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Solution of the Cauchy problem for anisotropic diffusion using stochastic and adaptive methods

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This paper considers the Cauchy problem for an anisotropic diffusion equation. A stochastic representation of the solution based on Wiener processes is employed. Within a unified framework, the classical Monte Carlo method and an adaptive stochastic algorithm are analyzed. It is shown that the use of adaptive procedures significantly reduces the variance of estimators and improves computational efficiency. The results of numerical experiments confirm the theoretical findings and demonstrate the advantages of the proposed method.

Keywords: anisotropic diffusion, Cauchy problem, stochastic methods, Monte Carlo method, adaptive algorithms.

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Diffusion problems with anisotropic coefficients often occur in mathematical physics, transport theory, thermal conductivity, and in simulation of processes in nonhomogeneous and direct-patterned media. Unlike isotropic models, anisotropic diffusion is characterized by directional dependence of transfer intensity, leading to considerable difficulties during analytical and numerical study of the corresponding boundary value problems and initial boundary value problems. Second-order parabolic equations with matrix diffusion coefficients, for which classical deterministic approaches often appear to be computationally expensive or instable, are of particular interest [1].

Stochastic methods based on probabilistic representations of solutions to differential equations, in particular the Monte Carlo methods, offer an alternative approach to solution to such problems [2,3]. Their important benefit is in low dependence of the computational complexity on the problem order, and natural adaptation to a complex region geometry. Meanwhile, the classical Monte Carlo method is characterized by slow convergence and high dispersion of estimates [4–6]. In recent years, adaptive stochastic algorithms have rapidly developed to reduce dispersion and increase computational efficiency [7,8], which constitute the aim of this work.

We consider the Cauchy problem for the linear parabolic second-order equation describing the anisotropic diffusion process in a bounded space region. Suppose that $\Omega \subset \mathbb{R}^d$ is an open bounded region with a sufficiently smooth boundary $\partial\Omega$, and $T > 0$ is a fixed time. Find $u(x, t)$ satisfying the following equation

$$\frac{\partial u}{\partial t} = \sum_{i,j=1}^d a_{ij}(x) \frac{\partial^2 u}{\partial x_i \partial x_j} + \sum_{i=1}^d b_i(x) \frac{\partial u}{\partial x_i} + f(x, t),$$

$$x \in \Omega, \quad t \in (0, T], \quad (1)$$

with the initial condition

$$u(x, 0) = u_0(x), \quad x \in \Omega. \quad (2)$$

Diffusion matrix $A(x) = \{a_{ij}(x)\}_{i,j=1}^d$ is assumed to be symmetric and uniformly positively definite, however, its elements can essentially depend on the spatial variable x , which defines the anisotropic nature of the diffusion process. The vector function $b(x) = (b_1(x), \dots, b_d(x))$ describes the drift term and is responsible for the directional mass or energy transfer in the fluid. $f(x, t)$ defines the density of internal sources or sinks.

For correct statement of stochastic representation, $a_{ij}(x)$ and $b_i(x)$ are assumed to be sufficiently smooth and limited, and the initial function $u_0(x)$ belongs to the class of continuous functions in closure of the region $\bar{\Omega}$. These conditions ensure the existence and uniqueness of the Cauchy problem solution in a classical or generalized sense.

For the bounded region Ω , the time, when the stochastic process first goes beyond the region boundaries, is considered

$$\tau = \inf\{t > 0 : X_t \notin \Omega\},$$

which makes it possible to naturally account for the boundary conditions in the probabilistic problem statement. Such approach is particularly suitable for numerical simulation because it does not require explicit discretization of the region boundary.

Thus, the set problem reduces to numerical computation of equations (1) and (2) in the anisotropic diffusion conditions using stochastic methods based on simulation of corresponding stochastic process paths.

To build a stochastic algorithm for the Cauchy problem solution, consider the stochastic process X_t associated with the differential operator on the right-hand side of equation (1). Suppose the process X_t satisfies the stochastic

differential equation

$$dX_t = b(X_t)dt + \sqrt{2A(X_t)}dW_t, \quad (3)$$

where W_t is the standard d -dimensional Brownian motion, $b(x)$ is the drift vector, and the matrix $A(x)$ defines the anisotropic diffusion intensity.

Link between the solution to equation (1) and the process X_t is established using the Feynman–Kac formula. For the Cauchy problem without explicit boundary conditions, the solution can be represented as a mathematical expectation

$$u(x, t) = E \left[u_0(X_t) + \int_0^t f(X_s, s)ds \right], \quad (4)$$

where the mathematical expectation is taken over all implementations of the stochastic process X_t starting at $X_0 = x$.

