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# NUMERICAL SOLUTIONS TO THE CAUCHY PROBLEM FOR THE GENERALIZED NON-ISOTROPIC DIFFUSION EQUATION

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ABSTRACT

*This article discusses one of the modern methods (Monte Carlo method) for solving boundary value problems for an ultraparabolic equation of mathematical physics. Based on the obtained results, some numerical estimates of the solution to the Cauchy type problem were carried out.*

When studying dynamic systems on a computer, the statistical testing method (Monte Carlo method) is often used. The application of this method to study systems defined by stochastic differential equations requires their replacement with Euler and Runge-Kutta difference schemes. Such replacements are considered in the works [1, 2]. However, known estimates of the error of solutions of deterministic equations using difference methods cannot be used in the digital modeling of stochastic equations due to the fact that their solutions are not differentiable almost everywhere.

If we keep in mind that the application of the Monte Carlo method, which has demonstrated its effectiveness in multidimensional problems, then the development of methods of numerical integration in a system with many noises is very relevant.

Let us consider the Cauchy problem in the classical formulation in the (n+1)-dimensional space $R^{n+1}$ in the layer $\Omega = R^n * [O,T]$:

$$(L_1 u)(x,t) = \frac{\partial u(x,t)}{\partial t} - \sum_{j=1}^{k} a^{ij} \frac{\partial^2 u(x,t)}{\partial x^l \partial x^j} +$$

$$+\sum_{j=1}^{k} \sum_{m=1}^{l} \beta_j^m x^j \frac{\partial u(x,t)}{\partial x^m} = f(x,t), \tag{1}$$

$$u(x,0) = \phi(x), \qquad x \in R^n,$$

where $\alpha^{ij}$ and $\beta_j^m$ (i=1,2,...,k , j=1,2,...,k, m=1,2,...,*l*) are constant coefficients, $n=k+l$. Let $\alpha=(\alpha^{ij})-$ be a matrix with dimension $k\times k$, $\beta=(\beta_j^m)-$ be a matrix with dimension $l\times k$.

Let us further assume that:

- $\alpha=(\alpha^{ij})$ is a symmetric matrix and positive definite;

- $\beta=(\beta_j^m)$ matrix such that, the Gram matrix sss - with dimension is positive definite, i.e. she is non-degenerate.

The functions $f(x,t)$ and $\phi(x)$ will be considered continuous in $R^n$. Assuming the existence and uniqueness of a solution to problems (1)-(2), we will construct an algorithm for its numerical implementation.

To simplify solutions to the problem, we introduce (in block notation) the following $n\times n$ matrices $a=a(s)=\begin{pmatrix} m_1 m_2 \\ m_2^T m_3 \end{pmatrix}$, $q=q(s)=a^{-1}(s)$,

$$C(s)=\begin{pmatrix} I_k & 0 \\ -s\beta_l & I_l \end{pmatrix}=\exp\begin{pmatrix} 0 & 0 \\ -s\beta & 0 \end{pmatrix},\quad d(\rho)=\begin{pmatrix} \rho^{1/2}I_k & 0 \\ 0 & \rho^{3/2}I_l \end{pmatrix}. \tag{2}$$

Here's a block $m_1=\frac{1}{4s}\left[\alpha^{-1}+3\beta^T\omega\beta\right]$ size $k\times k$, a block $m_2=\frac{3}{2s^2}\beta^T\omega$ size $k\times l$

A block $m_2^T$ size $l\times k$, $m_3=\frac{3}{s^3}\omega$ size $l\times l$, matrices $I_k,0,\beta,I_l$ also have similar dimensions. Here and below $I_r-$ is an identity matrix of size $r\times r$, $d(\rho)$ is a diagonal matrix, $s=t-\tau$.

Matrices $a(s)$ and $q(s)$, where *s>0,* are positively defined. Then the fundamental solution of the equation (1) with a singularity at a point $(y,\tau)$ has the form

$$Z(x,t;y,\tau)=\pi^{-\frac{n}{2}}\|a\|^{\frac{1}{2}}(t-\tau)^{-\frac{\gamma}{2}}\exp\left\{-(y-Cx)^T d\left(\frac{1}{t-\tau}\right)ad\left(\frac{1}{t-\tau}\right)(y-Cx)\right\} \tag{3}$$

where $\|a\|=\det(a)$, $\gamma=k+3l$.

