Closed-Form Solution for the Reconstruction Problem in Porous Media

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The statistical reconstruction of lattice models of real porous media is one of the basic engineering problems in the theory of porous structure and has a variety of applications in the study of transport, in mineral processing, and in material characterization. A systematic analysis of the reconstruction problem of porous media is presented, as well as a closed-form solution. The solution is presented in the form of a linear filter acting on Gaussian processes by means of a superposition of elementary correlated processes with prescribed correlation properties, and in the form of a memoryless process recalling the theory of Khinchin on the properties of correlation functions. The connection of this approach with models of correlated percolation is also discussed.

Introduction

Signal/image analysis by means of methods derived from fractal theory has produced many significant applications. The most significant result is certainly the approach to image compression by means of iterated function systems, first introduced by Barnsley (Barnsley, 1988; Barnsley and Hurd, 1993) and subsequently developed by many authors, including Forte and Vrscay (1994a,b).

Another interesting contribution comes from the analysis and filtering of stochastic fluctuations by applying fractional Brownian motion models or multifractal methods (for an overview of various approaches, see Baldo et al., 1994).

Image processing has important consequences in the theory of porous media with a view to describing the fine structure of the pore network, obtaining equivalent lattice models of real porous structures, analyzing transport phenomena on these models, and predicting the behavior of transport coefficients (Adler et al., 1990; Blumenfeld and Ball, 1992; Blumenfeld and Torquato, 1993). One of the most interesting results of image analysis in the study of porous structure, with a potential multiplicity of industrial applications, is the *reconstruction of porous media*, which involves the generation of lattice models possessing the same statistical properties as the real porous structure under investigation. The information on the porous medium is obtained from the optical analysis of the structure. This method has been applied mostly to geological macroporous media (sandstones) with a characteristic lengthscale ranging from 0.1 to 10 mm, but can also be applied to the macroporosity of packed columns, and in principle to microporous materials. This operation has been extensively studied by Joshi (1974), Quiblier (1984), and Adler et al. (1990) (the JQA approach) in connection with macroporous materials, borrowing a similar approach developed in electrical engineering for the filtering of a linear superposition of random Gaussian variables (Thompson, 1954; Barrett and Coales, 1955; Rugh, 1980). For further analysis on this topic, see also Yao et al. (1993) and Sallés et al. (1994).

The notion of equivalence between the original porous medium and the reconstructed lattice structure depends on the mathematical framework within which the reconstruction problem is tackled. In the JQA formulation, the reconstructed lattice is obtained by considering a linear superposition of Gaussian random variables. The equivalence of the original porous medium and the reconstructed lattice means that they have the same porosity and the same pore–pore correlation function (correlation function of the second order). The reconstruction of porous media is a typical inverse problem, like many other encountered in engineering applications. In the JQA formulation, this problem is recast in the form of a nonlinear functional equation that can be solved by applying parameter optimization.

In this article we show that the reconstruction problem can be solved in closed form by reducing the problem to a linear functional equation that can be solved by means of a Laplace inversion. The reduction of the reconstruction problem to the

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form of a linear functional equation is made possible by the choice of a suitable set of stochastic basis processes possessing an exponential decay in the correlation function. The analysis is further extended to consider memoryless reconstruction and its relationship with spectral representation and ergodicity. The connection between the reconstruction problem and the correlated percolation schemes is also discussed.

Statement of the Problem

Let us consider the experimental section of a porous medium as a two-dimensional image $\mathcal{I}$ and let $\mathcal{P}$ be the pore space, described by its characteristic function $\chi_{\mathcal{P}}(x)$

$$\chi_{\mathcal{P}}(x) = \begin{cases} 1 & x \in \mathcal{P} \\ 0 & \text{elsewhere.} \end{cases} \tag{1}$$

The porosity ϵ is given by $\epsilon = \langle \chi_{\mathcal{P}}(x) \rangle$, and the normalized pore-pore correlation function by

$$C_{2\chi}(x) = \frac{\langle (\chi_{\mathcal{P}}(y) - \epsilon)(\chi_{\mathcal{P}}(y+x) - \epsilon) \rangle}{\epsilon - \epsilon^2}. \tag{2}$$

Note that $\langle \chi_{\mathcal{P}}^n(x) \rangle = \langle \chi_{\mathcal{P}}(x) \rangle = \epsilon$, for every $n > 0$ ($\langle \cdot \rangle$ indicates statistical spatial average).

Under the assumption of isotropy, $C_{2\chi}(x)$ is solely a function of $x = |x|$ and a generic cross section of the material is representative of the entire three-dimensional structure. The statistical analysis is limited to the pore-pore correlation function, so that the lattice structure to be generated must have the same porosity and the same pore-pore correlation function as the original image.

A simple way to obtain this is to consider a continuous correlated random process $\mathcal{Y}(x)$

$$\mathcal{Y}(x) = \sum_{r'} a(r')\xi(r' + x), \tag{3}$$

where $\xi(x)$ is a normalized Gaussian random variable (with zero mean and unit variance), $a(r)$ is the kernel of the linear filter, and the summation is extended over the values r' belonging to the lattice representation of the periodic unit cell. Since $\mathcal{Y}$ is a linear superposition of Gaussian variables, $\mathcal{Y}$ is still Gaussian with zero mean. The transformation from the $\mathcal{Y}$ process to the binary (pore-pore matrix, 0/1) porous structure is given by a nonlinear filter $\mathcal{G}$, depending on the distribution function F_{y} of $\mathcal{Y}$ and on the porosity ϵ: for each point x, the reconstructed (0/1) porous structure $Z_R(x)$ is given by

$$Z_R(x) = \mathcal{G}(\mathcal{Y}(x), \epsilon) = \begin{cases} 1 & F_y(\mathcal{Y}(x)) < \epsilon \\ 0 & F_y(\mathcal{Y}(x)) > \epsilon \end{cases}. \tag{4}$$

Equation 4 ensures statistically that the reconstructed porous medium admits the porosity ϵ, so that the only condition to be further imposed is that $C_{2Z_R}(x) = C_{2\chi}(x)$.

