New Anisotropic Covariance Models and Estimation of Anisotropic Parameters Based on the Covariance Tensor Identity

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ABSTRACT

Many heterogeneous media and environmental processes are statistically anisotropic, that is, their moments have directional dependence. The term range anisotropy denotes processes that have variograms characterized by direction-dependent correlation lengths and directionally independent sill. We distinguish between two classes of anisotropic covariance models: Class (A) models are reducible to isotropic after rotation and rescaling operations. Class (B) models are separable and reduce to a product of onedimensional functions along the principal axes. We present a Class (A) model for multiscale processes and suggest applications in subsurface hydrology. This model is based on a truncated power law with short and long-range cutoffs. We also present a family of Class (B) models generated by superellipsoidal functions that are based on non-Euclidean distance metrics. We propose a new method for determining the orientation of the principal axes and the degree of anisotropy (i.e., the ratios of the correlation lengths). This information reduces the degrees of freedom of anisotropic variograms and thus simplifies the estimation procedure. In particular, Class (A) models are reduced to isotropic, and Class (B) models to one-dimensional functions. Our method is based on an explicit relation between the second-rank slope tensor (SRST), which can be estimated from the data, and the second-rank covariance tensor. The method is conceptually simple and numerically efficient. It is more accurate for regular (on-grid) data distributions, but it can also be used for irregular (off-grid) spatial distributions. We illustrate its implementation with numerical simulations.

Key Words: Anisotropy, random fields, covariance tensor, power law, simulation

I. INTRODUCTION

A central operation in spatial statistics is the estimation of the variogram. The variogram quantifies the spatial dependence of geophysical and environmental processes (e.g., Christakos, 1992). The estimation of spatial dependence is important in other scientific fields as well. For example, the structure function is a measure of two-point dependence that provides information about the microscopic structure of materials and helps to identify important length scales (e.g., Chaikin and Lubensky, 1995). Recent applications of the structure function in materials research include nanostructures, such as block copolymers (Jinnai et al., 2000a,b) and microemulsions (Choy and Chen, 2000), and paper (e.g., Provatas et al., 1996). The structure of most natural and engineered materials is anisotropic. Hence, their variograms (or of the physical processes that occur within them) exhibit anisotropic properties. There are various forms of variogram anisotropy (e.g., Erikson and Siska, 2000). In this work we focus on range anisotropy. The term is used for processes that have the same variogram sill in all directions but different correlation lengths. First, we propose new covariance functions with range anisotropy. They include a truncated power-law covariance for modeling multiscale processes, and separable covariance functions based on geometrical generalizations of the ellipse called superellipsoids. We discuss the relevance of the truncated power-law covariance for hydrological applications. The superellipsoidal covariance functions have anisotropic but non-ellipsoidal isolevel contours, and they can be used to model processes with non-Euclidean distance metrics (Christakos et al., 2000).

The estimation of spatial structure of materials is facilitated by the fact that multiple samples are usually available, and a statistical average over many realizations can be calculated. In contrast, in environmental applications the variogram is *de facto* estimated from the single available realization. Thus, the ergodic principle (e.g., Adler, 1981) is invoked, in order to justify estimation of the stochastic mean based on the spatial average. Since ergodicity is an asymptotic property a large number of data are required for good accuracy. Nonetheless, the ergodic principle is used by necessity as a working assumption, even if the sample size is small. The variogram estimation process requires the arbitrary definition of discrete separation classes (bins), each bin including a range of separations (lags). The bins must contain a minimum number of data pairs (at least 30) for a "good" approximation of the ensemble average. In the isotropic case the bins are defined with respect to the separation magnitude. In the anisotropic case a larger number of bins is required to account for the magnitude and orientation of the separation vector. The number of data pairs per bin and consequently the precision of the estimation are thus reduced. The estimated range anisotropy depends on the specific distribution of separation vectors and the binning scheme. The optimal anisotropic structure is selected among the various possibilities by means of an optimization criterion.

Anisotropic variogram estimation is simplified if a coordinate system exists in which the anisotropy is reduced. For range anisotropic processes such a system exists, and it can be accessed from the original system by means of rotation and rescaling We propose a new method for determining the necessary transformations. transformations. The method is based on the covariance tensor identity and uses the average of the second-rank slope tensor (SRST) of the random field, which can be estimated from the data. The SRST method estimates the orientation of the principal axes and d-1 correlation aspect ratios from the data. The aspect ratios are defined arbitrarily with respect to one of the correlation lengths. Determining the orientation of the principal axes requires d-1 angles. The aspect ratios and the orientation angles are the anisotropic parameters. The coordinate system is then accordingly rotated and rescaled. In the transformed system the variogram is isotropic for class (A) models, or a product of one-dimensional functions for class (B) models. The SRST method is conceptually simple and numerically efficient. The accuracy and computational efficiency of the method are better for data distributed on a regular grid, but the method can also be used with irregularly spaced data. Application in both cases is illustrated with synthetic examples.

The paper is structured as follows: In Section II we define the covariance classification and propose some new models. In Section III we introduce the covariance tensor identity, and we present a mathematical framework for the estimation of the anisotropic parameters. Methods of estimating the mean SRST from data are presented in Section IV. In Section V we illustrate the calculation of the anisotropic parameters using the SRST method. In Section VI we present our conclusions, and we discuss directions for future research.

II. RANGE ANISOTROPIC COVARIANCE FUNCTIONS

We will focus on statistically homogeneous, detrended Gaussian random fields X(s). The centered covariance function is denoted by $c_x(h)$, where h is the separation vector. Covariance models with range anisotropy involve functions that have the same sill but different correlation lengths in different directions. Due to the isotropy of the sill, the limiting value of the covariance at zero separation is independent of the direction along which the limit is approached. However, the derivatives at zero separation have directional dependence due to range anisotropy. In the SRST method we use information about the anisotropy contained in the derivatives of the random field to simplify the task of variogram estimation. With respect to the estimation of the reduced variogram, it helps to distinguish between two model classes. The models in the first class can be reduced to isotropic functions. The models in the second class can be reduced to onedimensional functions. The steps involved in the calculation of the SRST and the anisotropic parameters are identical for both classes. In this paper we will focus on the estimation of the anisotropic parameters from the full variogram estimation process.

