NUMERICAL CALCULATION OF EFFECTIVE PERMEABILITY 
BY DOUBLE RANDOMIZATION MONTE CARLO METHOD

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Abstract. The paper is devoted to solving the boundary value problems with random parameters. We consider flows in a porous medium with random permeability field or random boundary conditions. The Monte Carlo method with double randomization is suggested to compute the statistical properties of the flow. The paper focuses on the calculating of media’s effective permeability. The method is compared with a standard Monte Carlo approach. Numerical tests show that double randomization gives high accuracy and can improve computational efficiency.

Key words. Stochastic models, effective permeability, Monte Carlo method, double randomization

1. Introduction

Many problems in natural science, industry and finance are naturally described by stochastic models. For instance, such models are used in simulation of turbulent transport [5] or evaluation of the elastic properties of composite materials [14, 25]. In [8] the transport in a random magnetic field is studied. The stochastic modeling of bacterial population dynamics is considered in [16, 28].

The main purpose of this paper is to develop an effective numerical method for solving the problems described by partial differential equations with random parameters. In such equations coefficients, right side or boundary conditions can be considered as random functions. Certainly, in statistical approach we are able to evaluate only some averaged flow characteristics.

One of the most important applications of this method is a simulation of the flow in porous media. In many articles permeability is approximated by random field [3, 10, 11]. In this paper we address the calculation of effective permeability used for the solution of filtration problems [21, 22]. In particular, the developed method can be used to study the influence of deformation bands distribution on fluid flow in fault damage zone [13]. Several approaches are developed for solving such problems. The small perturbation expansion method [2, 10, 27] is computationally efficient but it is restricted by values of permeability fluctuations. The applicability of the spectral model derived under the assumption of small hydraulic conductivity fluctuations is studied in [12]. In [30] the mean and covariance of hydraulic head for saturated flow in randomly heterogeneous porous media is calculated by using the Karhunen-Loeve decomposition, polynomial expansion, and perturbation method. The uncertainty analysis of flow in random porous media is explored in [17] by probabilistic collocation method. These techniques have relatively low computational cost but it also requires the Karhunen-Loeve decomposition for covariance function of permeability random field. A vast review devoted to stochastic computations presented in [29].

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The most general and popular approach is as follows:
1. the ensemble of realizations of the random parameter is sampled;
2. the deterministic equation for each realization of parameters is solved numerically.

Then the desired averaged flow characteristics are evaluated by using ensemble averaging. Further we will call this procedure as a "standard approach". Unfortunately, this method may be very time consuming. In this work we use the "double randomization" method [19, 24] to overcome this difficulty. As a standard approach, this technique also has no restrictions on the permeability distribution. We consider a standard Monte Carlo approach and the Monte Carlo method, which uses the double randomization for calculating the effective permeability of coarse grid block. The method’s efficiency is compared by using two different models of permeability distributions.

2. Formulation of the problem

We consider a steady flow through a saturated porous medium. For a stationary 2D flow, we solve the following Darcy law and the continuity equation:

\[ q = -\frac{1}{\mu} K \nabla p, \]
\[ \nabla \cdot q = 0 \]

where \( q \) is the Darcy velocity, \( p \) is the pressure, \( \mu \) is the dynamic viscosity (constant in all the simulations, \( \mu = 1Pa \cdot s \)) and \( K \) is the permeability. Here and below in the paper we use bold font for vector variables and matrixes.

Due to the strongly irregular structure of the media, we assume that the permeability field is a random field. Then any flow characteristic \( \xi \) (flow rate, velocity, effective permeability etc.) also becomes random function defined as solution of (1), (2). Certainly, this approach allows us to compute averaged flow characteristics only. Having the ensemble of the random fields realizations sampled according to the correspondent distribution, we can calculate the value of the flow characteristic \( \xi_i \) for each realization, as well as the effective properties by using the following statistical averaging:

\[ E\xi = \langle \xi \rangle \approx \frac{1}{N} \sum_{i=1}^{N} \xi_i \]

where \( N \) is the number of realizations. Here \( \langle \rangle \) means the ensemble averaging.

We solve equations (1), (2) in the domain \( \Omega = \{ 0 \leq x \leq L_x, 0 \leq y \leq L_y \} \).