The correlation function $C_{2Z_R}(x)$ is related to the corresponding correlation function $C_{2y}(x)$ through the relation

$$C_{2Z_R} = \int_{-\infty}^{\infty} dy_1 \int_{-\infty}^{\infty} dy_2 \left[\frac{(\mathcal{G}(y_1,\epsilon) - \epsilon)(\mathcal{G}(y_2,\epsilon) - \epsilon)}{\epsilon - \epsilon^2} \right] \times p(y_1, y_2), \tag{5}$$

where

$$p(y_1,y_2) = \frac{1}{2\pi(1 - C_{2y}^2)^{1/2}} \exp\left[-\frac{y_1^2 + y_2^2 - 2C_{2y} y_1 y_2}{2(1 - C_{2y}^2)} \right]. \tag{6}$$

The normalized correlation function $C_{2y}(x)$ for $\mathcal{Y}$ given by Eq. 3 reads as

$$C_{2y}(x) = \sum_{r'} a(r') a(r' + x) / \sum_{r'} a^2(r'). \tag{7}$$

Therefore, for every $C_{2Z_R}(x)$, the corresponding value of $C_{2y}(x)$ is evaluated through Eqs. 5–6. In the work of Joshi (1974), Quiblier (1984), and Adler et al. (1990), C_{2Z_R} is expressed as a power series of C_{2y} by using an orthogonal expansion in terms of Hermite polynomials. This series expansion is computationally expensive and the convergence deteriorates for C_{2y} tending toward unity. For this reason, it is convenient to integrate numerically Eq. 5 with $p(y_1, y_2)$ of Eq. 6, for the prescribed value of the porosity ϵ. Starting from a set of values $\{C_{2y_i}\} \in [-1, 1]$ the corresponding values $\{C_{2Z_{Ri}}\}$ can be obtained in this way, and can be used as a calibration curve.) From the knowledge of $C_{2y}(x)$, the coefficients of the linear filter $\{a(r')\}$ are then calculated starting from Eq. 7 by means of optimization methods.

Closed-Form Solution with Linear Filters

In the previous section we have seen that the reconstruction problem reduces to the solution of the nonlinear functional Eq. 7. The approach followed to solve this equation is based on optimization methods.

In this section we show that the reconstruction problem can be recast in the form of a linear functional equation, analogous to a Laplace transform, which can be solved in closed form in many cases. This approach is based on the choice of a suitable set of basis processes with specified (exponential) decay in the correlation function. The choice of the basis processes depends on the domain of definition. For this reason, different cases are discussed separately.

In the theoretical development it is useful to recast the previous equation in integral form, by taking the continuous limit of Eqs. 3 and 7. The continuous counterparts of these equations are

$$\mathcal{Y}(x) = \int a(r')\xi(r' + x)\, dr',$$
$$C_{2y}(x) = \int a(r') a(r' + x)\, dr' / \int a^2(r')\, dr'. \tag{8}$$

Unless specified, we will always consider the continuous formalism.

One-dimensional case

The reconstruction of a 1-d Gaussian process with specified correlation properties is of limited interest in the theory of porous media [the reason is that it is impossible to represent nontrivial porous structures on the real line without inhibiting the existence of an end-to-end path; the only percolating cluster on the real line is for unit percolation probability (Stauffer and Aharony, 1992)], but is formally useful to highlight the method adopted.

Let $x \in (-\infty, \infty)$ and let us define as basis processes $\{\mathcal{Y}(x, \lambda)\}$, the Gaussian processes defined as

$$\mathcal{Y}(x,\lambda) = \int_0^\infty a(x',\lambda)\xi_\lambda(x+x')\,dx',$$

$$a(x,\lambda) = \sqrt{2\lambda}\exp^{(-\lambda x)}, \quad (9)$$

where $\xi_\lambda(x)$ is a Gaussian uncorrelated process with zero mean and unit variance. The correlation function $C_{2\mathcal{Y}}(x, \lambda)$ of $\mathcal{Y}(x, \lambda)$ is given by

$$C_{2\mathcal{Y}}(x,\lambda) = \langle \mathcal{Y}(x',\lambda)\mathcal{Y}(x'+x,\lambda)\rangle = e^{-\lambda x}, \quad (10)$$

that is, it exhibits an exponential decay in x. For example, Figure 1 shows the correlation function obtained numerically for the stochastic process, Eq. 9, compared with the predicted exponential relaxation, Eq. 10, for different values of λ.

We can expand a generic process $\mathcal{Y}(x)$ as the superposition of the basis processes $\{\mathcal{Y}(x,\lambda)\}$

$$\mathcal{Y}(x) = \int_0^\infty p(\lambda)\mathcal{Y}(x,\lambda)\,d\lambda. \quad (11)$$

By observing that $\langle \xi_\lambda(x)\xi_{\lambda'}(x')\rangle = \delta(x-x')\delta(\lambda-\lambda')$, it follows that

$$C_{2\mathcal{Y}}(x) = \int_0^\infty \pi(\lambda)C_{2\mathcal{Y}}(x,\lambda)\,d\lambda = \int_0^\infty \pi(\lambda)e^{-\lambda x}\,d\lambda, \quad (12)$$

where $\pi(\lambda) = p^2(\lambda)$.

Therefore, under the condition that $C_{2\mathcal{Y}} \geq 0$, it follows that $\pi(\lambda)$ is the inverse Laplace transform of the correlation function. The condition $C_{2\mathcal{Y}} \geq 0$ is not so restrictive in practical applications. The extension to d-dimensional structures is straightforward.