Class (A): Models Reducible to Isotropic

The first class includes all covariance functions that can be expressed as isotropic functions $c_x(\tilde{r})$, where \tilde{r} is the dimension-less separation in a coordinate system obtained by rotation and rescaling of the original axes. The separation in the original system, which is not in general aligned with the principal axes, is denoted by h. A coordinate system aligned with the principal axes is obtained by rotating the original system. The separation in the new system is denoted by r = Uh, where U is the rotation matrix. In the rotated system the covariance function is independent of cross products $r_i r_j$, $i \neq j$, but it is still anisotropic with correlation lengths ξ_i in each direction. For isotropic covariances there is no difference between h and r. If distances are rescaled in the new system according to $\tilde{r}_i = r_i / \xi_i$, the covariance function becomes isotropic. Conversely, the isotropic function $c_x(\tilde{r})$ generates the anisotropic function $c_x(h)$ by reversing the rescaling and rotation transformations. Thus, all isotropic covariance models are generators of anisotropic models by means of rotation and rescaling

transformations. Class (A) includes the standard geostatistical models (e.g, Abrahamsen, 1997): the Gaussian, spherical, cubic, rational quadratic, exponential, damped sine and cosine (with inverse distance or exponential damping), various Bessel functions, and the hole-effect models.

With the exception of the Bessel function models, the above covariances involve one or two distinct length scales. Such covariances are commonly used in groundwater hydrology (e.g., Gelhar, 1993) to model the correlations of the hydraulic conductivity and the velocity flow field. However, subsurface hydrological processes involve multiple scales (e.g., Cushman, 1984; 1986), because natural porous media are made of grains and pores of various sizes. Correlations that involve multiple scales are modelled using power law functions (Mandelbrot, 1982; Feder, 1988) that follow the general, power-law expression $c_{x}(\mathbf{r}) \propto r^{-\gamma}$ within a certain range of scales (e.g., Isichenko, 1992). Such functions are also called *scaling*, because a change of scale simply multiplies the function with a constant scale factor, i.e., $c_x(\lambda \mathbf{r}) = \lambda^{-\gamma} c_x(\mathbf{r})$. A major practical difficulty in determining if hydraulic conductivity covariances are scaling is the limited size of subsurface data sets. In contrast, scaling hypotheses can be tested for surface hydrological processes, for which data are more abundant. Thus, it has been established that rainfall involves multifractal correlations (e.g., Schertzer and Lovejoy, 1987; Lovejoy and Schertzer, 1995; Menadbe et al., 1999). In principle, power-law correlations can be obtained by a superposition of monoscale fluctuations at multiple scales (e.g., Koch and Brady, 1988). Experimental studies of porous rock in the range of scales between millimeters and meters (Makse et al., 1996a) indicate power-law correlations. In addition, certain analyses of experimental data suggest scaling behavior for the hydraulic conductivity at the field scale (Neuman, 1990; 1994). Power-law covariances with scaledependent variance have been used to model field-scale hydraulic conductivities (e.g., Di Federico and Neuman, 1997; 1998). The exact form of the power-law dependence is related to the degree of non-homogeneity of the hydraulic conductivity field. There are different views on this issue: If hydraulic conductivity is a homogeneous random field, appropriate power-law models are the fractional Gaussian noise (fGn) and the Lévystable distributions (LSD) (Painter, 1996; Liu and Molz, 1997). The fGn model has normal statistics and power-law covariances. Lévy-stable random fields are characterized by non-Gaussian, power-law tails in the probability density. If the logconductivity is non-homogeneous, appropriate models are the fractional Brownian motion (fBm) (Mandelbrot and Van Ness, 1968) and the fractional Lévy motion (fLm) (Molz et al., 1997). Then, the log-conductivity increments are homogeneous and have fGn and LSD statistics respectively. The reconstruction and permeability properties of porous media with fBm statistics are investigated in (Kikkinides and Burganos, 1999; 2000).

For power laws to be mathematically well defined, a cutoff is necessary to avoid the singularity at zero separation. The short-range cutoff is not only a mathematical convenience, since it is related to the smallest length scale with a physical role in the particular process. In the case of hydraulic conductivity this could be the size of the smallest pore. A modified power-law covariance with short-range cutoff based on the incomplete gamma function was proposed in (Christakos et al., 2000). At the opposite limit, asymptotic persistence of power-law correlations at large distances is a sign of long-range dependence. True long-range processes behave as power laws over the entire system. In this case, the power-law exponent should satisfy specific integrability conditions for the spectral density to be well defined (Isichenko, 1992). Also, true longrange correlations are a cause of anomalous diffusion behavior such as non-Gaussian tails (e.g., Bouchaud and Georges, 1990). However, it is also possible for a system to exhibit scaling behavior up to a maximum scale (determined from the largest physical feature) smaller than the system size. This implies a long-range cutoff of the scaling regime. The following covariance model is scaling for $w \ll r \ll \xi$ and has short and long-range cutoffs

$$c_{x}(\mathbf{r}) = \sigma^{2} \frac{\exp(-r/\xi)}{\left(1 + \frac{r^{2}}{w^{2}}\right)^{\nu/2}}.$$
(1)

The length w determines the short-range cutoff, since for $r/w \ll 1$ the covariance is approximately $c_r(\mathbf{r}) \cong \sigma^2 (1 - v r^2 / 2 w^2)$. The length scale ξ determines the longrange cutoff, since for $r > \xi$ the correlations are cut off by the exponential. The function $c_{r}(\mathbf{r})$ is an admissible covariance, if it satisfies Bochner's theorem (Bochner 1959) which requires that the spectral density be non-negative. This can be proved without evaluating the spectral density, because $c_x(\mathbf{r})$ is the product of the exponential $\exp(-r/\xi)$ and the rational function $(1 + r^2/w^2)^{-\nu/2}$. Both functions are permissible covariances, i.e., they have non-negative spectral densities. Hence, their product is also a permissible covariance. This follows since the spectral density of the product is given by the convolution of the spectral density of the components, and the convolution of two nonnegative functions is also non-negative. In Figure 1 we plot the covariance of Eq. (1) on a logarithmic scale. The scaling regime extends over the section of the plot where the covariance varies as a straight line. For comparison, we also plot the power law without the long-range cutoff. An anisotropic covariance function can be generated from Eq. (1). In two dimensions, in the coordinate system of the principal axes this is given by

$$c_{x}(\mathbf{r}) = \sigma^{2} \frac{\exp\left(-\sqrt{\frac{r_{1}^{2}}{\xi_{1}^{2}} + \frac{r_{2}^{2}}{\xi_{2}^{2}}}\right)}{\left(1 + \frac{r_{1}^{2}}{w_{1}^{2}} + \frac{r_{2}^{2}}{w_{2}^{2}}\right)^{\nu/2}}.$$
(2)