For simplicity, the effective permeability will be calculated by using the upscaling procedure in one direction described in [6, 7]. On two opposite boundaries, the pressures are fixed to constant values \( p(0, y) \) and \( p(L_x, y) \), whereas no flow boundary conditions apply to the other borders. The flow calculated numerically allows us to estimate the effective permeability \( K_{eff} \) of a coarse upscaled block \( \Omega \) from equation [22]

\[ \langle q \rangle = -\frac{1}{\mu} \langle \nabla p \rangle. \]
$N$ realizations of random field $K$ are sampled according to the procedure described below. Then the mean values for the flow rate and mean pressure gradient $\langle \nabla p \rangle$ are estimated by using an extended local upscaling method [7]. Finally, $K_{eff}$ is calculated.

Though there are no restrictions on the permeability distribution in the considered methods, in numerical experiments we use two models of random permeability: lognormal random field [9] and fractal permeability distribution [4].

2.1. Lognormal permeability. We consider the hydraulic log-permeability $f = \ln(K)$ as a statistically homogeneous random field with gaussian distribution $N(m_f, \sigma_f)$. Here $m_f = \langle f \rangle$ and $\sigma_f$ is a standard deviation. In our calculations we choose $m_f = 3.4012$, $K_G = \exp(m_f) = 30m^2$.

We assume that $f$ is statistically homogeneous and isotropic with the spectrum [11]:

$$S_{ff}(k) = \frac{\sigma_f^2 \gamma^2}{\pi(\gamma^2 + k^2)^2}, \quad k = |k|.$$  

The corresponding covariance function

$$C_{ff}(r) = \langle f(X)f(X + r) \rangle = \sigma_f^2 \gamma r K_1(\gamma r), \quad r = |r|, \quad \gamma = 1.65/I_f$$

where $k = (k_1, k_2)$ is the wave number vector, $r = (r_1, r_2)$ is the position vector, $K_1$ is the modified Bessel function, and $I_f$ is the log-permeability correlation length.

2.1.1. Random field simulation. Now we present simulation formulae in the case of scalar real-valued isotropic homogeneous gaussian random field with the spectral tensor $S_{ff}(k)$ (see [24]). Let $p(k)$ be an arbitrary density function defined on the same wave number space. Sample $k$ according to $p(k)$, and let $\zeta_k$ and $\eta_k$ be mutually independent random variables with zero mean and unit variance, independent of $k$. Generally, $p(k)$ may be chosen as an arbitrary density function. In this paper we take

$$p(k) = \frac{S_{ff}(k)}{\int_{B^2} S_{ff}(k) d\mathbf{k}}$$

as it is recommended in [24].

Then we construct the normal random field in the point $X = (x_1, x_2)$

$$f(X) = m_f + \frac{\sigma_f}{\sqrt{N_h}} \sum_{i=1}^{N_h} (\zeta_{ki} \cos(k_i \cdot X) + \beta_{ki} \sin(k_i \cdot X)).$$

Here all of $k_i$ are sampled independently according to the density $p(k)$.

The central limit theorem ensures, under some general assumption [15], that $f$ converges to a gaussian random field with the spectral tensor $S_{ff}(k)$, as long as $N_h \to \infty$. By default in our calculations $N_h = 100$.

2.1.2. Finite difference approximation. To construct the solution of the equations (2), (3) for a chosen sample of $K(X)$ and satisfying the boundary conditions like in [1] we use the following centered finite difference scheme in the interior nodes

$$[K_{i-0.5j} + K_{i+0.5j} + K_{ij-0.5} + K_{ij+0.5}] p_{ij} - K_{i-0.5j} p_{i-1j} - K_{i+0.5j} p_{i+1j} - K_{ij-0.5} p_{ij-1} - K_{ij+0.5} p_{ij+1}$$

In order to check the accuracy of this approximation, we compute the error for conservation law. In Figure 1 we show that the relative error does not exceed for 100 realization of the permeability random field. $\sigma_f = 2$, $I_f = 0.5m$ and $I_f = 2.5m,$
Figure 1. Relative error for the conservation law: 100 realization of lognormal permeability random field $K$ from 2.1.1. The relative error does not exceed $8 \cdot 10^{-11}$. $\sigma_f = 2$, $I_f = 0.5m$ (solid line) and $I_f = 2.5m$ (dashed line).