d-Dimensional isotropic structures

An isotropic porous medium is characterized by a pore–pore correlation function that depends exclusively on the distance $x = |\mathbf{x}|$, $C_{2\mathcal{Y}}(\mathbf{x}) = C_{2\mathcal{Y}}(x)$. For d-dimensional isotropic porous media it is convenient to define the basis processes $\{\mathcal{Y}(\mathbf{x},\lambda)\}$ in a slightly different way than in the preceding subsection, by convoluting a Gaussian uncorrelated process with a Gaussian kernel,

$$\mathcal{Y}(\mathbf{x},\lambda) = \int_{E^d} a(\mathbf{u},\lambda)\xi_\lambda(\mathbf{u}+\mathbf{x})\,d\mathbf{u}$$

$$= \left(\frac{4\lambda}{\pi}\right)^{d/4} \int_{E^d} e^{-2\lambda u^2}\xi_\lambda(\mathbf{u}+\mathbf{x})\,d\mathbf{u}, \quad (13)$$

where E^d is the Euclidean d-dimensional space, $E^d = \{\mathbf{x} \mid -\infty < x_i < \infty, (i=1,\ldots,d)\}$. The correlation function for the process given by Eq. 13 is Gaussian (Figure 2),

$$C_{2\mathcal{Y}}(x,\lambda) = e^{-\lambda x^2}. \quad (14)$$

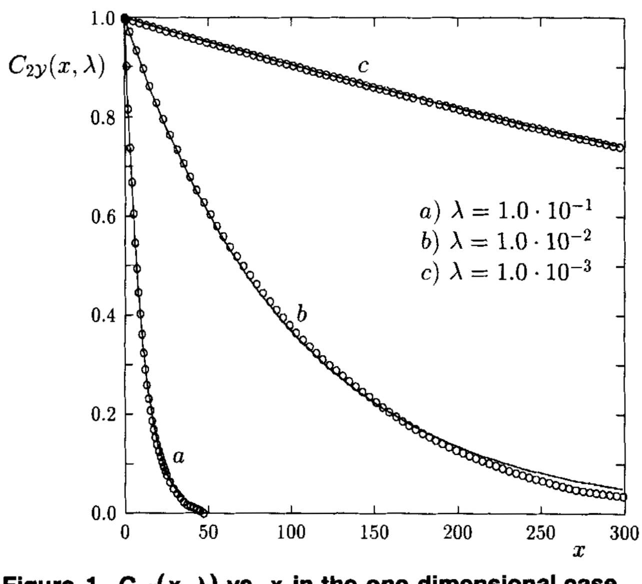


Figure 1. $C_{2\mathcal{Y}}(x, \lambda)$ vs. x in the one-dimensional case.
The correlation function obtained numerically for the stochastic process, Eq. 9, (points) is compared with the predicted exponential decay, Eq. 10, (continuous line) for different values of λ.

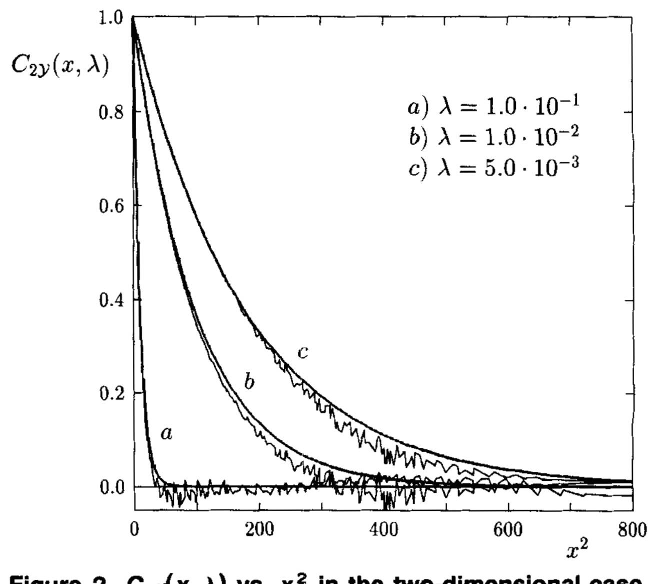


Figure 2. $C_{2\mathcal{Y}}(x, \lambda)$ vs. x^2 in the two-dimensional case.
The correlation function obtained numerically for the stochastic process, Eq. 13, (rough lines) is compared with the predicted exponential decay in x^2, Eq. 14, (continuous lines) for different values of λ.

As discussed earlier, by considering the linear superposition of basis processes, Eq. 11, and putting $z = x^2$, $C_{2\mathcal{Y}}(x) = \tilde{C}_{2\mathcal{Y}}(z)$, it follows that

$$\tilde{C}_{2\mathcal{Y}}(z) = \int_0^\infty \pi(\lambda) e^{-\lambda z} d\lambda. \tag{15}$$

Therefore, as in the 1-d case, Eq. 15 expresses the property that the weight function $\pi(\lambda)$ is the inverse Laplace transform of $\tilde{C}_{2\mathcal{Y}}(z)$.

It is important to observe that $\tilde{C}_{2\mathcal{Y}}(z)$ is defined for real z, while the Laplace inversion requires a Laplace transform on the complex plane. In order to apply Eq. 15, we therefore need an analytic continuation $\tilde{C}^{(p)}_{2\mathcal{Y}}(z)$ of $\tilde{C}_{2\mathcal{Y}}(z)$ valid for all complex z (whose restriction to real z coincides with $\tilde{C}_{2\mathcal{Y}}(z)$) such that

$$\pi(\lambda) = \frac{1}{2\pi i} \int_{x_o - i\infty}^{x_o + i\infty} \tilde{C}^{(p)}_{2\mathcal{Y}}(z) e^{\lambda z} dz. \tag{16}$$

The analytic continuation can be achieved by considering rational approximations (e.g., Padé approximants) or by means of other methods (e.g., orthogonal polynomial expansion). Examples will be given in the next section.

Two other topics deserve further attention. The aim of reconstruction methods is to obtain a stochastic characterization of a porous structure and to reproduce a three-dimensional lattice structure starting from a two-dimensional image. In the transition from $d = 2$ to $d = 3$ the formal apparatus remains unchanged as the prefactor of the kernel $a(\boldsymbol{u}, \lambda)$ in Eq. 13, which defines the basis functions, depends on d.