Equation (4) has a visual interpretation: solution value of $u(x, t)$ is defined by the mean contribution of the initial condition transferred along stochastic paths and by the accumulated action of sources $f(x, t)$ during the time $[0, t]$. Thus, solution to the differential equation reduces to calculation of statistical characteristics of the corresponding stochastic process.

This stochastic representation is a theoretical foundation for using the numerical Monte Carlo methods that enable the approximation of mathematical expectation (4) through a finite number of stochastic paths.

Stochastic representation of the solution to Cauchy problem (4) allows for using the numerical Monte Carlo method for approximate calculation of $u(x, t)$. The main idea of the method is in the mathematical expectation approximation by a finite number of random implementations of the stochastic process.

Suppose $\{X_t^{(k)}\}_{k=1}^N$ are independent implementations of process (3), starting from the same initial point $X_0^{(k)} = x$.

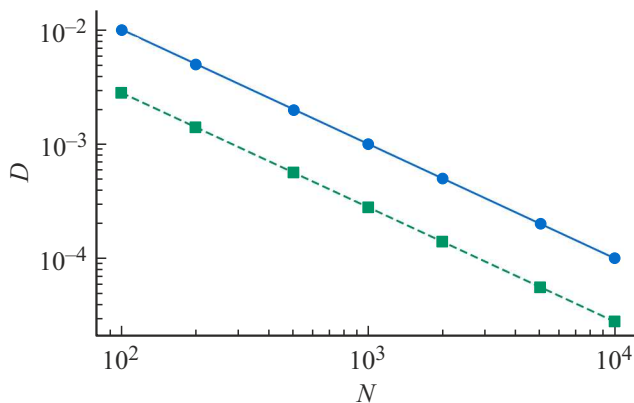


Figure 1. Dependence of the dispersion of estimate D on N (log-log scale). Solid line — classical Monte Carlo method, dashed line — adaptive stochastic method.

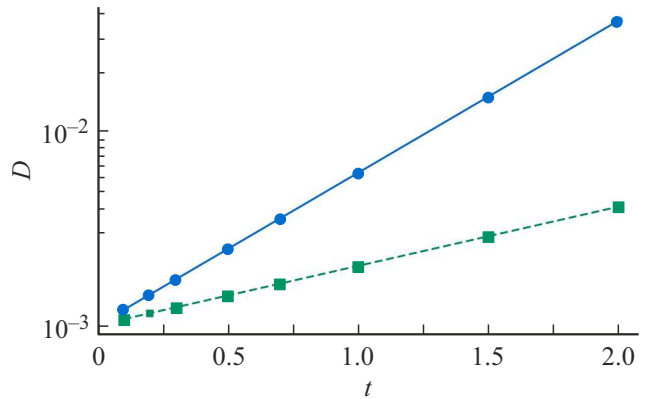


Figure 2. Dispersion vs. t at $N = 1000$ (semi-log scale). Solid line — classical Monte Carlo method, dashed line — adaptive stochastic method. At large times where anisotropy is most pronounced, the benefit of the adaptive method is manifested more significantly.

Then the approximate solution value of $u(x, t)$ is defined by

$$u_N(x, t) = \frac{1}{N} \sum_{k=1}^N \left[u_0(X_t^{(k)}) + \int_0^t f(X_s^{(k)}, s)ds \right], \quad (5)$$

where N is the number of stochastic paths.

For numerical implementation of equation (5), $[0, t]$ is broken into a uniform grid with the step Δt , and the stochastic process is approximated by the Euler–Maruyama scheme

$$X_{n+1}^{(k)} = X_n^{(k)} + b(X_n^{(k)})\Delta t + \sqrt{2A(X_n^{(k)})}\Delta W_n^{(k)}, \quad (6)$$

where $\Delta W_n^{(k)}$ are independent normally distributed random quantities with zero mathematical expectation and dispersion Δt .

The Monte Carlo method has a set of benefits such as simple implementation and weak dependence of the computational complexity on the problem order. However, statistical dispersion of estimate (5) decays in proportion to $N^{-1/2}$, resulting in a slow convergence and the need for using a large number of paths to achieve the acceptable accuracy.

This disadvantage is most pronounced during simulation of anisotropic diffusion processes where nonuniformity of diffusion coefficients leads to a significant spread of paths. This naturally necessitates using modified stochastic algorithms focused on reduction of the dispersion of estimates.

As noted above, the classical Monte Carlo method is characterized by slow convergence rate and high dispersion of statistical estimate, particularly in the case of anisotropic diffusion processes. To increase the numerical simulation efficiency, an adaptive stochastic method is proposed that is based on dynamic redistribution of computational resources.

