

# Random Walk Algorithms for Estimating Effective Properties of Digitized Porous Media\*

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**Abstracts** — In this paper we describe a Monte Carlo method for permeability calculations in complex digitized porous structures. The relation between the permeability and the diffusion penetration depth is established. The corresponding Dirichlet boundary value problem is solved by random walk algorithms. The results of computational experiments for some random models of porous media confirm the log-normality hypothesis for the permeability distribution.

## 1 Introduction

Determination of the effective transport, electromagnetic, or mechanical properties of disordered media, such as porous materials, is a long standing computational problem. Much effort has been expended to either estimate theoretically or to establish numerically a relation between geometric microstructure and macroscopic physical properties, such as the conductivity, dielectric constant, permeability, reaction rate, thermal or elastic properties of such disordered media.

For porous materials, permeability is the macroscopic parameter of basic practical interest, and its indirect measurement is very important for different environmental and technological applications. There now exists a vast variety of non-intrusive techniques making it possible to obtain three-dimensional images of the fine-scaled structure of composite materials. Availability of these digitized representations allows one to use different numerical methods for permeability computations based strictly on geometry. Our aim in this paper is to apply diffusion-based Monte Carlo algorithms to perform a series of such computational experiments in order to provide some hints for understanding the probabilistic behaviour of permeability.

The plan of the paper is the following. In §2 we review analytic formulas used with permeability. We also reacquaint the reader with the important concepts related to permeability and flow through porous media. In §3 we introduce the penetration depth based on the Debye-Brinkman equation, and show how knowing this quantity allows us to estimate permeability. The penetration depth is then measured using a random walk-based algorithm, as described in §4. We then apply this technique to some test problems to “calibrate” it in §5. In §6 we provide the bulk of our numerical results. Here we validate the method over a wide range of porosities (void space fraction), and use it to compute the distribution of permeabilities in random digitized media. Finally, in §7, we provide concluding remarks, discuss our results, and present possibilities for future work.

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## 2 Analytic Formulas for Permeability

Permeability is a measure of a medium's resistance to flow penetration. Intuitively, it is clear that the permeability is correlated with other properties of a porous medium, such as the capillary pressure and other geometric parameters [1]. However, it is quite obvious that any function relating different properties of porous material cannot be unique. The well-known relationship between the fluid permeability,  $k$ , and the porosity,  $n$ , established by the so called "Kozeny equations" [2]

$$k = cn(V/S)^2 \quad (1)$$

is exact for some of the simplest porous structures (see, e. g. [1]), such as a system of straight, parallel tubes penetrating a solid material. Here,  $V/S$  is the ratio of pore volume to their surface area, and  $c$  is some parameter. This constant, in fact, depends on the cross-sectional geometry of a capillary tube, and is determined by the Poiseuille flow velocity field.

Further attempts were aimed at modifying these formulas in order to make them applicable to different classes of porous materials. It is clear; however, that the introduction of arbitrary factors into (1) could help if it is possible to measure or calculate them. The most commonly used are 'tortuosity' or the formation factor which can be determined by measuring the effective electrical conductivity [3]. This property can be calculated by employing the Einstein relation for diffusion in the pore space with reflecting boundary conditions.

It has also been established that permeability can be estimated through some inequalities relating it to the solution of a diffusion-limited trapping problem. In particular, it has been determined that [4]

$$k \leq \eta n \bar{\tau} , \quad (2)$$

where  $\bar{\tau}$  is the mean exit (survival) time of a Brownian motion averaged over starting points in the whole void space of a porous sample with  $\eta$  being the diffusion coefficient of this Brownian process. This relation becomes an equality for the straight capillary model (and there coincides with the Kozeny equation). Later [5, 6], it was conjectured that by incorporating different parameters (such as the formation factor) into the right-hand side, (2) could provide more accurate estimates for the permeability of different porous formations. Computational experiments based on the simulation of diffusion via the walk on cubes algorithm in digitized porous media [7, 8] exploited the relation (2) and provided some suggestions for the choice of these parameters.