A final point is related to the presence of *localized* exponential solutions. In many applications, asymptotic exponential decay is observed in the correlation function $\tilde{C}_{2\mathcal{Y}}(z) \sim \exp(-\lambda_c z)$. In this case it is convenient to consider the process $\mathcal{Y}(\boldsymbol{x})$ defined as

$$\mathcal{Y}(\boldsymbol{x}) = \int_0^\infty \hat{p}(\lambda) \mathcal{Y}(\boldsymbol{x}, \lambda) d\lambda + A \mathcal{Y}(\boldsymbol{x}, \lambda_c), \tag{17}$$

where $\mathcal{Y}(\boldsymbol{x}, \lambda_c)$ and the basis processes $\{\mathcal{Y}(\boldsymbol{x}, \lambda)\}$ are uncorrelated to each other. The resulting correlation function, associated with the process defined by Eq. 17, is therefore given by

$$\tilde{C}_{2\mathcal{Y}}(z) = \int_0^\infty \hat{\pi}(\lambda) e^{-\lambda z} d\lambda + A^2 e^{-\lambda_c z}. \tag{18}$$

An example of the decomposition will be given in the subsequent section.

Examples and Applications

Closed-form solutions

Equations 15–16 state that the weight function $\pi(\lambda)$ is the inverse Laplace transform of the correlation function $\tilde{C}_{2\mathcal{Y}}(z)$. The entire apparatus of Laplace transform theory can therefore be applied to obtain $\pi(\lambda)$ in closed form in many situations. As an example, let us consider a correlation function with an exponential decay in x, and therefore,

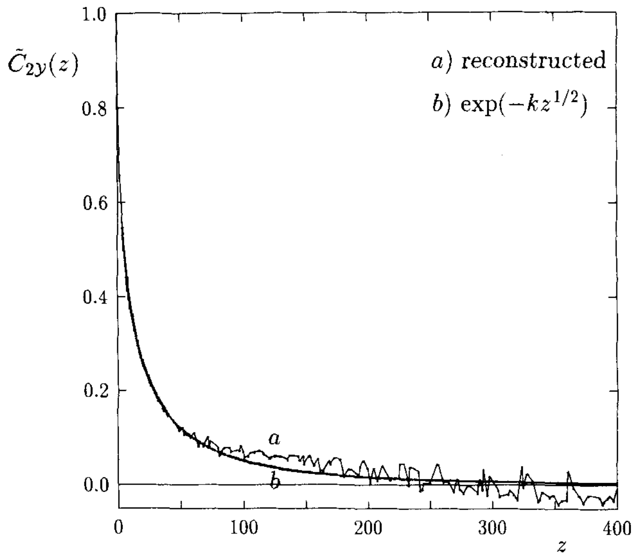


Figure 3. Comparison of the correlation function $\tilde{C}_{2\mathcal{Y}}(z)$ obtained numerically for the stochastic process, Eq. 11, and the predicted exponential decay, Eq. 19.

Simulation was performed on 200×200 lattice with $k = 1/3$.

$$\tilde{C}_{2\mathcal{Y}}(z) = e^{-k\sqrt{z}}. \tag{19}$$

By recalling Eq. 16, it follows that the corresponding inverse Laplace transform is given by (Abramowitz and Stegun, 1974)

$$\pi(\lambda) = \frac{k}{2\sqrt{\pi\lambda^3}} \exp(^{-k^2/4\lambda}). \tag{20}$$

Figure 3 shows the comparison of Eq. 19 and the correlation function obtained from a reconstructed 2-*d* 200×200 lattice by applying Eq. 11.

A numerical case study

In dealing with the reconstruction of real porous media, closed-form expressions for the weight function $\pi(\lambda)$ cannot be obtained in general and Eqs. 15–16 should therefore be solved numerically.

The correlation functions $C_{2\mathcal{Y}}(x)$ or $\tilde{C}_{2\mathcal{Y}}(z)$ are defined for real x or z: in order to apply Eq. 16 we need the analytic continuation of the correlation function on the complex plane. Orthogonal polynomial expansion can be useful to avoid numerical problems associated with the Laplace inversion.

As a case study we consider a two-dimensional lattice obtained by means of fractal percolation. This case reflects exactly the same difficulties as can be encountered in connection with a 2-*d* analysis of a real porous medium. A fractal percolation lattice is a random fractal generated by an iterative procedure (Falconer, 1990). The unit square $\mathcal{E}_o = [0,1] \times [0,1]$ is divided into b^2 squares of side $1/b$. A subset of these squares is selected to form $\mathcal{E}_1$ in such a way that each square has the independent probability p of being chosen as a square of $\mathcal{E}_2$. The iterative procedure continues so that $\mathcal{E}_n$ is a random collection of squares of side $(1/b)^n$. This iterative proce-

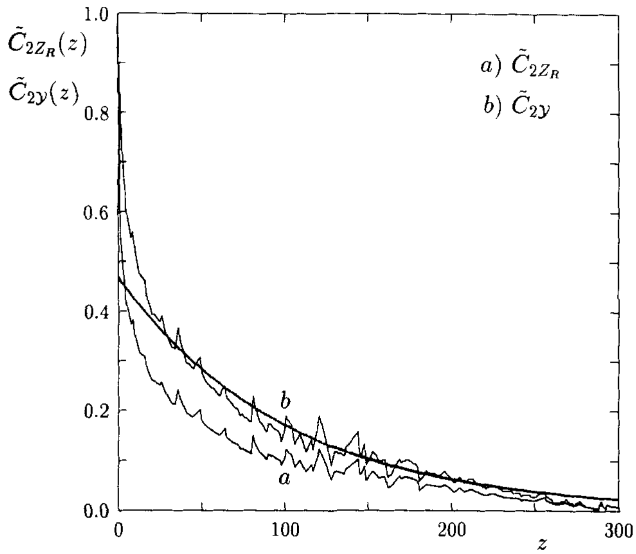


Figure 4. $\tilde{C}_{2Z_R}(z)$ and $\tilde{C}_{2\mathcal{Y}}(z)$ vs. z for a 128×128 fractal percolation lattice ($n=7$, $b=2$, $p=0.90$).
The bold line is the asymptotic decay, $\tilde{C}_{2\mathcal{Y}}(z) \sim A^2 \exp(-\lambda_c z)$.