Note that the covariance of Eq. (2) has anisotropic cutoffs but an isotropic power-law exponent. A more general covariance with anisotropic exponents v_1 and v_2 is given by

$$c_{x}(\mathbf{r}) = 2\sigma^{2} \frac{\exp\left(-\sqrt{\frac{r_{1}^{2}}{\xi_{1}^{2}} + \frac{r_{2}^{2}}{\xi_{2}^{2}}}\right)}{\left(1 + \frac{r_{1}^{2}}{w_{1}^{2}}\right)^{v_{1}/2} + \left(1 + \frac{r_{2}^{2}}{w_{2}^{2}}\right)^{v_{2}/2}}.$$
(3)

From the numerical viewpoint, simulation of random fields with long-range correlations that span the entire system is not trivial (e.g., Makse et al., 1996). An explicit long-range cutoff that limits the extent of the scaling regime, like the one suggested above, alleviates numerical difficulties. However, we emphasize that using a long-range cutoff should be justified by the analysis of the data or by the physics of the modelled process.

Class (B): Separable Models

The second class includes all separable covariance functions with one-dimensional components of the same functional form. In a coordinate system aligned with the principal axes these covariances are expressed as $c_x(\tilde{r}) = \sigma_x^2 \prod_{i=1}^d g(\tilde{r}_i)$, where $g(\cdot)$ is a permissible one-dimensional covariance function (Christakos, 1992). Classes (A) and (B) are not completely disjoint since the Gaussian model belongs to both of them. However, with this notable exception, the models in class (B) can not be reduced to isotropic functions. An example of a class (B) covariance is the hole-effect model, defined by $g(\tilde{r}_i) = \sin(\tilde{r}_i)/\tilde{r}_i$.

Superellipsoidal Covariance Models

A new family of separable covariance models can be defined based on superellipsoids (Wallace, 1968). The superellipsoids are geometrical generalizations of the ellipse. In two spatial dimensions they obey the following equation

$$\left|\frac{r_1}{|\xi_1|}\right|^{2/n} + \left|\frac{r_2}{|\xi_2|}\right|^{2/n} = |\tilde{r}_1|^{2/n} + |\tilde{r}_2|^{2/n} = c.$$
(4)

Let us consider the following separable superellipsoidal function

$$c_{x}(\tilde{r}) = \sigma_{x}^{2} g(|\tilde{r}_{1}|^{2/n}) g(|\tilde{r}_{2}|^{2/n}).$$
(5)

The function $c_x(\tilde{r})$ is a covariance if it satisfies Bochner's theorem. In view of the separability property, it is sufficient that the one-dimensional spectral density of $g(|\tilde{r}_1|^{2/n})$ be non-negative. The shape of isolevel contours and the smoothness of individual realizations depend on the value of the index *n*. According to a familiar theorem (e.g., Adler, 1981; Yaglom, 1987), a Gaussian random field is differentiable (in the mean square sense) at every point if the second-order derivative of the covariance exists and is finite at zero separation. The second-order derivative of the superellipsoidal function at zero separation is given by (see Appendix I)

$$\frac{\partial^{2} c_{x}(\tilde{\boldsymbol{r}})}{\partial r_{1}^{2}} = \sigma_{x}^{2} \left(|\tilde{r}_{2}|^{2/n} \right) \left\{ \left[\frac{2}{n\xi_{1}} |\tilde{r}_{1}|^{2/n-1} \operatorname{sgn}(r_{1}) \right]^{2} g''(\omega) + \frac{2g'(\omega)}{n\xi_{1}^{2}} \left(\frac{2}{n} - 1 \right) |\tilde{r}_{1}|^{2/n-2} \operatorname{sgn}^{2}(r_{1}) + \frac{2g'(\omega)}{n\xi_{1}^{2}} |\tilde{r}_{1}|^{2/n-1} \delta(r_{1}) \right\}.$$
(6)

In Eq. (6) the prime denotes differentiation with respect to $\omega \equiv |r_1/\xi_1|^{2/n}$, and $\operatorname{sgn}(r_1)$ denotes the sign function. The first and second terms on the right hand-side of Eq. (6) are proportional to $\operatorname{sgn}^2(r_1) = 1$. Thus they are well defined at zero separation. The third

term is potentially singular due to the delta function. However, this term vanishes if 2/n-1>1 or g'(0) = 0. These conditions guarantee a finite derivative at zero separation. Hence, a superellipsoidal random field with covariance given by Eq. (5) is differentiable if n < 2 or $g'(0) \neq 0$. Note that the condition n < 2 is necessary but not sufficient. The index may need to satisfy additional conditions for the function (5) to be a permissible covariance, as shown below.

Exponential Superellipsoidal

A special case of superellipsoidal covariance is the exponential superellipsoidal that is expressed as follows

$$c_{x}(\mathbf{r}) = \sigma_{x}^{2} \exp\left(-\left|\frac{r_{1}}{\xi_{1}}\right|^{2/n} - \left|\frac{r_{2}}{\xi_{2}}\right|^{2/n}\right).$$
(7)

The functions defined by Eq. (7) are not, in general, reducible to an isotropic form, and hence they differ from the isotropic exponential models $c_x(\mathbf{r}) = \sigma_x^2 \exp\left[-(r/\xi)^v\right]$ (Abrahamsen, 1997) in which $r = ||\mathbf{r}||$ is the Euclidean distance. The only exception is the Gaussian case v = 2/n = 2. The function $c_x(\mathbf{r}) = \sigma_x^2 \exp\left(-|r_1/\xi_1| - |r_2/\xi_2|\right)$ is known to be a permissible covariance function (Christakos et al., 2000). This is a special case of the exponential superellipsoidal family with index n = 2. In Figure 2 we plot the isolevel contours of the functions (7) for index values n = 0.5, 1, 1.5, 2, 2.5 and 3. These plots show the deviation of the isolevels from the ellipsoidal shape. The isolevel contours are rounded rectangles for n < 1, ellipses for n = 1, concave diamonds for 1 < n < 2, diamonds for n = 2, and convex ("pinched") diamonds for n > 2. In Figure 3 we plot the one-dimensional spectral density of the six exponential superellipsoidals with the above values of the index. The spectral density calculations used the Fast Fourier Transform (e.g., Press et al., 1986). All densities are non-negative except for n = 0.5. Hence, the exponential superellipsoidal with n = 0.5 is not a permissible covariance. It can be shown more generally that the non-negativity condition is true for $\infty > n \ge 1$ (Schoenberg, 1938).