Using the fundamental solution of the $Z(x,t;y,\tau)$ in space, we define domains (spheroids) as follows. Let the number (parameter) be positive, i.e. $r>0$. Next domain

$$B_r(x,t)=\left\{(y,\tau):Z(x,t;y,\tau)>\pi^{-\frac{n}{2}}\|a\|^{\frac{1}{2}}r^{-\gamma},t>\tau\right\}$$

we will call it a spheroid with radius r, the center of which is located at the point $(x,t)$. Then $B_r,(x,t)$ we can rewrite it in the form

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

From (4) it is clear that $\tau$ satisfies the following conditions: $\tau<t,\tau>t-r^2$. Each section of the spheroid by the horizontal plane $\tau=const$, $t-r^2<const<t$, is an n-dimensional ellipsoid centered at the point $e^{-(t-\tau)\beta}x,\tau$. 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 converge towards the center $(x,t)$. Therefore, there is such a thing $r>0$ that when $(x,t)\in\Omega$ $\overline{B_r(x,t)}\subset\overline{\Omega}$. Let $r>0$ be that $\overline{B_r(x,t)}\subset\overline{\Omega}$. Then to solve problem (1)-(2) the following relation is valid:

$$u(x,t)=(E_r,u)(x,t)+\overline{f}(x,t), \quad (5)$$

where

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

$$\overline{f}(x,t)=\int_{B_r(x,t)}\int\left[Z(x,t;y,\tau)-\pi^{-\frac{n}{2}}\|a\|^{\frac{1}{2}}r^{-\gamma}\right]f(y,\tau)dyd\tau.$$

Here $S_1(0)$ -is $(n-1)$ - dimensional unit sphere with usual orthogonal coordinates: $\theta=(\theta_2,\theta_3,\dots,\theta_n)$, $0\le\theta_j\le\pi$ for $2\le j\le n-1$, $0\le\theta_n\le 2\pi$. $H(\theta)\in S_1(0)$ is a unit n-dimensional vector,

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

$$\tau(\lambda)=t-r^2\lambda^2, \quad (6)$$

From (6) it follows that if $r(x,t)\le t^{\frac{1}{2}}$, then for $(x,t)\in\Omega$ we have $\overline{B_r(x,t)}\subset\overline{\Omega}$.

Let's proceed to constructing a Markov chain $\left\{(x^j,t^j)\right\}_{j=0}^{\infty}$, on which we will construct an unbiased estimate of the solution $u(x,t)$ to problem (1)-(2).

For $u(x,t)=1$, applying formula (5) we obtain

$$\left(\frac{\gamma}{\pi}\right)^{\frac{n}{2}}\int_0^1 \lambda^{\gamma-1}\left(\ln\left(\frac{1}{\lambda}\right)\right)^{\frac{n}{2}} d\lambda \int\int_{s_1(0)} H^T(\theta)4b\alpha b^T H(\theta)ds=1.$$

It follows that the kernel of the integral equation (5) can be considered as a distribution density.

Consider the integral

$$J=\int_0^1 \lambda^{\gamma-1}\left(\ln\left(\frac{1}{\lambda}\right)\right)^{\frac{n}{2}} d\lambda.$$

By replacing the variables $\lambda=e^{-\frac{\rho}{\gamma}}$, we get

$$J=\frac{1}{\gamma^{\left(1+\frac{n}{2}\right)}}\int_0^\infty e^{-\rho}\rho^{\frac{n}{2}}d\rho=\frac{\Gamma\left(1+\frac{n}{2}\right)}{\gamma^{\left(1+\frac{n}{2}\right)}},$$

where $\Gamma(n)$ is the gamma function. Now, we can represent the $(E_r u)(x,t)$ as follows

$$(E_r u)(x,t)=\int_0^\infty P_1(\rho)d\rho\int_{S_1(0)} P_2(H)u\left(y\left(e^{-\frac{\rho}{\gamma}},\theta\right),\tau\left(e^{-\frac{\rho}{\gamma}}\right)\right)d\rho,$$

where $P_1(\rho)$ is the density of a gamma-distributed random variable with parameter $1+\frac{n}{2}$, $P_2(H)=H^T 4B\alpha B^T \frac{H}{\gamma\sigma_n}$.