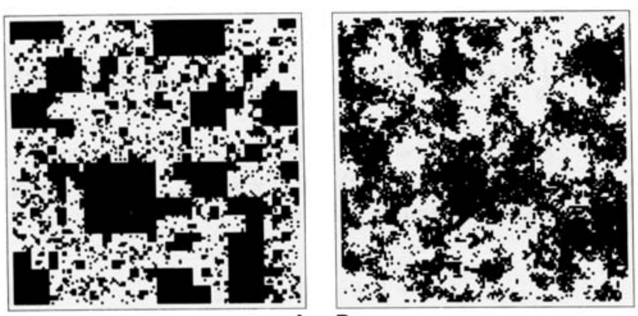
dure, which depends on the parameters p and b, defines a random fractal $\mathfrak{F}_{p,b} = \cap_{n=0}^{\infty} \mathcal{E}_n$. The fractal dimension of $\mathfrak{F}_{p,b}$ is $D = \log(b^2 p)/\log(b)$. Figure 4 shows the behavior in a log-normal plot of $\tilde{C}_{2Z_R}(z)$, $\tilde{C}_{2\mathcal{Y}}(z)$ for a 2-d fractal percolation lattice with $b=2$, $n=7$, $p=0.90$ (128×128 lattice units, see Figure 5A). These two correlation functions are related to each other by means of transformation, Eq. 5. The bold line represents the asymptotic decay $\tilde{C}_{2\mathcal{Y}}(z) \sim A^2 \exp(-\lambda_c z)$. For numerical reasons it is therefore convenient to develop the correlation function $\tilde{C}_{2\mathcal{Y}}(z)$ as

$$\tilde{C}_{2\mathcal{Y}}(z) = A^2 e^{-\lambda_c z} + \hat{C}_{2\mathcal{Y}}(z),$$

$$\hat{C}_{2\mathcal{Y}}(z) = \int_0^{\infty} \hat{\pi}(\lambda) e^{-\lambda z} d\lambda, \quad (21)$$

and to approximate the new weight function $\hat{\pi}(\lambda)$.

The estimate of $\hat{\pi}(\lambda)$ and its analytic continuation can be achieved by means of an orthogonal polynomial expansion.



A B

Figure 5. (A) Fractal percolation lattice (128×128 lattice units, $p=0.90$, $n=7$, $b=2$); (B) its reconstruction by means of the method discussed in the text.

Let us define the new variable $y = 1/(z+1)$ so that the positive real line $z \in [0,\infty)$ is mapped into $y \in [0,1]$ and put $\hat{C}^*_{2\mathcal{Y}}(y) = \hat{C}_{2\mathcal{Y}}(1/y - 1)$. In this way $\hat{C}^*_{2\mathcal{Y}}(y)$ can be easily approximated by means of an orthonormal polynomial expansion

$$\hat{C}^*_{2\mathcal{Y}}(y) = \sum_{n=0}^{N} c_k \hat{P}_k(y), \quad (22)$$

where $\hat{P}_k(y) = \sum_{h=0}^{k} \alpha_h^{(k)} y^h$ are the modified orthonormal Legendre polynomials on [0,1], $\hat{P}_k(y) = \sqrt{2k+1} P_k(2y-1)$, where $P_k(x)$ are the Legendre polynomials, orthogonal in $x \in [-1, 1]$. Once the coefficients c_k are evaluated from the moment hierarchy $\{m_k\}$,

$$c_k = \sum_{h=0}^{k} \alpha_h^{(k)} m_h, \qquad m_h = \int_0^1 \hat{C}^*_{2\mathcal{Y}}(y) y^h \, dy, \quad (23)$$

$\hat{C}_{2\mathcal{Y}}(z)$ can be written as

$$\hat{C}_{2\mathcal{Y}}(z) = \sum_{k=1}^{N} d_k \frac{1}{(z+1)^k}, \qquad d_k = \sum_{h=k}^{N} c_k \alpha_k^{(h)}. \quad (24)$$

Note that the zeroth-order term is vanishing since for $z \to \infty$, $\hat{C}_{2\mathcal{Y}}(z)$ is vanishing. This expression can be easily inverted to give

$$\hat{\pi}(\lambda) = \sum_{k=0}^{N-1} \frac{d_{k+1} e^{-\lambda} \lambda^k}{k!}. \quad (25)$$

Figure 6 shows that the reconstructed $\hat{\pi}(\lambda)$ with $N=5$, and Figure 7 shows the comparison of the original and reconstructed correlation functions. The comparison of the original structure and the reconstructed lattice is shown in Figure

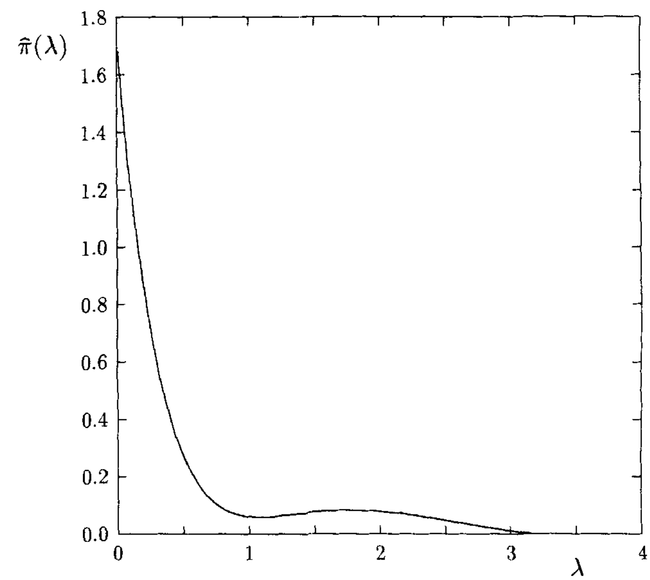


Figure 6. $\hat{\pi}(\lambda)$ vs. λ for the fractal percolation lattice of Figure 5A, obtained from Eq. 25 with $N=5$.

