried out at the world level lead to the problems of creating mathematical models of initial-boundary value problems for diffusion equations, therefore, the

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numerical solution of such problems by the method of statistical modeling (Monte Carlo method) is of great importance [7–10].

Algorithms of the Monte Carlo method for problems with initial conditions have been little studied even in the case of ordinary differential equations. The only study with examples of Monte Carlo solutions for systems of ordinary differential equations was considered in [10]. In these cases, Monte Carlo methods can be more efficient than classical computational methods. If we bear in mind that the application of the Monte Carlo method, which has shown its effectiveness in multidimensional problems, then the development of methods of numerical integration in a system with many noises is highly relevant.

Formulation of the problem

Consider in $(n+1)$-dimensional space of $\mathbb{R}^{n+1}$ points (y,z,t), $y \in \mathbb{R}^k$, $z \in \mathbb{R}^l$, $t \in \mathbb{R}^1$, $k+l=n$ equation

$$Lu = \frac{\partial u(y,z,t)}{\partial t} - \sum_{i,j=1}^{k} a_{ij} \frac{\partial^2 u(y,z,t)}{\partial y_i \, \partial y_j} + \sum_{j=1}^{k} \sum_{m=1}^{l} \beta_j^m \, y_j \frac{\partial u(y,z,t)}{\partial z_m} = f(y,z,t)$$

with constant coefficients α_{ij} and β_j^m $(i = 1,2,\dots,k, j = 1,2,\dots,k, m = 1,2,\dots,l)$.

Let $\alpha = (\alpha_{ij})$ be a $k \times k$ matrix, $\beta = (\beta_j^m)$ be an $l \times k$ matrix.

We assume:

• Matrix $\alpha = (\alpha_{ij})$ symmetric and positive definite.

• Matrix $\beta = (\beta_j^m)$, such that $l \times l$ the Gram matrix $\omega = (\beta\alpha\beta^T)^{-1}$ is positive definite (non-degenerate).

Let $D \subset \mathbb{R}^n$ – bounded area with border ∂D. Let's combine the variables (y,z) into one space variable - column $x = (y^T, z^T)^T \in \mathbb{R}^n$ (T – transpose operation).

Consider in space $\mathbb{R}^{n+1}$ variables $(x,t) = (x_1, x_2, \dots, x_n, t)$ cylinder $\Omega = D \times [0,T]$.

For functions $\psi(x,t) \in C(\partial D \times [0,T])$ and $\varphi(x) \in C(\overline{D})$ the following initial and creative problem is posed: find the function $u(x,t) \in C(\overline{\Omega}) \cap C^{2,1}(\Omega)$ satisfying in the cylinder Ω equation

$$(Lu)(x,t) = f(x,t) \qquad (1)$$

with a condition

$$u(x,t) = \psi(x,t), \quad x \in \partial D, \quad t \in [0,T] \qquad (2)$$

and the initial condition

$$u(x,0) = \varphi(x), \quad x \in D. \qquad (3)$$

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Function $f(x,t)$ will be considered continuous in $\overline{\Omega}$. Agreement condition $\varphi(x) = \psi(x,0)$ for $x \in \partial D$, necessary for the solvability of the problem, we will assume that it is satisfied.

Assuming that there is a solution to problem (1) - (3), we construct an algorithm for its numerical implementation.

Representation of probabilistic problem solving and construction of a Markov chain

The most common Monte Carlo algorithm is based on modeling Markov chains.

Using a fundamental solution to the equation (1) with a singularity at the point (y,τ) in space $\mathbb{R}^{n+1}$ we define domains (spheres) as follows.

$$B_r(x,t) = \left\{(y,\tau): (y-Cx)^T d\left(\frac{1}{t-\tau}\right) ad\left(\frac{1}{t-\tau}\right)(y-Cx) \le \gamma^2 \ln\frac{r^2}{t-\tau},\ t > \tau\right\}. \qquad (4)$$

From (4) it can be seen that satisfies the following conditions: $\tau < t$, $\tau > t - r^2$. Each section of a spherical plane by a horizontal plane $\tau = \text{const}$, $t - r^2 < \text{const} < t$, is an n-dimensional ellipsoid centered at the point $\left(e^{-(t-\tau)\beta}x, \tau\right)$. If $\rho < r$, then $B_\rho(x,t) \subset B_r(x,t)$. At $r \to 0$, $B_r(x,t)$ and $\partial B_r(x,t)$ monotonically shrink to the center (x,t). Therefore, there is such $r > 0$ what with $(x,t) \in \Omega$, $B_r(x,t) \subset \Omega$.