Thus, the *permissibility condition* for the exponential superellipsoidals defined by Eq. (7) is $\infty > n \ge 1$. In addition, as we showed above the *differentiability condition* is $2 > n \ge 1$. As it is seen in Figure 3, the covariance functions of the differentiable random fields are smoother (more rounded) at the edges. A realization of a two-dimensional superellipsoidal random field with unit variance, correlation lengths $\xi_1 = \xi_2 = 5$, and index n = 3 is shown in Figure 4.

III. THE COVARIANCE TENSOR IDENTITY

The covariance tensor is the second-rank tensor generated by the second order derivatives of the covariance at zero separation i.e., $\partial^2 c_x(h) / \partial h_i \partial h_j$. If the covariance tensor exists at the origin the random field is differentiable in the mean square sense. The second-rank slope tensor (SRST) $X_{ij}(s)$ is generated by the products of the local slope vectors $\nabla X(s)$,

i.e.,
$$X_{ij}(s) = \frac{\partial X(s)}{\partial s_i} \frac{\partial X(s)}{\partial s_j}$$
. Thus, the SRST is also a random field. Its mean value is

denoted by $\langle X_{ij}(s) \rangle \equiv Q_{ij}$, where the brackets denote the stochastic average. If the first derivative of the covariance vanishes at zero separation, the following tensor identity (e.g., Swerling, 1962) relates the mean SRST to the covariance tensor as follows

$$Q_{ij} = \left\langle \frac{\partial X(s)}{\partial s_i} \frac{\partial X(s)}{\partial s_j} \right\rangle = -\frac{\partial^2 c_x(\boldsymbol{h})}{\partial h_i \partial h_j} \bigg|_{\boldsymbol{h} = (0,0)}.$$
(8)

Eq. (8) is valid in all coordinate systems. It is not valid for the exponential covariance, the first derivative of which does not vanish. The covariance tensor identity can be used to estimate the anisotropic parameters from the mean SRST. The latter is estimated from the available data. When the anisotropic parameters are known, it is possible to transform into a coordinate system in which the covariance function is either isotropic or can be expressed as a separable product of identical one-dimensional functions. The transformation involves a rotation that aligns the coordinate system with the principal axes, and a rescaling that makes all the correlation lengths equal. To estimate a variogram that becomes isotropic in the transformed system standard geostatistical methods can be used (e.g., Christakos, 1992; Olea, 1999). To estimate a separable variogram, one of its components along a principal direction should be determined. In both cases the estimation is simplified, because there is no need to consider many directions in space. Once the variogram is estimated in the transformed system, the inverse set of transformations should be used to obtain the variogram in the original coordinate frame.

If ξ_i , i = 1,...,d denote the correlation lengths along the principal axes, d-1 aspect ratios can be defined based on the equation

$$R_{i(1)} \equiv \frac{\xi_1}{\xi_i}, \quad i \neq 1.$$
(9)

The selection of ξ_1 as the reference length is arbitrary. The correlation length in any of the principal directions can be used to anchor the ratios. Note that $\mathbf{R}_{(1)} = (1, R_{2(1)}, ..., R_{d(1)})$ is a vector in \Re^d with d-1 independent components. Next, we determine the orientation of the principal axes and the correlation aspect ratio from the SRST. We consider first a coordinate system that is aligned with the principal axes.

Principal Axes Coordinate System

In a coordinate system the axes of which coincide with the principal directions of anisotropy we can express the covariance function in terms of the dimensionless separation \tilde{r} , where $\tilde{r}_i = r_i/\xi_i$ and ξ_i is the correlation range in the direction r_i . Then, the covariance tensor identity leads to the following expression

$$Q_{ij} = -\frac{1}{\xi_i \xi_j} \frac{\partial^2 c_x(\tilde{\boldsymbol{r}})}{\partial \tilde{r}_i \partial \tilde{r}_j} \bigg|_{\boldsymbol{r}=(0,0)}.$$
(10)

In this system the covariance tensor for both Class (A) and (B) models is isotropic at zero separation, that is, $-\partial^2 c_x(\tilde{r})/\partial \tilde{r}_i \partial \tilde{r}_j \Big|_{r=(0,0)} \equiv \sigma_x^2 \zeta^2$ for all directions *i*, *j*, where ζ is a dimensionless number. Then, based on Eq. (10) we obtain the following d-1 equations for the aspect ratios

$$\sqrt{\frac{Q_{ii}}{Q_{11}}} = \frac{\xi_1}{\xi_i} = R_{i(1)}, \quad i \neq 1.$$
(11)

The roots of the Eqs. (11) are the correlation aspect ratios. A coordinate system aligned with the principal axes is not always practical for applications. Nonetheless, it is useful for testing the accuracy of anisotropic simulation methods, and it is often the most natural choice for engineered materials.

General Coordinate System

In general the axes of the coordinate system do not coincide with the principal axes. The covariance tensor identity is valid regardless of the coordinate system alignment. As discussed above, if \mathbf{r} is the separation vector in the system of the principal axes and $\tilde{\mathbf{r}}$ the rescaled (isotropic) separation, then $\mathbf{r} = \mathbf{U}\mathbf{h}$ where \mathbf{U} is a rotation matrix, and $\tilde{r}_i = r_i/\xi_i$, for i = 1,...,d. Using the chain rule for partial derivatives $\partial/\partial h_i = (\partial r_k/\partial h_i)\partial/\partial h_k = U_{ki}\partial/\partial r_k$ and $\partial/\partial r_i = \xi_i^{-1}(\partial/\partial \tilde{r}_i)$. In these expressions and in the following summation is implied over repeated indices. The second-order derivative operator in the original system is expressed in terms of its equivalent in the principal axes system as follows

$$\frac{\partial^2}{\partial h_i \partial h_j} = \frac{U_{ki} U_{lj}}{\xi_k \xi_l} \frac{\partial^2}{\partial r_k \partial r_l},\tag{12}$$