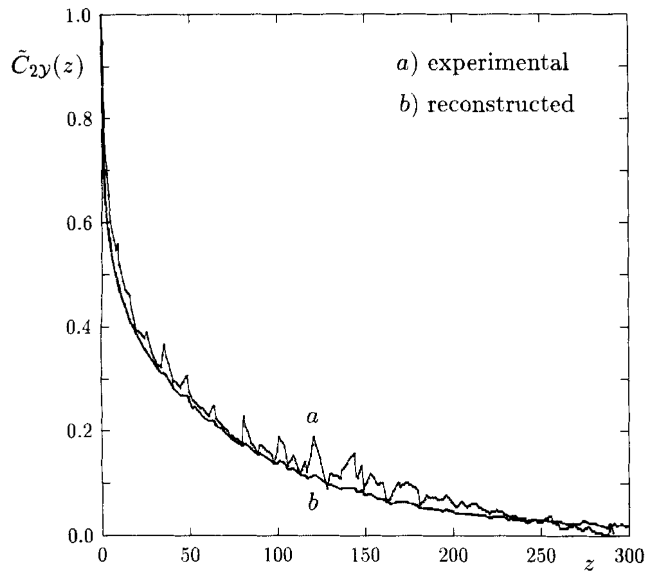


Figure 7. Comparison of the experimental and the reconstructed $\tilde{C}_{2\mathcal{Y}}(z)$ for the fractal percolation lattice of Figure 5A.

5A, 5B, where the close statistical similarity between the original and reconstructed structures can be appreciated. A snapshot of the corresponding three-dimensional reconstructed lattice is shown in Figure 8.

The method just outlined to obtain the kernel $\hat{\pi}(\lambda)$, based on orthogonal polynomial expansion in a transformed variable y, is a simple and effective way to avoid numerical problems. Other approaches can also be proposed, for example, by borrowing the results obtained in the theory of adsorption

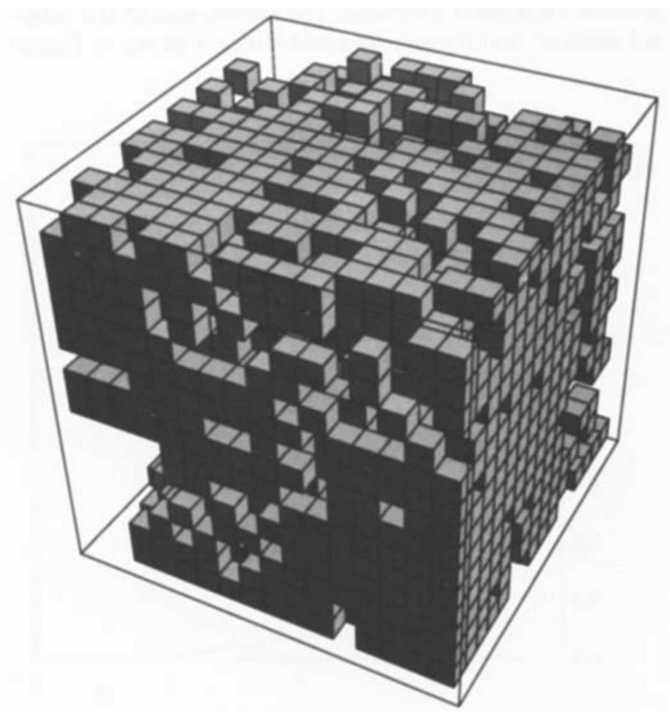


Figure 8. Three-dimensional reconstructed lattice with the same statistical features as in Figure 5B.

on heterogeneous solids, which is based on a similar continuum approach considering a spectrum of adsorption energies. For more details, see the review article of Cerofolini and Re (1993).

Memoryless Processes and Khinchin Theorem

The approach followed so far is based on linear convolutory functionals with prescribed kernels. However, it is possible to address the reconstruction problem by means of memoryless processes that are stationary in a wide sense. This method was originally proposed by Adler (1992). In this section we focus mainly on the statistical properties of this approach compared with the convolution method discussed in the preceding sections.

Let us first consider the case of a periodic porous medium whose statistical properties are fully characterized within a unit cell. We develop the analysis in the 1-d case. The results obtained can be easily extended to arbitrary dimensions. In this case, the unit cell is defined for $x \in [0, L]$, in which we define a stochastic process $\mathcal{Y}(x)$ as

$$\mathcal{Y}(x) = \sum_{k=0}^{\infty} b_k \left[\xi_{1k} \cos\left(2\pi k \frac{x}{L}\right) + \xi_{2k} \sin\left(2\pi k \frac{x}{L}\right) \right], \quad (26)$$

where for each k, ξ_{1k} and ξ_{2k} are stochastic variables uncorrelated with each other ($\langle \xi_{1i} \xi_{1j} \rangle = \langle \xi_{2i} \xi_{2j} \rangle = \delta_{ij}$, $\langle \xi_{1i} \xi_{2j} \rangle = 0$) having zero mean, and the coefficients b_k are to be determined. The correlation function associated with the stochastic process is given by

$$C_{2\mathcal{Y}}(x) = \sum_{k=0}^{\infty} b_k^2 \cos\left(2\pi k \frac{x}{L}\right), \quad (27)$$

and the coefficients b_k^2 are therefore the Fourier coefficients of $C_{2\mathcal{Y}}(x)$ in a cosine Fourier expansion

$$b_0^2 = \frac{1}{L} \int_0^L C_{2\mathcal{Y}}(x)\,dx, \qquad b_k^2 = \frac{2}{L} \int_0^L C_{2\mathcal{Y}}(x) \cos\left(2\pi k \frac{x}{L}\right) dx,$$
$$k = 1, 2 \ldots. \quad (28)$$

The series approach, Eqs. 26–28, can be extended by removing the condition of periodicity and by considering a process defined as

$$\mathcal{Y}(x) = \int_0^{\infty} b(\omega)[\xi_1(\omega)\cos(\omega x) + \xi_2(\omega)\sin(\omega x)]\,d\omega, \quad (29)$$

where $\langle \xi_i(\omega) \rangle = 0$ ($i = 1, 2, \forall\omega$), $\langle \xi_i(\omega_1)\xi_i(\omega_2) \rangle = \delta(\omega_1 - \omega_2)$ ($i = 1,2$), $\langle \xi_i(\omega_1)\xi_j(\omega_2) \rangle = 0$ ($i \neq j, \forall\omega_1, \omega_2$), for which the correlation function is given by

$$C_{2\mathcal{Y}}(x) = \int_0^{\infty} b^2(\omega)\cos(\omega x)\,d\omega, \quad (30)$$

and therefore

$$b^2(\omega) = \frac{2}{\pi} \int_0^{\infty} C_{2\mathcal{Y}}(x)\cos(\omega x)\,dx. \quad (31)$$

The introduction of a memoryless process to solve the reconstruction problem of porous media permits us to highlight several important aspects.