Let $r > 0$ such that $B_r(x,t) \subset \Omega$. Then the solution to problem (1) - (3) satisfies the following relation

$$u(x,t) = (E_r u)(x,t) + f(x,t). \qquad (5)$$

where

$$(E_r u)(x,t)$$

$$= \left(\frac{\gamma}{\pi}\right)^{\frac{n}{2}} \int_0^1 \lambda^{\gamma-1}\left(\ln\frac{1}{\lambda}\right)^{\frac{n}{2}} \int_{S_1(0)} u\left(y(\lambda,\theta),\tau(\lambda)\right) T(\theta) 4b\alpha b^T(\theta)\, ds\, d\lambda,$$

$$f(x,t) = \iint_{B_r(x,t)} \left(Z(x,t;y,\tau) - \pi^{-\frac{n}{2}} a^{\frac{1}{2}} r^{-\gamma}\right) f(y,\tau)\, dy\, d\tau$$

$$y(\lambda,\theta) = e^{-r^2\lambda^2\beta}x + \left(\gamma \ln\frac{1}{\lambda}\right)^{\frac{1}{2}} d\left(\frac{r}{2\lambda^2}\right) b^{-1} H(\theta)$$

$$\tau(\lambda) = t - r^2\lambda^2. \qquad (6)$$

It follows from (6) that if $r(x,t) \le t^{\frac{1}{2}}$, then at $(x,t) \in \Omega$ we have $B_r(x,t) \subset \Omega$. We define in Ω Markov chain $\left\{\left(x^j, t^j\right)\right\}_{j=0}^{\infty}$ by the following recurrence relations:

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$$x^0 = x, \quad t^0 = t, \quad t^j = t^{j-1} - r_{j-1}^2 \exp\left(-\frac{2\xi_j}{\gamma}\right),$$

$$x_i^j = x_i^{j-1} + r_{j-1}^2 \exp\left(-\frac{\xi_j}{\gamma}\right) \xi_j^{\frac{1}{2}} \sum b_{im} \omega_i^j, \qquad (7)$$

$$x_{k+p}^j = x_{k+p}^{j-1} - r_{j-1}^2 \exp\left(-\frac{2\xi_j}{\gamma}\right) \sum_{o=1}^{k} \beta_{po}\, x_o^j$$

$$+ r_{j-1}^3 \exp\left(-\frac{3\xi_j}{\gamma}\right) \xi^{\frac{1}{2}} \sum_{\nu=1}^{n} b_{k+p,\nu}\, \omega_i^j.$$

where $i = 1,2,\dots,k$, $p = 1,2,\dots,l$, $j = 1,2,\dots$, $r_{j-1} = r\left(x^{j-1}, t^{j-1}\right)$.

Relations (7) are derived from formula (6). Now we can write formula (5) in the following form

$$u\left(x^{j-1}, t^{j-1}\right) = E_{\left(x^{j-1}, t^{j-1}\right)} u\left(x^j, t^j\right) + f\left(x^{j-1}, t^{j-1}\right)$$