In the future we will simulate a random vector with a distribution density

$$P_2(H)=P_2(H_1,H_2,....,H_n)=-\frac{1}{\gamma\sigma_n}\sum_{ij=1}^{n}K_{ij}H_iH_j\chi_{s_1(0)}(H), \qquad (7)$$

where $\chi_{s_1(0)}(H)$ is the indicator of the set $S_1(0)$, $\sigma_n$ is the surface of the unit sphere, $K_{ij}$ is the elements of the matrix $K=4bab^T$ of size $n\times n$. Since $H_1,H_2,....,H_n$ are the coordinates of the unit vector and $H_1^2+H_2^2+...+H_n^2=1$, we obtain that $H^TKH\le\mu_1$, where $\mu_1$ is the largest eigenvalue of the matrix K. Then we can model a random vector with distribution density (7) using the Neumann method.

Below we present the modeling algorithm.

**Algorithm:**

1. A $\omega=(\omega_1,\omega_2,...,\omega_n)$ isotropic vector and $\gamma_2$ -random variable uniformly distributed in (0,1) are modeled.

2. $E=\mu_1\gamma_1$.

3. If $\dfrac{\left(\sum_{ij=1}^{n}K_{ij}\omega_i\omega_j\right)}{\gamma}\geq E$, then $\omega$ is accepted, otherwise point (1) is repeated.

Let $\{\xi_j\}_{j=1}^{\infty}$ be a sequence of independent gamma distributed random variables with parameter $\left(1+\frac{n}{2}\right)$, $\{\omega^j\}_{j=1}^{\infty}$ be a sequence of independent vectors with distribution density $P_2(H)$. Now, we define a Markov chain with the following recurrence relations:

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

$$x_i^j=x_i^{j-1}+t_{j-1}\exp\left(-\frac{\xi_j}{\gamma}\right)\xi_j^{\frac{1}{2}}\sum_{m=1}^{n}b_{im}\omega_i^j,$$

(8)

$$x_{k+p}^j=x_{k+p}^{j-1}-t_{j-1}\exp\left(-\frac{2\xi_j}{\gamma}\right)\sum_{c=1}^{k}\beta_{pc}x_c^j+t_{j-1}^{\frac{3}{2}}\exp\left(-\frac{3\xi_j}{\gamma}\right)\xi_j^{\frac{1}{2}}\sum_{\nu=1}^{n}b_{k+p,\nu}\omega_i^j,$$

where $i=1,2,\ldots,k$, $p=1,2,\ldots,l$, $j=1,2,\ldots,$ $r\left(x^{j-1},t^{j-1}\right)=\left(t_{j-1}\right)^{\frac{1}{2}}$ and relation (8) is obtained from (6). Now, we can write (5) in the form

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

(9)

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

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

(10)

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

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

$$h(x,t)=\iint\limits_{B_r(x,t)}\left[Z(x,t;y,\tau)-\pi^{-\frac{n}{2}}\|a\|^{\frac{1}{2}}r^{-\gamma}\right]dyd\tau.$$

where

Assuming that $u(x,t)=t$ and applying formula (9) for $j=1$ from (8) we obtain

$$h(x,t)=r^2(x,t)(\gamma/(\gamma+2))^{\left(1+\frac{n}{2}\right)}. \quad (11)$$

Let $\{\Im_l\}_{l=0}^{\infty}$ be a sequence of $\sigma$ - algebras generated by random variables $\xi_1,\xi_2,...,\xi_l$ and a sequence of vectors $\omega^0,\omega^1,...,\omega^l$ and random points $(y^0,\tau^0),(y^1,\tau^1),...,(y^{l-1},\tau^{l-1})$. Let us denote the solutions to problem (1)-(2) corresponding to the given $f,\varphi$ as $u_{f,\varphi}(x,t)$.