## 3 Penetration Depth Versus Direct Calculations

With the geometrical structure of the void space inside porous material given, one could try to calculate the permeability by the direct simulation of fluid flow in this geometrical structure. In the cases of interest, the Reynolds number of flow inside porous medium is very low, and thus the inertial term is comparatively small. Hence, it suffices to solve the linear steady-state Stokes equation for the fluid velocity on the microscopic scale. This must be combined with the incompressibility constraint and boundary conditions on the pore-skeleton interface. Usually, the velocity on the boundary is set to zero (no-slip). To evaluate the macroscopic permeability, a rectangular porous sample is considered and

a pressure gradient  $p_1 - p_0$  is applied along one of the axes (say  $x_i$ ). Next the microscopic velocity field is obtained by solving the boundary value problem for Stokes equation. Finite-difference or lattice-Boltzmann computational methods are commonly used to solve this problem. Next, the macroscopic velocity (specific discharge)  $V^{(i)}$  is calculated as an average of the microscopic field. Finally, the application of the Darcy's law makes it possible to obtain the permeability tensor row by row:

$$k_{i,j} = \frac{\eta}{p_1 - p_0} V_j^{(i)}, j = 1, 2, 3 . \tag{3}$$

There are a number of papers that make use of this computational routine (see, e. g. [6, 9, 10, 11]).

Another approach to estimating permeability was adopted in [12]. It is based on calculation of the mean survival distance of the Brownian motion in the void space of a porous medium where the porous medium is viewed as absorbing. It was conjectured that the permeability can be estimated as the mean square value of the macroscopic penetration depth of a diffusion started randomly on the surface of a porous sample. In [12], the sample was taken to be a sphere, and the penetration depth was calculated as the average of radial distances between the boundary and the points where the particles diffusing inside a microscopic pore structure were captured.

Following the expositions of Brinkman [13], we assume that the macroscopic velocity satisfies the Navier-Stokes equations. For low Reynolds numbers, it is possible to consider only frictional forces exerted by the porous medium on the fluid. These forces are supposed to depend linearly on the velocity. In the stationary case, these two assumptions lead to the Debye-Brinkman equation (see e. g. [14, 1]):

$$\nabla p = \eta \Delta V - \frac{\eta}{k} V . \tag{4}$$

Here,  $\eta$  is the fluid viscosity and  $k$  is, as always, the constant permeability coefficient;  $p$  and  $V$  are the macroscopic pressure and velocity, respectively.

Suppose there is no pressure gradient (or, equivalently, the fluid viscosity is infinite). For a porous medium occupying the half-space  $\{X \equiv (x, y, z) : X \in \mathbb{R}^3, z > 0\}$  and with a constant inflow velocity  $V = (0, 0, U_0)$  for  $z < 0$ , only  $U$ , the  $z$ -component of the macroscopic velocity inside porous material, is non-zero. From (4) it follows that  $U$  exponentially decays with the distance  $z$  as:

$$U(z) = U_0 \exp\left(-\frac{z}{\sqrt{k}}\right) . \tag{5}$$

Let  $L(X)$  be the microscopic penetration depth of a diffusion started at  $X$ . On the pore scale, this function satisfies the Laplace equation in the void space of the porous medium with Dirichlet boundary conditions on the pores' surface:

$$\Delta L(X) = 0 , \quad L|_S = z . \tag{6}$$

Consider the integral  $I(z) \equiv \int_0^z U(X') dz'$ .

By definition,  $U(X) = \frac{1}{S \Delta z} \int_S \int_{\Delta z} u(X')$ , where  $S \times \Delta z$  is a representative volume centered at the point,  $X$ , inside a porous sample (see, e. g. [15]). With a specific definition

of macroscopic velocity at the sample-fluid interface,  $z = 0$ , we have:

$$I(z) = \int_0^z \frac{1}{S} \int_S u(X') + O(u(z)) .$$

For a zero pressure gradient,  $u(X)$  can be thought of as a solution of the following Dirichlet problem:  $\Delta u = 0$ ,  $u|_S = 0$ ,  $u|_{z=0} = U_0$ . Hence  $u = U_0 \left(1 - \frac{\partial L}{\partial z}\right)$ . Therefore,

$$I(z) = U_0 \left( z - \frac{1}{S} \int_S L(x', y', z) + \frac{1}{S} \int_S L(x', y', 0) \right) + O(u(z)) .$$

Both the difference,  $z - \frac{1}{S} \int_S L(x', y', z)$ , and  $u(z)$  tend to zero as  $z \rightarrow \infty$ . From (5) we have

$$I(z) = \sqrt{k} U_0 \left( 1 - \exp\left(-\frac{z}{\sqrt{k}}\right) \right) .$$

Hence, taking the limit as  $z \rightarrow \infty$  we obtain

$$k = (\bar{L})^2 , \quad \text{where} \quad \bar{L} = \frac{1}{S} \int_S L(x', y', 0) . \quad (7)$$

Our subsequent permeability estimates will be based on this relation.