We define a sequence of random variables $\{\eta_l\}_{l=0}^{\infty}$ by the following equality,

$$\eta_l = \sum_{j=1}^{l-1} h\left(x^j, t^j\right) f\left(y^j, \tau^j\right) + u(x^l, t^l), \qquad (8)$$

where $\left(y^j, \tau^j\right)$ is a random point of the spheroid $B_r(x,t)$ with fixed $\left(x^j, t^j\right)$, having a distribution density of

$$\frac{Z\left(x^j, t^j; y, \tau\right) - \pi^{-\frac{n}{2}} a^{\frac{1}{2}} r^{-\gamma}}{h(x^j, t^j)}$$

where

$$h(x,t) = \iint_{B_r(x,t)} \left(Z(x,t;y,\tau) - \pi^{-\frac{n}{2}} a^{\frac{1}{2}} r^{-\gamma}\right) dy\, d\tau.$$

Let $\{\Im_l\}_{l=0}^{\infty}$ - sequence σ-algebras generated by random variables $\xi_1, \xi_2, \dots, \xi_l$, sequence of vectors $\omega^0, \omega^1, \dots, \omega^l$ and random points $(y^0, \tau^0), (y^1, \tau^1), \dots, (y^{l-1}, \tau^{l-1})$, $u_{f,\psi,\varphi}(x,t)$.

The solution to problem (1) - (3) corresponding to the data f, ψ, φ.

Theorem [10]

a) The sequence $\{\eta_l\}_{l=0}^{\infty}$ forms a martingale with respect to the sequence σ-algebras $\{\Im_l\}_{l=0}^{\infty}$.

b) If $\| u_f \|_{2,0,0}\ (x,t) < +\infty$, then η_l is square integrable.

Let $N_\varepsilon = \min\{l: (x^l, t^l) \in (\partial\Omega)_\varepsilon\}$ - moment of the first hit of the process (x^l, t^l) in $(\partial\Omega)_\varepsilon$, i.e. N_ε is the moment of stopping the process (Markov moment).

Lemma [5]

The inequality

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$$E_{(x,t)}N_\varepsilon \le \frac{\gamma-2}{\gamma}\left(1+\frac{n}{2}\right)\frac{t}{\varepsilon}$$

holds.

NUMERICAL EXPERIMENT AND CONCLUSION.

As is typical for the numerical calculation of diffusion problems, the choice of a random spherical radius for the algorithm of wandering spheres creating trajectories of the Markov chain is essential, which characteristically preserves the properties of a finite propagation velocity, spatial localization, boundedness and destruction.

Solutions, which guarantees convergence with a given accuracy to the solution of the problem with the minimum number of trajectories. Note that due to the ambiguity of solutions in the numerical study, problem (1) - (3). Therefore, the question arises about the choice of the optimal radius of the approximation of the ball, which preserves the properties of convergent boundary value problems. Comparison of the statistical modeling method for solving boundary value problems by known grid methods suggests the following advantages of the first:

- simplicity and physical clarity;
- the ability to solve problems without significant simplifications (problems with complex multidimensional geometry and taking into account physical effects that have to be neglected when using other methods can be solved);
- the possibility of evaluating individual functionals without memorizing decision tables as a whole;
- the possibility of an empirical assessment of the error of the results under sufficiently broad assumptions;
- the possibility of parallel tracking of independent trajectories on multiprocessor computers, the algorithm is naturally parallelized.

As the area D we choose the unit cube with

$$f(x,y,z,t) = e^t\left(5\sin(x+y+z) + (x+y)\cos(x+y+z)\right)$$

$$\varphi(x,y,z) = \sin(x+y+z)$$

at $\alpha = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$, $\beta = \begin{pmatrix}1\\ 1\end{pmatrix}$.

Exact solution $u(x,y,z,t) = e^t\sin(x+y+z)$.

Table I.

Results of a numerical experiment

Number of trajectories	Point (x,y,z,t)	ε	Exact solution	Selective assessment	3-sigma
100	0.7, 0.7, 0.7, 0.7	0.005	1.738	1.732	0.017

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500	0.6, 0.6, 0.6, 0.6	0.005	1.774	1.647	0.005
100	0.6, 0.6, 0.6, 0.3	0.005	1.315	1.317	0.005
100	0.8, 0.8, 0.8, 0.8	0.005	1.503	1.513	0.020
100	0.5, 0.5, 0.5, 0.3	0.005	1.349	1.358	0.0058

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