**Theorem 1.**

a) the sequence $\{\eta_l\}_{l=0}^{\infty}$ forms a martingale relative to the sequence of $\sigma$-algebras $\{\Im_l\}_{l=0}^{\infty}$;

b) if $u_{f,0}(x,t)<+\infty$ and $u_{|f|,0}(x,t)<+\infty$, then it is $\eta_l$ square integrable.

**Proof:** First we prove that $\{\eta_i\}_{l=0}^{\infty}$ forms a martingale. From the definition of $\Im_l$ it is clear that $\eta_l$ is $\Im_l$ - measurable, then using the property of conditional mathematical expectation and formulas (9, 11) we get

$$E_{(x,t)}[\eta_{l+1}/\zeta_l]=\sum_{j=0}^{l-1}h(x^j,t^j)\mathrm{f}(y^j,\tau^j)+u(x^l,t^l)=\eta_l$$

Hence, it follows that $\{\eta_l\}_{l=0}^{\infty}$ is martingale with respect to $\{\Im_l\}_{l=0}^{\infty}$. We will prove that $E_{(x,t)}\eta_l^2\leq\infty$.

$$I=E_{(x,t)}(\sum_{j=0}^{l-1}h(x^j,t^j)f(y^j,t^j))^2<+\infty$$

Dividing $I$ into two terms, from the final condition $r^2(x,t)\leq t$ we obtain that $h(x,t)\leq\left(\frac{\gamma}{\gamma+2}\right)^{1+n/2}t$ of these conditions we obtain the proof of the theorem.

Now we will show one of the ways to estimate the value from one random node

$$\bar{f}(x,t)=\iint\limits_{B_r(x,t)}\left[z(x,t;y,\tau)-\pi^{-\frac{n}{2}}\|a\|^{\frac{1}{2}}r^{-\gamma}\right]f(y,\tau)dyd\tau.$$

**Lemma 1.** The function $\overline{f}(x,t)$ has the following relation:

$$\overline{f}(x,t)=\left(\frac{\gamma}{\gamma+2}\right)^{\left(1+\frac{n}{2}\right)} r^2 Ef\left(y(\xi,\zeta,\omega),\tau(\xi,\zeta)\right),$$

where

$$y(\xi,\zeta,\omega)=e^{-r^2\exp\left(-\frac{2\xi}{\gamma+2}\right)\zeta^{2/\gamma}}\beta x+\left(\frac{\gamma}{\gamma+2}\xi\right)^{1/2}\alpha\left(r^2\exp\left(-\frac{2\xi}{\gamma+2}\right)\zeta^{2/\gamma}b^{-1}\omega\right),$$
$$\tau(\xi,\zeta)=t-\exp\left(-\frac{2\xi}{\gamma+2}\right)\zeta^{2/\gamma}. \qquad (12)$$

Here $\xi-$ is a gamma distributed random variable with parameter $\left(n/2\right)$, $\zeta$ beta distributed random variable with parameter $\left(2/\gamma,\ 2\right)$, $\omega-$ is a random unit vector.

**Proof:** Let's introduce the domain $B_r=\left\{(y,\tau): y^T a(1/\tau)ad(1/\tau)y<\gamma/2\ln r^{2/\tau},\ \tau>0\right\}$,

The resulting mirror image of spheroids $B_r(0,0)$ relative to the plane $\tau=0.$. These domains will also be called spheroids (radius ). Then we have

$$f(x,t)=\frac{\|a\|^{1/2}}{\pi^{n/2}r^{\gamma}}\iint_{B_r}\left[r^{\gamma}\tau^{\gamma/2}\exp\left(-y^T d(1/\tau)ad(1/\tau)y\right)-1\right]\times$$
$$\times f\left(e^{-\tau\beta}x+y,t-\tau\right)dyd\tau.$$

Let us make a change of variables and some integral transformation and obtain the proof of Lemma 1.

Let us consider the question of the computational feasibility of estimate (10). Let's take ε small enough and consider $(\partial\Omega)_\varepsilon=(R^n*[0,\varepsilon])$.

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

**Lemma 2.** The inequality holds: $E_{(x,t)}N_\varepsilon\le\left(\frac{\gamma=2}{\gamma}\right)^{1+\frac{n}{2}}\frac{t}{\varepsilon}$.