## 4 Random Walk Algorithms

In calculating the permeability based on formula (7), there is no need to compute the solution of (6) in the whole computational domain. For Monte Carlo computational methods this is exactly the case where we expect them to be the most efficient. There are several Monte Carlo algorithms that could be used here; all of them based on some constructive simulation of Brownian motion. The choice of which to use depends on the representation of the computational domain and the void space of the porous sample in this case. Our approach is based on the assumption that the structure of the porous material is given by a digitized three-dimensional image. Every cubic voxel of this image is either part of the impervious skeleton of the porous medium or an element of the fully saturated pore space. Given this information, we select a square  $S = \{Nx \text{ pixels} \times Ny \text{ pixels}\}$  centered at a point  $(x, y)$  on the sample's boundary, simulate  $(x_0, y_0)$  uniformly distributed in  $S$  and construct a Monte Carlo estimate  $\xi[L]$  for  $L(x_0, y_0, 0)$ . By the double randomization principle,  $\mathbb{E}\xi[L](x, y) = \bar{L}(x, y)$ . As a macroscopic parameter,  $k(x, y) = \bar{L}^2(x, y)$  has to be a slowly varying function of coordinates, and so must tend to a constant value of permeability as the size of the surface of the square,  $S$ , goes to infinity.

On the macroscopic scale, every voxel can be thought of as a point, and as a part of the grid of voxels. This makes it possible to simulate the standard random walk on this grid starting at  $(x_0, y_0, 0)$ . A random walker is absorbed when it first hits the skeleton. Let  $z_N$  be the  $z$ -coordinate of the last position before absorption. Then we set  $\xi[L] = z_N$ . This estimate is rather crude, and, clearly, it highly overestimates the value of  $L$ .

Coming down to the pore's scale, one could discretize the Laplace operator and randomize the resulting equation. With the Neumann boundary condition  $\frac{\partial L}{\partial z} = 0$  at  $z = 0$ ,

the reflected random walk on the grid in the void space provides estimates for the point values of  $L$ . We found; however, that this algorithm still gives biased results, and the difference has the same order of magnitude as the size of the grid. For higher accuracy estimates, this results in prohibitively time-consuming computations.

Note, that in this setting the function values are calculated on the boundary of the computational domain. This can't be done with the Green's-function-based algorithms. To be able to apply more powerful Monte Carlo algorithms such as "walk on spheres," we have to reformulate the boundary value problem (6). Let  $L$  satisfy the Laplace equation in the whole space  $\mathbb{R}^3$  with the exception of the solid porous matrix.<sup>1</sup> This means that  $\xi[L](X_0) = g(X_\tau)$ , by using the probabilistic representation. Here,  $X_\tau$  is the exit point of the diffusion started at  $X_0$ , and the boundary condition is  $g(x, y, z) = z$ .

The specific structure of the boundary given by the voxel-wise representation of the porous material hints at the preference for using "walk on cubes" for constructing approximations for  $X_\tau$  in this case. There are several distinctive features between the construction of cube-based and sphere-based random walks. The main difficulty in simulating "walk on spheres" is in finding the distance from the current position to the boundary of the computational domain. To a great extent this task can be simplified by the "walk in subdomains" approach [16]. In several cases, we have found that despite the  $\varepsilon$ -bias in the boundary conditions, and the larger number of steps required, the "walk on spheres" computations were faster than the cube-based ones. The main reason is the apparent simplicity of simulating an isotropic random vector. The calculation of the distribution of exit points on the cube's surface is not as straightforward. The separation of variables technique gives us a formula for their density in the form of the double infinite series

$$pc(x, y) = 12 \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} (-1)^{n+m} \frac{\sin((2n-1)\pi x) \sin((2m-1)\pi y)}{\cosh\left(\frac{\pi}{2}((2n-1)^2 + (2m-1)^2)^{1/2}\right)}$$

for every face of the unit cube. To generate a random point according to  $pc$ , we approximated this function by a finite sum and used the acceptance-rejection technique with the help of the simulation density  $pc_0(x, y) = \frac{\pi^2}{4} \sin(\pi x) \sin(\pi y)$ .

## 5 Calibration of the Algorithms

To calibrate our computational algorithms, we applied them to a model problem with an analytically calculated permeability value. For the simple porous medium represented by a bundle of straight, parallel capillaries with square cross-section  $a \times a$ , the Kozeny equation gives the permeability as

$$k = nc \frac{a^2}{16},$$

where  $c = 0.562308\dots$ , and the porosity  $n$  is the fraction of capillaries in the whole cross-section of the porous sample (see, e. g. [1, 17]). This result follows from the available exact solution for steady-state Navier-Stokes flow in straight ducts (Poiseuille flow). Hence, for one channel ( $n = 1$ ) we must have  $k = 0.035144\dots \equiv k_1$  (dimensionless, scaled by  $a^2$ ). The same separation of variables technique provides us with the exact solution of the problem (6) with a reflection condition at  $z = 0$ . Substitution of  $L$  in (7) gives  $k = 0.028936\dots$

<sup>1</sup>Note that this model is physically more viable since we don't assume that the velocity is constant up to the 'fluid - porous media' interface.