Finally, by using Eq. (12) and rescaling the lengths the covariance identity is expressed as

$$Q_{ij} = \frac{\sigma_x^2 \zeta^2}{\xi_1^2} U_{ki} R_{k(1)} U_{lj} R_{l(1)} \delta_{kl} = \frac{\sigma_x^2 \zeta^2}{\xi_1^2} U_{ki} U_{kj} R_{k(1)}^2, \quad i, j = 1, ..., d.$$
(13)

The expression (13) of the covariance identity constitutes a system of equations. The unknowns of the system are the components of the rotation matrix U and the vector R. These should be determined from the mean SRST elements Q_{ij} . The parameter ζ^2 and ξ_1^2 are not determined by the solution of the system. The number ζ^2 depends on the value of second-order derivative of the covariance at zero separation. For example, in the Gaussian case one finds $\zeta^2 = 2$. The value of ζ^2 is not required for the rotation and rescaling transformation. The correlation length ξ_1 is determined from the estimation of the experimental variogram in the transformed system.

Two-dimensional Random Field

We derive specific expressions based on the Eqs. (13) that apply to two-dimensional random fields. The rotation matrix U in two dimensions is given by

$$\boldsymbol{U} = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix},\tag{14}$$

and $\mathbf{R}_{(1)} = (1, R_{2(1)})$. The equations (13) are then expressed as follows

$$Q_{11} = \frac{\sigma_x^2 \zeta^2}{\xi_1^2} \left(\cos^2 \theta + R_{2(1)}^2 \sin^2 \theta \right), \tag{15}$$

$$Q_{22} = \frac{\sigma_x^2 \zeta^2}{\xi_1^2} \left(R_{2(1)}^2 \cos^2 \theta + \sin^2 \theta \right)$$
(16)

$$Q_{12} = Q_{21} = \frac{\sigma_x^2 \zeta^2}{\xi_1^2} \left[\sin \theta \cos \theta (1 - R_{2(1)}^2) \right].$$
(17)

The orientation of the principal axes is determined by the angle θ , and the aspect ratio is determined by $R_{2(1)}$. By dividing both sides of Eqs. (16) and (17) with the terms on the respective sides of Eq. (15) we obtain the following set of equations

$$\frac{Q_{22}}{Q_{11}} = \left(\frac{R_{2(1)}^2 + \tan^2 \theta}{1 + R_{2(1)}^2 \tan^2 \theta}\right),\tag{18}$$

and

$$\frac{Q_{12}}{Q_{11}} = \frac{\tan\theta(1 - R_{2(1)}^2)}{1 + R_{2(1)}^2 \tan^2\theta}.$$
(19)

Eqs. (18) and (19) constitute a nonlinear system, the roots of which are the anisotropic parameters. The nonlinear system can be solved by the minimization of the following objective function

$$\Phi(\theta, R_{2(1)}) = \left[\frac{Q_{22}}{Q_{11}} - \left(\frac{R_{2(1)}^2 + \tan^2 \theta}{1 + R_{2(1)}^2 \tan^2 \theta}\right)\right]^2 + \left[\frac{Q_{12}}{Q_{11}} - \frac{\tan \theta (1 - R_{2(1)}^2)}{1 + R_{2(1)}^2 \tan^2 \theta}\right]^2,$$
(20)

The function $\Phi(\theta, R_{2(1)})$ is non-negative, and it becomes zero when both terms inside the brackets are zero. Hence, the minimization of the objective function yields the anisotropic parameters.

IV. ESTIMATION OF THE MEAN SRST

In this section we discuss the estimation of the mean SRST from the data. For practical estimates of the SRST the derivative operators in $X_{ij}(s)$ are replaced by discrete differences. Hence, the accuracy and precision of the SRST estimation depend on the

spatial distribution of the data. Accuracy refers to how closely the mean estimate $\langle \hat{X}_{ij}(s) \rangle$ approximates the actual stochastic mean $\langle X_{ij}(s) \rangle$. Precision is a measure of the uncertainty of each estimate $\hat{X}_{ij}(s)$. For a data point located at position s_k (k = 1, ..., Nwhere N is the number of data points) the nearest-neighbor distance $r_{nn}(s_k)$, is defined as $r_{nn}(s_k) = \min\{\|s_l - s_k\|, l \neq k, l = 1, ..., N\}$. In general $r_{nn}(s_k)$ is a distributed variable. The data distribution is spatially dense if the average nearest-neighbor distance $\overline{r_{nn}(s_k)} = N^{-1} \sum_{k=1}^{N} r_{nn}(s_k)$ is sufficiently small for the discrete difference approximation to be accurate. Hence, a data set is dense if the shortest correlation length is a multiple of the maximum nearest-neighbor distance $r_{nn,max} = max[r_{nn}(s_k)], k = 1,...,N$. We define a density index by means of $\mu_{de} = \xi_{min}/r_{nn,max}$, where $\xi_{min} = min(\xi_i)$, i = 1,...,d. Large values of the index imply higher sampling density. Ideally, the density index should be larger than one. However, note that very small distances in the distribution of $r_{nn}(s_k)$ could lead to numerical instabilities in the calculation of the derivatives, as discussed below. The data distribution is *uniform* if the nearest-neighbor distance is approximately uniform from site to site. The variation of the nearest-neighbor distance is measured by $\operatorname{Var}(r_{nn}) = N^{-1} \sum_{k=1}^{N} \left[r_{nn}^2(s_k) - \overline{r_{nn}(s_k)}^2 \right]$. We define the *uniformity index* as the inverse coefficient of variation of the nearest-neighbor distance distribution, i.e., $\mu_{\rm un} = \overline{r_{\rm nn}} / \sqrt{\operatorname{Var}(r_{\rm nn})}$. Hence, uniformity increases for higher values of the index.