First of all, Eqs. 27 and 30 are the most general expressions for the correlation function of a continuous stationary process with a discrete or continuous spectrum. Indeed, the coefficients of the Fourier expansions (b_k^2 or $b^2(\omega)$) should be strictly positive in accordance with the theorems of Slutskij and Khinchin (Doob, 1953). (The Khinchin theorem states that a function $f(x)$ is correlation function of a continuous stationary process (possessing a continuous spectrum) if it can be presented by

$$f(x) = \int \cos(\omega x)\, dF(\omega),$$

where $F(\omega)$ is a distribution function. The Slutskij theorem states the same properties of a continuous stationary process with a discrete spectrum.)

It should also be noted that the processes represented by Eqs. 26 and 29 are stationary but in a wide sense. This implies that the ergodic theorem of Birkhoff and Khinchin cannot be applied, and therefore spatial averages do not coincide with ensemble averages.

The following example illustrates this property. Let us consider a one-dimensional periodic structure on $x \in [0, 1]$ and a correlation function $C_{2\mathcal{Y}}(x) = \exp(-kx)$, $x \in [0, 1/2)$ with an exponential decay in x. The periodicity of the structure implies that $C_{2\mathcal{Y}}(x) = C_{2\mathcal{Y}}(1-x)$. Figure 9 shows the reconstructed correlation function starting from Eq. 26, with the coefficients given by Eq. 28, averaged over 10^4 realizations of the process, for $k = 5.0$. The comparison between the reconstructed process and the original is fairly good. Nevertheless, a single realization of the process may possess a correlation function that differs significantly from the averaged correlation function: this is a consequence of the lack of ergodicity.

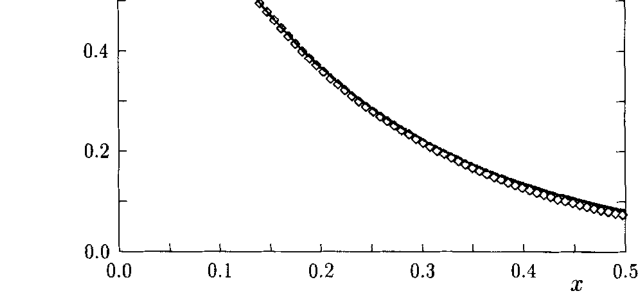


Figure 9. $C_{2\mathcal{Y}}(x)$ vs. x for a one-dimensional periodic porous medium.

The line represents $C_{2\mathcal{Y}}(x) = \exp(-kx)$ with $k = 5.0$; the points are the results of the memoryless reconstruction, Eq. 26, averaged over $N = 10^4$ realizations of the process. The spectral expansion, Eq. 26, is truncated up to the coefficient of the fiftieth order.

This situation does not arise when we apply the convolutory approach presented in the previous sections, for which spatial and ensemble averages do coincide. From this observation we may conclude that in the overwhelming majority of applications the convolutory approach is to be preferred. The memoryless reconstruction is indeed interesting for its simplicity and for its relationships with the spectral decomposition of a porous medium.

Connection with Correlation Percolation

The reconstruction of porous media is a typical inverse problem aimed at obtaining a way to generate lattice structures with the same geometrical features as the original sample.

However, many ideas developed to solve the reconstruction problem can be applied to approach the topic of percolation models with correlation (*correlated percolation*) by assuming a given functional expression for the stochastic process $\mathcal{Y}(x)$ and letting the porosity ϵ vary. In this case, the porosity plays the role of the percolation probability.

Models of correlated percolation have been discussed by Weinrib and Halperin (1983), Weinrib (1984), Prakash et al. (1992), and recently by Sahimi (1994). In this section we do not intend to analyze the physics of correlated percolation (which would fall outside the scope of this work) but to highlight the relationships between correlated percolation and the reconstruction problem. Let us consider a generic random process $\mathcal{Y}(x)$ expressed by Eq. 11 or by Eq. 26. In a formal way, a correlated percolation process can be viewed as the triplet ($\mathcal{L}$, $\mathcal{Y}$, p), where $\mathcal{L}$ is a discrete lattice (with prescribed dimensionality and topology of neighbors), $\mathcal{Y} = \mathcal{Y}(x)$ a stochastic process, and p a nonnegative number $0 \leq p \leq 1$. For every point $x \in \mathcal{L}$, the state of the system $Z_R(x)$ is specified by the relationship

$$Z_R(x) = \mathcal{G}(x,p). \qquad (32)$$

As an example, Figure 10 shows four different realizations of a 2-*d* correlated percolation cluster obtained by considering $\mathcal{Y}$ given by Eq. 13 with $p = \epsilon = 0.5$ for different values of λ. The parameter λ is related to the correlation length $L_c = 1/\sqrt{\lambda}$. Models of exponentially correlated percolation cluster are interesting for studying nonuniversal transport properties (e.g., permeability) of real porous materials far from criticality. As discussed by Weinrib and Halperin (1983) and Weinrib (1984), an exponential correlation does not change the universality properties, so that close to the criticality, exponentially correlated percolation clusters show the same universal features of usual uncorrelated percolation. Nevertheless, in most of the cases, macroporous materials show an exponential decay in the correlation function. There are, however, some examples of long-range correlated porous materials. An interesting property related to the closed-form solution presented in the previous sections is that it is easily possible to simulate models of correlated percolation having correlation functions that decay slower than any power. Indeed, if we choose for $\pi(\lambda)$ the expression $\pi(\lambda) = [\exp(-a\lambda) - \exp(-b\lambda)]/\lambda$, with $0 < a < b$, then the corresponding correlation function becomes $C_{2\mathcal{Y}}(z) = \log[(z+b)/(z+a)]/\log(b/a)$, that is, exhibit a logarithmic decay.