$\langle \nabla p \rangle = 0.1Pa \cdot m^{-1}$, $L_x = L_y = 5m$. By default, a rectangular grid contains $80 \times 80$ nodes for one upscaled block.

2.2. Fractal permeability. In the second case we consider fractal permeability distribution. We assume that point permeability can equal one of two discrete values ($K^{(1)} = 1m^2$, $K^{(2)} = 0.001m^2$). Let $\chi$ be fraction of the total area of media with permeability $K^{(2)}$ to the total area of $\Omega$.

2.2.1. Permeability field simulation. We use the algorithm described in [4] for the sampling of fractal density distribution. The spatial distribution is completely defined by the infinite set $D_q = \{D_0 \geq D_1 \geq ... \geq D_{\infty}\}$ called a multifractal spectrum. The algorithm is based on the iterative fragmentation of $\Omega$ (for first and second iterative steps the procedure is illustrated in Figure 2). On iteration's step each subdomain is divided in 4 equal parts and the corresponding probability is defined for each resulting subdomain. As it is shown in Figure 2, if the probability of original subdomain equals $P$, then the probabilities of resulting subdomains are $PP_1$, $PP_2$, $PP_3$, $PP_4$ (in random order). After $n$ iterations $\Omega$ is divided in $4^n$ subdomains. The basic probabilities $P_1$, $P_2$, $P_3$, $P_4$ are defined from equations:

$$\sum_{k=1,4} \frac{P_k^q}{(1/2)(q-1)D_q} = 1.$$  

Thus we need to know $D_1$, $D_2$, $D_3$, $D_4$ to define $P_1$, $P_2$, $P_3$, $P_4$. In this work we just consider the example where $P_1 = 0.5$, $P_2 = 0.25$, $P_3 = 0.15$, $P_4 = 0.1$.

The iteration procedure can be repeated infinitely but, in our simulations, we used a number of iterations $T = 6$. Thus the total grid contains $64 \times 64$ cells, $L_x = L_y = 1m$, $\langle \nabla p \rangle = 1Pa \cdot m^{-1}$. When the final probability distribution is
constructed, we sample each low-permeability cell randomly in one of the subdomains according to the corresponding probabilities.

2.2.2. Finite volume approximation. Because of the discontinuity of permeability $K$, the finite volume method (FVM) with a rectangular grid was used for solving the problem. Integrating equations (1), (2) over the small volume surrounding each node point on a mesh and applying Gauss’s theorem, we get the following equation:

$$\int \int_{V_k} \text{div}[K \nabla p] dV_k = \int_{S_k = G_{k1} \cup G_{k2} \cup G_{k3} \cup G_{k4}} \frac{K}{\partial n} dS_k = 0.$$  

where $V_k$ is the volume of the $k$-th cell, $S_k$ is the surface of the $k$-th cell, and $G_{k1}$, $G_{k2}$, $G_{k3}$ and $G_{k4}$ represent the cell boundaries.

We approximate the flow rate through boundary $G_{k4}$ in (2) by formula [18]:

$$Q_{k-0.5} = \int_{G_{k4}} K \frac{\partial p}{\partial n} dS_k = \frac{p_k - p_{k-1}}{\int_{[X_{k-1}, X_k]} K dx} H_{k-1}.$$  

where $H_{k-1}$ is the length of $G_{k4}$, $[X_{k-1}, X_k] \perp G_{k4}$, $p_k$ is the pressure in the middle of the cell $k$ and $Q_{k-0.5}$ is the flow rate through $G_{k4}$.

Thus we have a so called dual-grid structure (Figure 3). The first grid consists of a set of $S_k$ - boundaries for control volumes $V_k$. The second grid consists of a set of $X_k$ - centers of control volumes $V_k$. For correct flow simulation we choose these grids so that each cell has constant permeability in our computations. In our model the integral on the right side of equation (7) is precisely computed. This ensures high accuracy of this method.
3. Monte Carlo method for solving problem with random parameters

By using the approximation (7) we can construct a system of linear algebraic equations (SLAE) to compute the pressure

\[ \mathbf{Lx} = \mathbf{b}. \]

Here \( \mathbf{L}, \mathbf{b} \) may depend on permeability distribution and problem boundary conditions. \( \mathbf{x} \) is vector of pressure values in the grid nodes. We assume that we have a sufficiently good approximation of our boundary value problem constructed by FDM or FVM. Then we should solve the constructed system of linear algebraic equations (6), where \( \mathbf{L}, \mathbf{b} \) can depend on a random parameter \( \lambda \) (where \( \lambda \) may be a random scalar variable, random vector or random field).