SRST on Regular Grid

Absolute uniformity, $\mu_{un} = \infty$, is achieved for regularly distributed data on a grid. Regularly spaced data are not the rule in environmental applications. However, uniform spacing is often a natural choice for laboratory studies of porous materials (e.g., Henriette et al., 1989). Regular grids are also used for simulations of environmental processes. In addition, they are useful for testing how accurately random field simulators generate specific anisotropic properties. Let us assume that X(s) is distributed on a Cartesian grid G with N points. The mean SRST is estimated by means of a discrete estimator \hat{Q}_{ij} based on forward differences as follows

$$\hat{Q}_{ij} = \frac{1}{N b_i b_j} \sum_{k=1}^{N} \left[X(s_k + b_i \hat{e}_i) - X(s_k) \right] \left[X(s_k + b_j \hat{e}_j) - X(s_k) \right].$$
(21)

The grid step is b_i and \hat{e}_i denotes the unit vector in direction s_i . The right hand-side of Eq. (21) can be calculated very efficiently numerically. The spatial distribution is dense if $b_i < \xi_i$. Dense distributions give better accuracy than sparse ones, because the latter introduce systematic errors due to inadequate discretization.

Numerical Example

We illustrate the estimation process by means of a synthetic numerical example. Assume a random field with a Gaussian covariance function

$$c_x(\mathbf{r}) = \sigma_x^2 \exp\left(-\frac{r_1^2}{\xi_1^2} - \frac{r_2^2}{\xi_2^2}\right).$$
 (22)

The SRST in system of the principal axes is given, according to Eq. (8) above, by

$$\boldsymbol{Q} = 2\sigma_x^2 \begin{bmatrix} \xi_1^{-2} & 0\\ 0 & \xi_2^{-2} \end{bmatrix}.$$
(23)

We simulate a random field with $\sigma_x^2 = 1$, $\xi_1 = 6$, $\xi_2 = 4$ on a square grid with *L* nodes per side using the Fourier Filtering Method (FFM) (e.g., Makse et al., 1996b; Le Ravalec et al., 2000). The "true" values of the mean SRST tensor for the above values of the variance and correlation lengths are $Q_{11} = 0.0556$ and $Q_{22} = 0.1250$. The anisotropic ratio is $R_{2(1)} = 1.5$. A typical realization of the random field on a domain with 100 nodes per side is shown in Figure 5. We estimate the mean SRST for different values of *L* using Eq. (21). The SRST components and the aspect ratio $R_{2(1)}$ are plotted in Figure 6. The components of the SRST approach stable values for L>100. The aspect ratio tends to a stable value faster. The difference is probably due to the dependence of the SRST on the variance that makes it sensitive to deviations of the sample variance from the theoretical value. In contrast, the aspect ratio is independent of the variance. The accuracy of the aspect ratio estimate depends on the departure from perfect ergodic conditions, i.e., on the ratio of the domain length over the correlation length. Similarly, precision improves as the domain size increases and spatial averaging suppresses the fluctuations.

SRST for Irregular Spatial Distribution

X

For data that are not distributed on a grid various approximate estimators of the SRST can be defined. We assign to each point s_k a nearest neighbor denoted by $s_{nn(k)}$ such that the Euclidean distance $r_{nn}(s_k) = ||s_{nn(k)} - s_k||$ is minimized. There are other ways to define the neighbors, and some possibilities are discussed in Section VI. The discretization step at s_k in direction s_i , i = 1,...,d, is given by

$$\Delta s_{k,i} = s_{\mathrm{nn}(k),i} - s_{k,i}.\tag{24}$$

A location s_k is used in the calculation of Q_{ij} if the values of the separation magnitudes $|\Delta s_{k,i}|$ and $|\Delta s_{k,j}|$ are within a specified interval. Separations exceeding an upper cutoff α_u introduce smoothing effects in the calculation of the slope. Separations smaller than a lower cutoff α_1 can introduce large errors due to numerical fluctuations. Hence, the number of data points used in the estimation of Q_{ij} is given by the following expression

$$N_{\text{eff},ij} = \sum_{k=1}^{N} \pi \left(|\Delta s_{k,i}|; \alpha_{u}, \alpha_{l} \right) \pi \left(|\Delta s_{k,j}|; \alpha_{u}, \alpha_{l} \right),$$
(25)

where $\pi(x;\alpha_u,\alpha_l)$ is the unit pulse function that equals one if $\alpha_u > x > \alpha_l$ and zero otherwise. Consequently, the mean SRST is estimated as follows

$$\mathcal{Q}_{ij} = \frac{1}{N_{\text{eff},ij}} \sum_{k=1}^{N} \left[\frac{X(s_{\text{nn}(k)}) - X(s_k)}{\Delta s_{k,i}} \pi \left(|\Delta s_{k,i}|; \alpha_u, \alpha_l \right) \right] \left[\frac{X(s_{\text{nn}(k)}) - X(s_k)}{\Delta s_{k,j}} \pi \left(|\Delta s_{k,j}|; \alpha_u, \alpha_l \right) \right].$$
(26)

The cutoffs are not *a priori* specified. Ideally, the upper cutoff should satisfy $\alpha_u \ll \min(\xi_1, ..., \xi_d)$ to avoid excessive smoothing of the random field derivatives. However, the correlation lengths are unknown before the variogram is known. It is often possible to guess an initial estimate for the correlation length(s) by visual inspection of contour plots of the data. The initial "guess" for α_u can be used to calculate the SRST. Ultimately, this will have to be confirmed by comparing with the estimated correlation lengths. A comprehensive study of the accuracy and precision of the estimator with respect to the data distribution and the cutoffs is beyond the scope of this study.

Numerical Example

We illustrate the calculation of the SRST for an irregular data distribution using a synthetic random field. We select N random sites within a square domain of length L. The FFT simulation method used above works only for regular grids. Hence, we use instead a harmonic superposition method (Drummond, 1987; Jinnai et al., 2000) which is less efficient numerically but can generate a random field at any set of locations. In this method the random field is represented as follows

$$X(s) = \sigma_x \left(\frac{2}{N_{\rm m}}\right)^{1/2} \sum_{n=1}^{N_{\rm m}} \cos(\boldsymbol{k}_n \cdot \boldsymbol{s} + \boldsymbol{\phi}_n).$$
(27)

The phase variables ϕ_n are distributed uniformly in $[0, 2\pi]$. The wavevectors \mathbf{k}_n are randomly distributed with probability density $f_x(\mathbf{k}_n) = A \tilde{c}_x(\mathbf{k}_n)$, where $\tilde{c}_x(\mathbf{k}_n)$ is the spectral density of the covariance $c_x(\mathbf{r})$ and $f_x(\mathbf{k}_n) = A = \left[\int d\mathbf{k}_n \tilde{c}_x(\mathbf{k}_n)\right]^{-1}$. In particular, the probability density corresponding to the Gaussian covariance of Eq. (22) is given by

$$f_x(\mathbf{k}_n) = (\xi_1 \xi_2 / 4\pi) \exp\left[-(k_1^2 \xi_1^2 + k_2^2 \xi_2^2)/4\right]$$
. Based on the central limit theorem, the superposition given by Eq. (27) approaches asymptotically the normal distribution with Gaussian covariance as the number of modes $N_{\rm m}$ tends to infinity.