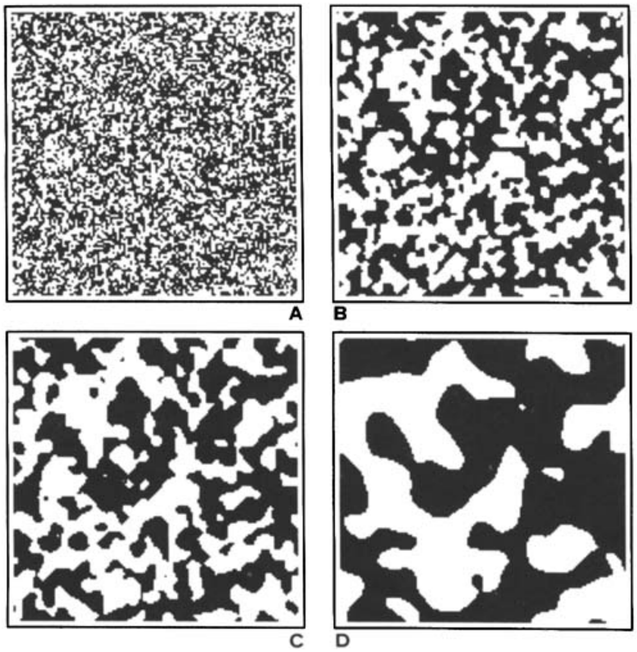


Figure 10. Correlated percolation lattices (130×130 lattice units, porosity $\epsilon = 0.5$) for different values of λ: (A) $\lambda = 1$; (B) $\lambda = 0.1$; (C) $\lambda = 0.05$; (D) $\lambda = 0.01$.

As noted by Sahimi (1994), correlated percolation models are very useful in application to porous media and transport because they mimic the structure of real materials better than the usual (uncorrelated) percolation schemes. This observation can be regarded as a simple consequence of the results previously obtained by Joshi et al. and further discussed here, since the inverse reconstruction problem and correlated percolation are two aspects of the same theory.

The same analysis can be generalized to generic stochastic processes given by the convolution of Gaussian processes. The most general way to construct such a process is by considering a Wiener-series expansion for $\mathcal{Y}(x)$ (Rugh, 1980) of the form

$$\mathcal{Y}(x) = \sum_{k=1}^{N} \mathcal{A}^{(n)}[\xi, x], \tag{33}$$

where $\mathcal{A}^{(n)}$ are n-ary functionals of the form

$$\mathcal{A}^{(n)}[\xi, x] = \int_{E^d} a(u_1, \ldots, u_n)\xi(u_1 + x)\cdots\xi(u_n + x)du_1\cdots du_n. \tag{34}$$

The introduction of a nonlinear functional relation of the form of Eq. 33 breaks down the Gaussianity of $\mathcal{Y}$, thus making the theoretical analysis of the properties of the resulting structure much more difficult. As emerges from this brief discussion, the range of applicability of correlated percolation models is practically unlimited. The scaling properties of correlated percolation schemes depend on the functional expression for the kernels defining $\mathcal{Y}$.

Concluding Remarks

We have presented a detailed analysis of the analytical results underlying the closed-form solution of the inverse reconstruction problem of porous media. The introduction of the correlated processes $\mathcal{Y}(x, \lambda)$, see Eq. 13, enables us to reduce the problem (which in its usual formulation is intrinsically nonlinear) to the form of a linear functional equation.

We have presented a functional approach to solve the inverse problem based on the convolution of uncorrelated Gaussian processes. This approach has been compared with the memoryless Fourier analysis discussed in the section on memoryless processes and the Khinchin theorem. The corresponding reconstructed processes present different statistical properties. In the former case, the resulting $\mathcal{Y}(x)$ is stationary in the strict sense and the ergodic theorem can therefore be applied to it. In the latter case, $\mathcal{Y}(x)$ is stationary in a wide sense, and spatial averages do not therefore necessarily coincide with ensemble averages. In principle, the convolutory approach should be preferred in practical applications. Nevertheless, Fourier expansion is theoretically important for highlighting the spectral properties of the process and could be of use in some special cases.

Deeper examination of practical applications shows that there are many theoretical problems still to be solved. Two aspects are particularly interesting: the extension of the inverse reconstruction procedure to the case of nonlinear filters of the form of Eqs. 33 and 34, and the analysis of n-component reconstruction. The first problem represents the generalization of the reconstruction analysis developed here. The main difficulty in this extension to the nonlinear case is that the Gaussianity of $\mathcal{Y}(x)$ is lost.

The second problem arises in many separation processes, for example, in mineral processing in connection with leaching (Dixon and Hendrix, 1993). While the study of transport in porous media requires the analysis of a two-component system, pores, and pore matrix, the analysis of metal extraction by the leaching of porous particles requires the introduction of a three-component system: pores and both mineral and metallic clusters. A similar situation arises in connection with the fine description of catalytic particles in which the catalytic clusters are distributed neither uniformly nor in a purely uncorrelated way, but present some specific correlation properties. Correspondingly, the inverse problem involves the reconstruction of several independent correlation functions. These aspects will be discussed in future works.

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Notation

$\{b_k\}$ = coefficients of the stochastic process, Eq. 26
d = space dimension
$\{d_k\}$ = see Eq. 24
L = unit-cell characteristic length
N = order of polynomial expansion
$p(y_1, y_2)$ = bivariate Gaussian probability density function
$p(\lambda)$ = see Eq. 11
$\{P_k\}$ = Legendre polynomials, orthogonal in $x \in [-1, 1]$

$\{\hat{P}_k\}$ = modified orthonormal Legendre polynomials on [0, 1]
x = position vector
$y = 1/(z+1)$

Greek letters

$\{\alpha_k^{(k)}\}$ = see Eq. 23
$\delta(x)$ = Dirac's delta function
λ = exponential decay parameter, Eqs. 10 and 14
λ_c = localized exponential decay parameter, Eqs. 17 and 18
$\chi_{\mathcal{P}}(x)$ = characteristic function of the pore space $\mathcal{P}$

Superscript

(p) = analytic continuation on the complex plane

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