**Proof.** Taking $u(x,t)=t$ and applying formulas (10) and (11), we get

$$t = U_{1,0}(x,t) \ge E_{(x,t)} \sum_{j=1}^{N_\varepsilon - 1} h\left(x^j, t^j\right) = \left(\frac{\gamma}{\gamma+2}\right) E_{(x,t)} \sum_{j=1}^{N_\varepsilon - 1} r^2\left(x^j, t^j\right).$$

From the definition of $r(x,t)$ it follows that $r^2(x^j, t^t) = \left\{t^j\right\} \ge \varepsilon$.

From here we get that $t \ge \left(\frac{\gamma}{\gamma+2}\right)^{1+n/2} \varepsilon E_{(x,t)} N_\varepsilon$.

Hence $E_{(x,t)} N_\varepsilon \le \left(\frac{\gamma+2}{\gamma}\right)^{1+n/2} \frac{t}{\varepsilon}$. The lemma has been proved.

**Theorem 2.** Let the conditions of Theorem 1 be satisfied. Then $\eta_{N_\varepsilon}$ is an unbiased estimate for $u(x,t)$. Its variance is finite.

**Proof**. From Theorem 1 it follows that it is $\eta_t$ quadratically integrable and hence $\eta_t$ is uniformly integrable and $N_\varepsilon < +\infty$. Further, the moment the process stops is a Markov moment. Therefore, ac cording to Doob's theorem "On the transformation of free choice" and formula (9) $E\eta_{N_\varepsilon} = E\eta_t = u(x,t)$ i.e. $\eta_{N_\varepsilon}$ is an unbiased estimate for $u(x,t)$. From the definition of random variables $\eta_{N_\varepsilon}$ and $\eta_\infty$ it is clear that $D\eta_{N_\varepsilon} \le D\eta_\infty$. From $\eta_{N_\varepsilon}$ a mixed one is built using the standard method, but practically realizable estimate $\overset{*}{\eta}_{N_\varepsilon}$. Let $\varphi_1(x,0) = \phi(x)$ $x \in R^n$ and $(x,t^*)$ be the point closest to $\partial\Omega$. Estimated

$$\eta_{N_\varepsilon} = \sum_{j=0}^{N_\varepsilon - 1} h(x^j, t^j) f(y^j, \tau^j) + u(x^{N_\varepsilon}, t^{N_\varepsilon})$$

replace $u(x, t^{N_\varepsilon})$ and $u(x, t^{*N_\varepsilon})$ and get

$$\overset{*}{\eta}_{N_\varepsilon} = \sum_{j=0}^{N_\varepsilon - 1} h(x^j, t^j) f(y^j, \tau^j) + \varphi_1(x, t^{*N_\varepsilon}).$$

**Theorem 3.** Let $u(x,t)$ satisfy the Lipschitz condition and $A(\varepsilon)$ the modulus of continuity $u(x,t)$. Then the random variable is $\overset{*}{\eta}_{N_\varepsilon}$ is a biased estimate for $u(x,t)$. $D\overset{*}{\eta}_{N_\varepsilon}$ limited parameter function $\varepsilon$.

**Proof.** Since $E_{(x,t)}\eta_{N_\varepsilon} = u(x,t)$ $u(x,t)$, then

$$|u(x,t) - E_{(x,t)}\overset{*}{\eta}_{N_\varepsilon}| = |E_{(x,t)}\eta_{N_\varepsilon} - E_{(x,t)}\overset{*}{\eta}_{N_\varepsilon}| = |E_{(x,t)} u(x, t^{N_\varepsilon}) -$$

$$- E_{(x,t)}\varphi_1(x, t^{*N_\varepsilon})| \le E_{(x,t)} |u(x, t^{N_\varepsilon}) - u(x, t^{*N_\varepsilon})| = A(\varepsilon).$$

The theorem 3 has been proved.

Let us present the results of the computational experiment.

Numerical experiment:

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

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

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

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

The results of the numerical experiment are given in the table.

| Number of tracks | Point x,y,z,t | $\varepsilon$ | exact solution | Selective assessment | 3-sigma |
|---|---|---|---|---|---|
| 100 | 0.7, 0.7, 0.7, 0.7 | 0.005 | 1.738 | 1.732 | 0.017 |
| 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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