Monte Carlo estimates for the function  $L$  that satisfies the Laplace equation in the half-space  $\{z < 0\}$  and in the void space of a porous medium with channels positioned on the regular quadratic grid ( $n = 0.5$ ) provide the value 0.102990... for  $\bar{L}$ , the penetration depth averaged over the entrance of one capillary. This means that for the whole porous sample the average value of  $L$  equals  $n\bar{L} = 0.051495...$ . By using the permeability estimate (7), we obtained  $k = 0.0026517...$ . On the other, hand the Poiseuille flow solution gives us  $k = 0.5k_1 = 0.017577...^2$ .

To take this bias into account, in our further computations we suppose that

$$k = CL^2, \quad (8)$$

where the factor  $C \approx 6.63$ , and depends weakly on the geometry of the void space and, possibly, on the viscosity. To elucidate the real nature of this dependence and to provide the possibility of using some additional parameters that can be calculated while simulating the diffusion process, further investigations are needed. It is clear; however, that, as always, this formula cannot be exact for all conceivable configurations of porous medium.

## 6 Numerical Results

Here we present results of some computational experiments we performed with the stochastic computational methods described in the previous sections. These algorithms were applied to investigating the behavior of the permeability in some of the simplest models of random porous structures. We are very well aware of the large number of microscopic models that have been proposed to represent the microstructure of porous media, and to predict its macroscopic parameters and properties. There are a vast number of publications on this subject (see, e. g. [6, 18, 9, 10]). The algorithms used and the models described are intricate, and simulation procedures are rather time-consuming. So, the apparent reason for our choice was that we did not want to obscure the properties of the computational methods by specific features of some complex model.

The samples of porous material we used in our computations were generated voxel-wise, independently in the simplest case. This means that the local porosity has the binomial distribution. The second model was based on the multilevel simulation of voxels. We also carried out some experiments for a sample with the porosity distribution correlated in one direction.

In the choice of size of the sampling square we are guided by the statistical properties of some real porous materials. Data from direct measurements suggest that the distribution of local porosity is approximately normal with the standard deviation of order of several percent (see, e. g. [15]). This corresponds to a digital sample having at least  $ns = 10$  voxels in every dimension. In [18] in particular, it was conjectured that the statistics of sedimentary rocks corresponds to samples with linear measurements twice as that. The permeability distribution data gives approximately the same order of sample sizes.

To check the dependence between the permeability and porosity, we simulated random digital structures for different values of  $n$ . Next we randomly choose the position of the

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<sup>2</sup>Usually it is assumed that permeability is totally determined by the geometric properties of a porous medium and does not depend on the properties of the fluid that flows through it. It is clear, however, that this supposition is valid only for some range of viscosity values. Here, the bias we have in the values of  $k$  can be accounted by our assumption of an infinite viscosity coefficient.

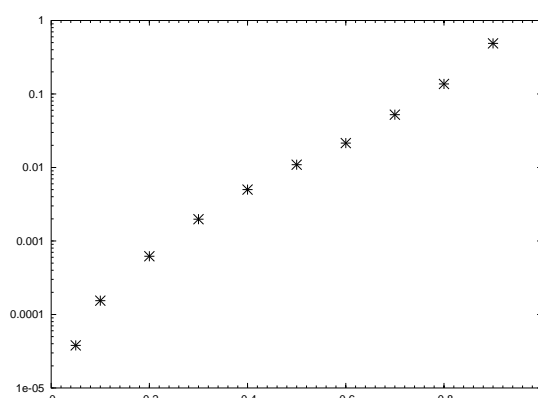


Figure 1: Dimensionless permeability  $k/(Ca^2)$  vs porosity (logarithmic scale).