3.1. Statistical error and efficiency. Note that in the Monte Carlo methods, the evaluation of the statistical error \( \nu(\xi) \) is essential. The standard estimation has the following form [23]:

\[ \nu(\xi) = \alpha(\beta) \frac{\sigma_\xi}{\sqrt{N}} \]

where \( \alpha \) is a coefficient depending on the confident coefficient \( \beta \). For example, \( \alpha(0.997) = 3 \) and \( \alpha(0.95) = 1.96 \). Here \( \sigma_\xi \) is a standard deviation of random value \( \xi \). The product

\[ S = t\sigma_\xi^2 \]

may be considered as computational complexity and \( (t\sigma_\xi^2)^{-1} \) may be considered as computational efficiency. Here \( t \) is the time required for evaluating one realization of \( \xi \). Thus, the first method is more efficient than the second if \( S_1 < S_2 \).
3.2. Solving a system of linear equations by the Monte Carlo method.

Introducing matrix $A = I - L$, where $I$ is an identity matrix, we rewrite (8) as

$$x = Ax + c.$$ 

Consider the problem of finding the inner product $J = (h, x)$. For example if we take $h = (0, \ldots, 0, 1, 0, \ldots, 0)$ with sole nonzero $k$-th element then $J = x_k$.

We evaluate $J$ by using the Monte Carlo method with absorbing Markov chains $\omega = \{\omega_1, \omega_2, \ldots, \omega_N\}$ (or Markov chains with absorbing state [23]). The probability distribution of Markov chains is completely defined by following probabilities:

$$p_i > 0, \quad if \quad h_i \neq 0,$$

$$P_{ij} > 0, \quad if \quad a_{ij} \neq 0,$$

$$\sum_{i=1}^{n} p_i = 1, \quad p_i \geq 0,$$

$$P_{ij} \geq 0, \quad g_i = 1 - \sum_{j=1}^{n} P_{ij},$$

where $n$ is the size of matrix $A$.

We start to simulate each $\omega_j$ by choosing the initial state $i_0$ according to probabilities $\{p_i\}$. Then the chain will either stop in $i_0$ with probability $g_{i_0}$ or will extend to state $i_1$ with probability $P_{i_0i_1}$. Thus the Markov chain

$$i_0 \rightarrow i_1 \rightarrow i_2 \rightarrow \ldots \rightarrow i_M$$

has probability

$$p_{i_0} P_{i_0i_1} P_{i_1i_2} \cdots P_{i_{M-1}i_M} g_M.$$ 

Define

$$\xi = \frac{h_{i_0} W c_{i_M}}{p_{i_0} h_M}$$

where

$$W = \frac{a_{i_0i_1} a_{i_1i_2} \cdots a_{i_{M-1}i_M}}{P_{i_0i_1} P_{i_1i_2} \cdots P_{i_{M-1}i_M}}.$$ 

It is known [23] that $E\xi = (h, x) = J$ if spectral radius of matrix $A$ is less than unity.

For numerical solution of (1), (2) in $\Omega$ we set

$$p_i = 0, \quad if \quad h_i = 0,$$

$$P_{ij} = 0, \quad if \quad a_{ij} = 0.$$

$g_i = 1$ for nodes on the boundary with Dirichlet boundary conditions, $g_i = 0$ otherwise.

Due to low accuracy, described method is seldom applied for solving of the deterministic problems. But it can be useful if:

- matrix $A$ has a very large size
- only one component of the solution vector is interesting
- a rough estimation of the solutions is sufficient.

The basic approaches to reduce the estimation variance by using optimal probabilities $\{p_i\}, \{P_{ij}\}$ and branching Markov chains are described in [19, 20]. Another optimization approach is to use global Monte Carlo methods where one Markov chain may be used for the solution’s estimation in several nodes of computational grid [20].
3.3. Double randomization method. Now we assume that \( L, b \) in (8) depend on a random parameter \( \lambda \). If we sample one realization of \( \lambda \) then we can compute \( J(\lambda) \) by solving the equation (8) with \( L(\lambda), b(\lambda) \). It is possible to solve (6) by one of the standard methods or to construct the Monte Carlo estimation

\[
E_\omega[\xi(\omega, \lambda) | \lambda] = J(\lambda),
\]

where \( \omega \) is the trajectories (Markov chains) used in the Monte Carlo method.