In Figure 7 we show 500 random sites on a 80×80 square domain. Each site is connected with a straight line to its nearest neighbor. We generate the "data set" from a random field with $\sigma_x = 1$, Gaussian covariance, $\xi_1 = 4$, $\xi_2 = 6$, and principal axes oriented along the domain sides. Hence, the mean SRST values corresponding to this field according to Eq. (12) are: $Q_{11} = 0.1250$, $Q_{22} = 0.0556$, and $Q_{12} = 0$. The number of modes used in the simulation is $N_{\rm m} = 14000$. The "data set" obtained is shown in Figure 8. The plot is based on a map of estimated values on a regular grid obtained from the "data" using linear interpolation. The distribution of the nearest neighbor distances $r_{nn}(s_k)$ is shown in the histogram of Figure 9. The mean of the distribution is $\overline{r_{nn}(s_k)} \cong 1.79$, and the variance is $\sqrt{Var(r_{nn})} \cong 0.98$, giving a uniformity index $\mu_{un} \cong 1.83$. The maximum nearest neighbor distance is $r_{nn,max} \cong 5.40$, which gives a density index $\mu_{de} \cong 0.56$. This means that the "data set" is fairly uniform, but not very dense. The sparseness of the spatial distribution is expected to have a negative impact on the estimation of the SRST. We show in Table I the estimates of the SRST components for different values of the lower cutoff. The upper cutoff used in these calculations is $\alpha_{\mu} = 2$, i.e., one half of the shortest correlation length. The best agreement with the

theoretical values is obtained for $\alpha_l \in [1-1.5]$. However, the number of data points involved in the average for these values of the cutoff is small, implying reduced precision of the estimation. In conclusion, the relatively small number of points in the data set imposes strong constraints on predictability. This is, however, an inherent limitation of all spatial statistics methods when the size of the available data set is small.

V. ESTIMATION OF ANISOTROPIC PARAMETERS

Estimation of the anisotropic parameters is based on the solution of the general Eqs. (13). In particular, in two dimensions the anisotropic parameters are determined from the minimization of the objective function (20), as discussed in Section III. This procedure requires estimates of the mean SRST, which can be obtained from the data as discussed in Section IV. Below we illustrate the numerical procedure using synthetic random field examples.

Numerical Examples

Let us consider the Gaussian covariance function of Eq. (22) with correlation lengths $\xi_1 = 4.5$ and $\xi_2 = 3$. We assume that the principal axes are rotated by $\theta = 45^\circ$ with respect to the coordinate system. We calculate the ratios of the SRST elements from Eqs.

(18) and (19), obtaining $Q_{22}/Q_{11} = 1$ and $Q_{12}/Q_{11} = -5$. We minimize the objective function $\Phi(\theta, R_{2(1)})$ with the above values of the mean SRST ratios using the MATLAB routine FMINS with initial values $\theta_0 = 0^\circ$ and $R_{2(1)} = 1$. The minimization is based on the simplex search method of Nelder and Mead (e.g., Press et al., 1986). The solutions are $R_{2(1)} = 1.5000$ and $\theta = 45.0002^\circ$ in excellent agreement with the exact values.

Next, we calculate the SRST for the synthetic random field on a grid shown in Figure 10. The random field has correlation lengths $\xi_1 = 7.5$ and $\xi_2 = 5$. The principal axes are rotated by 45° as it can be seen from the orientation of the correlated regions in Figure 10. The SRST elements are estimated numerically based on Eq. (21). Then, they are used in Eq. (27) to estimate the anisotropic parameters. The results for three different realizations with the same aspect ratio and orientation angle (i.e., $R_{2(1)} = 1.5$ and $\theta = 45^{\circ}$) but different correlation lengths are compared in Table II with the theoretical values. The latter are given for the SRST elements from Eqs. (15)-(17) using $\zeta^2 = 2$ for the Gaussian covariance. The estimates for the aspect ratio and the orientation angle are very accurate, especially for the two smaller correlation lengths. As the correlation length increases the accuracy of the estimates is reduced. This is attributed to departure from the ergodic conditions, due to the finite size of the sample. The estimates of the mean SRST elements are not as accurate. This is due, as we discussed above, to fluctuations of the sample variance.

VI. CONCLUSIONS AND DISCUSSION

In this paper we discuss issues related to the modeling of range anisotropy in environmental processes. We present an anisotropic, truncated power-law covariance with short-range and long-range cutoffs. This model can be used for stochastically homogeneous processes that exhibit scaling behavior over a range of scales. We also introduce a family of separable covariances based on superellipsoids. These functions have non-elliptical isolevel contours and are useful if the distance metric is non-Euclidean. We also propose a new method for estimating the anisotropic parameters (i.e., the correlation aspect ratios and the orientation of the principal anisotropy axes) of an random field. This method is based on the covariance tensor identity and employs the mean Second-Rank-Slope Tensor (SRST), which can be estimated from the available data. We propose SRST estimators for both regular (on-grid) and irregular (off-grid) data distributions. We also formulate a general system of equations that relate the mean SRST to the anisotropic parameters in any number of dimensions. In two spatial dimensions we derive an explicit system of nonlinear equations that determines the anisotropic parameters. We solve the system using a minimization method. We demonstrate how to calculate the mean SRST and the anisotropic parameters using simulated random fields.

Approaches for optimizing the mean SRST estimates for irregular data distribution merit further investigation. How to determine the optimal value of the lower cutoff to be used in the discrete approximation of random field derivatives is an open issue. Calculations using very low cutoff values are sensitive to numerical fluctuations that compromise the accuracy of the estimate. On the other hand, by increasing the lower cutoff precision is reduced following a reduction in the number of nearest neighbor pairs. We have based the SRST estimation on the Euclidean distance between points. However, the point with the nearest value of the x (or y) coordinate is not necessarily the nearest neighbor based on the Euclidean distance. An alternate approach is to define nearest neighbors separately in each direction. In addition, next nearest neighbors can be considered if the distance between two nearest neighbors is smaller than the lower cutoff. These changes will increase the number of points that can be used in the spatial average. Another issue is the maximum aspect ratio that can be accurately estimated. This obviously depends on the domain size. Since the estimation procedure is based on the ergodic principle, the domain size should significantly exceed the largest correlation length. Otherwise, the estimates will be inaccurate.