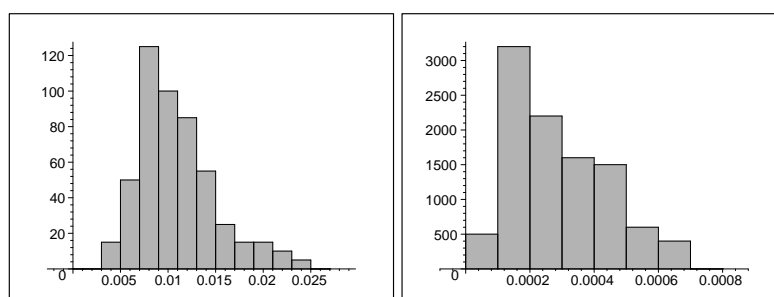


Figure 2: Distribution of permeability for the simplest random model. **1.**  $n = 0.5, ns = 10$ . For the log-normal distribution the  $\chi^2$  criterion gives  $p = 0.81 \gg 0.1$ . **2.**  $n = 0.1355, ns = 10$ . Here  $p = 0.12$ .

square,  $S = ns \times ns$ , and simulated random points uniformly distributed in  $S$ . Values for different positions gave us the statistics of sample values for permeability. Clearly, the behavior of this data depends on  $ns$ . The total permeability for the given porosity comes through the averaging of these sample values. The results presented in Figure 1 clearly show the predicted functional dependence (see, e. g. [12] for reference).

Numerous direct measurements corroborate the hypothesis that the permeability of various porous materials have a log-normal distribution given a normal porosity distribution. To investigate this phenomenon, we carried out a series of numerical experiments with different sample square sizes of  $ns = 1, 2, 5, 10, 15, 20, 30$ . First, we considered the simplest model of porous medium. Clearly, for  $ns = 1$  and  $2$  the behaviour is chaotic, and for small porosities the sample is often a complete solid. For  $ns = 10$ , statistical tests strongly support the log-normality hypothesis for the porosities in the interval  $[0.3, 0.6]$ . For smaller porosities the statistical results are marginal. As for large values of  $n$ , the chi-squared test gives a hint that sample values of permeability are normally distributed. For larger sizes of the sample, the variability of the calculation results becomes small. This makes both the normality and log-normality hypotheses equally viable. However, in these cases the Gamma distribution also fits well.

Given the results of [18, 10], we apply our algorithms to calculations of permeability for the particular values of porosity ( $n = 0.1355$ ) and voxel size ( $a = 7.5 \mu m$ ) that were considered there.

For the simplest uncorrelated model we obtained a permeability of  $k = 107$  Darcy.

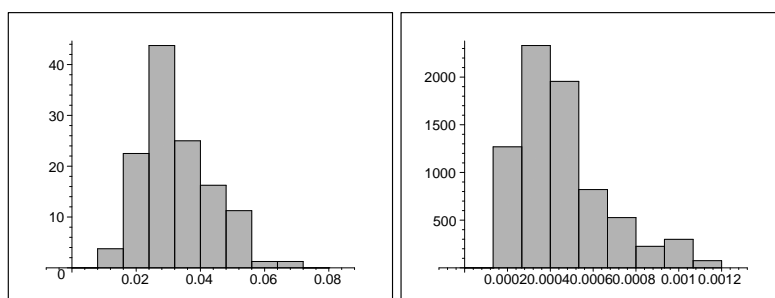


Figure 3: Distribution of permeability for the hierarchical model. **1.**  $n = 0.5, ns = 20$ . For the log-normal distribution the  $\chi^2$  criterion gives  $p = 0.51$ . **2.**  $n = 0.1355, ns = 20$ . Here  $p = 0.80$ .

For the model with three digital scales of simulated voxel sizes, our computations gave a permeability of  $k = 191$  Darcy. Note that for the digital sample of real sandstone, the finite-difference calculations of [10] gave a permeability value of 1150 Darcy. It would be irrelevant to compare such different results. However, it is worth noting that Gaussian and simulated annealing reconstruction models of porous material with the same porosity provide much more biased values: 24 Darcy and 38 Darcy respectively.

## 7 Discussion, Conclusions, and Future Directions

The results of computational experiments with the Monte Carlo algorithms we presented here clearly show that even for the simplest models of digital porous material the distribution of calculated values of permeability conforms with the log-normal statistical law. Note that the same computations for the regular capillary structure provides statistics that are approximately normally distributed. It is essential, however, to recall that statistical tests do not provide us with the exact criterion for choosing the exact distribution. In many cases these results are marginal and some distributions other than the log-normal distribution fit as well.

This work shows the utility of the penetration depth used in concert with Monte Carlo in computing permeabilities. More specifically, we were able to show that a simple geometrical set of assumptions on the statistical structure of a porous medium results in a statistical distribution in the resulting permeabilities consistent with the empirical, log-normal, findings. This not only validates the use of penetration depth, but the Monte Carlo approach in general for these class of problems.

In future work, we will study the application of these techniques to a wider class of permeability problems. We will study different geometrical models of porous media along with applying the penetration depth algorithm described here to calculations of permeability in non-isotropic cases.

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