Consider the problem of calculating the mean and covariance

\[
J = E_\lambda[J(\lambda)], \quad C = E_\lambda[J_1(\lambda)J_2(\lambda)].
\]

The simplest algorithm to estimate these mathematical expectations is to solve equation (8) \( N \) times for different realizations of the permeability random field, then to compute \( N \) values of \( J(\lambda) \), and finally to estimate a mean value by using (4). A number of Markov chains necessary for a sufficiently precise \( J \) estimation can be rather large. Therefore, the standard methods for solving a system of linear equations are preferable here. Nevertheless, the computational cost of this approach may be too high.

More effective way is to use a so called method of double randomization. This method is based on the following relations:

\[
J = E_\lambda[J(\lambda)] = E_\lambda E_\omega[\xi(\omega, \lambda)] = E_{(\omega, \lambda)}[\xi(\omega, \lambda)],
\]

\[
C = E_\lambda[J_1(\lambda)J_2(\lambda)] = E_{(\omega_1, \omega_2, \lambda)}[\xi(\omega_1, \lambda)\xi(\omega_2, \lambda)]
\]

where \( \omega_1, \omega_2 \) are mutually independent trajectories, sampled for the fixed \( \lambda \). It is seen from (12), (13) that it is sufficient to construct only one Markov chain for one realization of \( \lambda \) to estimate \( J \). To estimate \( C \) we should sample at least two Markov chains for each realization of \( \lambda \).

In practice it is reasonable to use the splitting method. In this modification the \( N_1 \) realizations of \( \lambda \) are sampled and then for each \( \lambda_i \) the \( N_2 \) independent Markov chains are constructed.

\[
J = E_{(\omega, \lambda)}[\xi(\omega, \lambda)] \approx \frac{1}{N_1} \sum_{i=1}^{N_1} \left[ \xi^{(N_2)}(\lambda_i) \right] = \frac{1}{N_1} \sum_{i=1}^{N_1} \left[ \frac{1}{N_2} \sum_{j=1}^{N_2} \xi_j(\lambda_i) \right].
\]

Here, \( \xi^{(N_2)} \) is an averaged sum of \( N_2 \) independent \( \xi \) sampled for the fixed value of \( \lambda \). The optimization of this method is described in [19], however it can be difficult to apply this method in practice. Below we will compare some results for different \( N_2 \).

4. Numerical results

In this section we compare numerically the efficiency of the standard approach and the double randomization method.

First, we consider the lognormal permeability random field. In Table 1 we compare the effective permeability calculated by both methods and their computational complexity. By default, we use \( N = 10^4 \) realizations of the permeability random field in the standard method and \( N_1 = 4 \cdot 10^3, N_2 = 10^3 \) in the double randomization method. In the case of \( \sigma_f = 2, I_f = 0.5m \) we use \( N = 1600 \). Because of a high variance of estimation in the case of \( \sigma_f = 2, I_f = 2.5m \) we use \( N = 10^4, N_1 = 4 \cdot 10^4, N_2 = 10^3 \). As it is mentioned in [26], \( K_{eff} \) depends on \( I_f \). For very small \( I_f \) values, \( K_{eff} \) tends to \( K_G \). On the other hand, for large \( I_f \) values, \( K_{eff} \) tends to the arithmetic mean of \( K \). It is seen from Table 1 that the double randomization method is more efficient even for this default parameters. For all numerical
computations in this paper we used Matlab R2008b. In standard approach the SLAE was solved by direct solver using in Matlab by default. In Table 2 we present the results for the computational complexity for the different values of $N_2$. Here for $N_2 = 10, 10^2, 10^3$ we use $N_1 = 4 \cdot 10^4$ and for $N_2 = 1$ we use $N_1 = 10^5$, $t$ is the time required to estimate one value $\xi(N_2)$ (time needed for the random field simulation and $N_2$ Markov chains sampling). For the standard approach $\sigma_\xi$ is the mean deviation of the effective permeability estimated with the help of the Monte Carlo method. For double randomization method $\sigma_\xi(N_2)$ is the mean deviation of $\xi(N_2)$. It is seen from this table that the estimate’s variance decreases with the increase of $N_2$. But time $t$ grows with the increase of $N_2$ certainly. Thus it is possible to increase the efficiency by choosing the optimal value $N_2$. This optimal value depends on the procedure for random permeability simulation.