The main idea of the adaptive approach is in the fact that contribution of various stochastic paths to the final estimate

Computational efforts for achievement of the specified accuracy of ε (parameters: $\Omega = [0, 1] \times [0, 1]$ — two-dimensional region (unit square), diffusion matrix $D_{11} = 2.0$, $D_{22} = 0.5$, Euler–Maruyama scheme, $\Delta t = 0.01$)

ε	Number of paths N		Time, s		Saving, %
	Classical Monte Carlo method	Adaptive stochastic method	Classical Monte Carlo method	Adaptive stochastic method	
10^{-1}	500	180	0.8	0.3	63
$5 \cdot 10^{-2}$	2000	620	3.2	1.1	66
10^{-2}	50 000	12 500	80	21	74
$5 \cdot 10^{-3}$	200 000	43 000	320	72	77

of solution differs considerably. In phase space regions where high solution sensitivity or sudden change of diffusion coefficients is observed, a denser statistical averaging is required.

Suppose a limited number N_0 of stochastic paths is simulated at the first stage, which are used for calculating the preliminary dispersion estimate

$$\sigma^2(x, t) = \frac{1}{N_0} \sum_{k=1}^{N_0} \left(\Phi^{(k)}(x, t) - \bar{\Phi}(x, t) \right)^2, \quad (7)$$

where

$$\Phi^{(k)}(x, t) = u_0(X_t^{(k)}) + \int_0^t f(X_s^{(k)}, s) ds, \quad \bar{\Phi} = \frac{1}{N_0} \sum_{k=1}^{N_0} \Phi^{(k)}.$$

According to estimate (7), adaptive strategy is built for increasing the number of paths in those time intervals or spatial regions where the dispersion exceeds the specified threshold ε^2 . Additional paths are simulated only in these regions allowing essential reduction of the total computational efforts.

Final adaptive solution estimate becomes

$$u_{ad}(x, t) = \sum_{i=1}^M w_i \left[\frac{1}{N_i} \sum_{k=1}^{N_i} \Phi_i^{(k)}(x, t) \right], \quad (8)$$

where M is the number of adaptive subdomains, N_i is the number of paths in the i -th subdomain, and w_i are selected such that the unbiased statistical averaging is maintained.

The proposed method retains stochastic solution interpretation and does not require a change of the integration scheme of the stochastic differential equation. In addition, considerable reduction of the dispersion is achieved compared with the classical Monte Carlo method with comparable computational efforts. Numerical experimental results are provided here to compare the efficiency of the classical Monte Carlo method and proposed adaptive stochastic method for solving the Cauchy problem for the anisotropic diffusion equation.

A problem of the bounded region $\Omega \subset \mathbb{R}^d$ with uniform boundary conditions and the specified initial function $u_0(x)$ is considered. Diffusion coefficients are selected such

that a pronounced process anisotropy is ensured, which considerably hinders the numerical simulation.

Stochastic paths are simulated using the Euler–Maruyama scheme with the fixed time step Δt . All experiments use the same discretization parameters to ensure correct comparison of the methods.

Accuracy of numerical solution is evaluated using the RMS error

$$\text{Err}(t) = \left(E |u_{num}(x, t) - u_{ref}(x, t)|^2 \right)^{1/2}, \quad (9)$$

where u_{num} is the numerical solution obtained by the stochastic method, and u_{ref} is the reference solution calculated using a large number of paths.

Calculation results show that with the same total number of simulated paths, the adaptive stochastic method provides a much smaller dispersion compared with the classical Monte Carlo method, in particular, at large times where the anisotropy effect is most pronounced (Figure 1, 2). Computational efficiency analysis based on the inclusive CPU time measurement shows that the adaptive approach allows the specified accuracy level to be reached with lower computational efforts (see the table).

The gain in time is achieved via redistribution of the number of stochastic paths in regions with high dispersion, while in the classical Monte Carlo method resources are evenly distributed. The numerical experiments support the theoretical conclusions and show that the adaptive stochastic method maintains unbiasedness of solution estimate and simultaneously reduces the dispersion without increasing the computational algorithm complexity.

The study uses a common stochastic approach to address the Cauchy problem solution for the anisotropic diffusion equation on the basis of the probabilistic solution representation. It is shown that the classical Monte Carlo method and proposed adaptive stochastic algorithm are successive steps of a common computational scheme, while the adaptive method makes it possible to reduce the dispersion of estimates and increase the computational efficiency without violation of correct stochastic representation. Numerical experiment results confirm the benefit of the adaptive approach, in particular, in pronounced anisotropy conditions,

which makes the proposed method suitable for practical simulation of transfer processes in anisotropic media.

Conflict of interest

The author declares no conflict of interest.

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