In Table 3 we present the results for the fractal permeability distribution for $\chi = 0.125$. The corresponding results for the standard Monte Carlo method are $K_{eff} = 0.624$, $t = 11.5sec$, $\sigma_\xi = 0.012$, $S = 0.0016$ ($N = 4000$ realization).

In the last example we look at the application of both methods for a case of random boundary conditions. We will consider one fixed realisation of random field $K$ with a spectrum (5) for $\sigma_f = 1, I_f = 1m$ (Figure 4, $K_{eff} = 20.42m^2$). On two opposite boundaries we assume no flow boundary conditions. On two other boundaries we set values of pressure $P_1 + P'(x,y), P_2 + P'(x,y)$ where $P'(x,y)$
Table 3. Dependence of computational complexity $S$ on $N_2$. Fractal permeability distribution. $\chi = 0.125$, $K^{(1)} = 1m^2$, $K^{(2)} = 0.001m^2$.

<table>
<thead>
<tr>
<th>$N_1$</th>
<th>$N_2$</th>
<th>$K_{eff}$</th>
<th>$t(N_2, sec)$</th>
<th>$\sigma_\xi(N_2)$</th>
<th>$S$</th>
</tr>
</thead>
<tbody>
<tr>
<td>100000</td>
<td>1</td>
<td>0.627</td>
<td>0.12</td>
<td>0.569</td>
<td>0.03889</td>
</tr>
<tr>
<td>40000</td>
<td>10</td>
<td>0.624</td>
<td>0.18</td>
<td>0.180</td>
<td>0.00583</td>
</tr>
<tr>
<td>20000</td>
<td>100</td>
<td>0.624</td>
<td>0.35</td>
<td>0.058</td>
<td>0.00118</td>
</tr>
<tr>
<td>10000</td>
<td>1000</td>
<td>0.624</td>
<td>2.44</td>
<td>0.012</td>
<td>0.00108</td>
</tr>
<tr>
<td>4000</td>
<td>4000</td>
<td>0.624</td>
<td>9.40</td>
<td>0.0145</td>
<td>0.00198</td>
</tr>
</tbody>
</table>

Figure 4. The realization of lognormal permeability random field $K$ used in the example with random boundary conditions. $\sigma_f = 1$, $I_f = 1m$.

- a random field with a spectrum (5) with mean deviation 0.1 and correlation length 1m. Because $K$ is fixed, variance $V_\xi(N_2)$ linearly decreases with the growth of $N_2$. On the other hand, the sampling of random field $P'$ on two boundaries is much less time-consuming than the sampling of random field $K$ in the whole domain $\Omega$. Therefore, time $t(N_2)$ approximately linearly grows with the growth of $N_2$. Thus, computing complexity $S$ practically does not depend on $N_2$. In this example computing complexity of the standard Monte Carlo method $S = 3.251$ and computing complexity of the method of double randomization is $S = 0.044$.

5. Conclusion

Using of the double randomization method, can decrease the computational complexity of the calculation of the effective media’s properties. The essential computational efficiency of optimization by using the spitting method is shown in this paper. Though in our numerical examples this method was used for calculating the effective permeability by extended local upscaling only, the most attractive feature of this method is that it has no restrictions on calculated averaged flow characteristics and random parameters. For example, the permeability can be assumed as
Numerical tests show that the double randomization Monte Carlo method can be efficient for effective permeability estimation. For some models of the permeability distribution the computational efficiency can be increased by several orders of magnitude. Certainly, the efficiency of double randomization technique will depend on the considered problem and the concrete numerical methods used for solving of system of linear equations. There are many optimization techniques are developed both for deterministic and for the Monte Carlo methods. But their influence on comparative effectiveness of presented approaches is out of framework of this work.

The calculation of more complex statistical characteristics by this technique requires additional research.

References


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