We have presented numerical simulations based on the Gaussian covariance, which is a Class (A) model. Other types of covariances from both classes and random fields with larger variances should be investigated. Finally, extension of the method to threedimensional random fields is straightforward, based on the general Equations (13).

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APPENDIX I

We calculate the second partial derivative of the covariance function $c_x(\tilde{r}) = \sigma_x^2 g(|\tilde{r}_1|^{2/n}) g(|\tilde{r}_2|^{2/n})$. It follows that

$$\frac{\partial c_x(\tilde{\boldsymbol{r}})}{\partial r_1} = \sigma_x^2 g\left(\left|r_2/\xi_2\right|^{2/n}\right) \frac{dg\left(\left|r_1/\xi_1\right|^{2/n}\right)}{dr_1} \,. \tag{I.1}$$

Let us define $\omega \equiv |r_1/\xi_1|^{2/n}$. Then, we find that

$$\frac{dg\left(\left|r_{1}/\xi_{1}\right|^{2/n}\right)}{dr_{1}} = \frac{dg(\omega)}{d\omega}\frac{d\omega}{dr_{1}} = \frac{2g'(\omega)}{n\xi_{1}}\left|\frac{r_{1}}{\xi_{1}}\right|^{2/n-1}\operatorname{sgn}(r_{1})$$
(I.2)

where $g'(\omega) = dg(\omega)/d\omega$. Similarly,

$$\frac{\partial^2 c_x(\tilde{\boldsymbol{r}})}{\partial r_1^2} = \sigma_x^2 g\Big(|r_2/\xi_2|^{2/n}\Big) \frac{d^2 g\Big(|r_1/\xi_1|^{2/n}\Big)}{dr_1^2} = \sigma_x^2 g\Big(|r_2/\xi_2|^{2/n}\Big) \frac{d}{dr_1} \left[\frac{2g'(\omega)}{n\xi_1} \left|\frac{r_1}{\xi_1}\right|^{2/n-1} \operatorname{sgn}(r_1)\right]$$
(I.3)

The derivative is given by

$$\frac{d}{dr_{l}} \left[\frac{2g'(\omega)}{n\xi_{l}} \left| \frac{r_{l}}{\xi_{l}} \right|^{2/n-1} \operatorname{sgn}(r_{l}) \right] = \left[\frac{2}{n\xi_{l}} \left| \frac{r_{l}}{\xi_{l}} \right|^{2/n-1} \operatorname{sgn}(r_{l}) \right]^{2} g''(\omega) + \frac{2g'(\omega)}{n\xi_{l}^{2}} \left(\frac{2}{n} - 1 \right) \left| \frac{r_{l}}{\xi_{l}} \right|^{2/n-2} \operatorname{sgn}^{2}(r_{l}) + \frac{2g'(\omega)}{n\xi_{l}^{2}} \left| \frac{r_{l}}{\xi_{l}} \right|^{2/n-1} \delta(r_{l})$$
(I.4)

Finally, we obtain

$$\frac{\partial^{2} c_{x}(\tilde{\boldsymbol{r}})}{\partial r_{1}^{2}} = \sigma_{x}^{2} g\left(\left|r_{2}/\xi_{2}\right|^{2/n}\right) \left\{ \left[\frac{2}{n\xi_{1}}\left|\frac{r_{1}}{\xi_{1}}\right|^{2/n-1} \operatorname{sgn}(r_{1})\right]^{2} g''(\omega) + \frac{2g'(\omega)}{n\xi_{1}^{2}} \left(\frac{2}{n}-1\right) \left|\frac{r_{1}}{\xi_{1}}\right|^{2/n-2} \operatorname{sgn}^{2}(r_{1}) + \frac{2g'(\omega)}{n\xi_{1}^{2}} \left|\frac{r_{1}}{\xi_{1}}\right|^{2/n-1} \delta(r_{1})\right\} \right].$$
(I.5)

FIGURE CAPTIONS

Figure 1: Plot of the power-law covariance with short-range cutoff w = 5 and exponent $\gamma = 1.5$. Function with long-range cutoff $\xi = 4000$ (solid line) and without (broken line).

Figure 2: Plot of the isolevel contours of exponential superellipsoidal functions for six different values of the exponent n.

<u>Figure 3:</u> Plot of the power spectral density for the six exponential superellipsoidal functions with exponents as shown in Figure 1.

<u>Figure 4:</u> Realization of an exponential superellipsoidal random field with n = 3

<u>Figure 5:</u> Realization of a Gaussian random field with anisotropic Gaussian correlation on a grid aligned with the principal axes.

<u>Figure 6:</u> Plot of the diagonal elements of the SRST and the anisotropic ratio obtained by spatial average over one realization as a function of the grid size (number of RF points) for sizes ranging from 40 to 161 nodes per side.

Figure 7: Plot of 500 randomly selected locations and of their nearest neighbors

<u>Figure 8:</u> Grayscale plot of the irregularly-spaced random field based on linear interpolation. The positions of "data" are marked with stars.

Figure 9: Histogram of nearest neighbor distances.

Figure 10: Plot of a two-dimensional random field with Gaussian covariance and unit variance, $\xi_1 = 6.5$, $\xi_2 = 5$. The principal axes are at 45° with respect to the coordinate system.

TABLE CAPTIONS

<u>Table I</u>: Estimates of the mean SRST tensor as a function of the lower cutoff. Results are obtained from sampling a zero-mean random field with $\sigma_x = 1$, $b_1 = 4$, $b_2 = 6$ at 500 random locations on a square domain 80×80 . Theoretical values of the mean SRST elements are $Q_{11} = 0.1250$, $Q_{22} = 0.0556$ and $Q_{12} = 0$. The number of sites used in the calculation of each element is also shown. The upper cutoff is $\alpha_u = 2$.

<u>Table II</u>: Estimates and theoretical values of the mean SRST, the aspect ratio and the orientation angle (in degrees) for three realizations of a two-dimensional random field with different correlation lengths. The aspect ratio is 1.5 and the orientation angle 45° for all the realizations.

$lpha_l$	\dot{Q}_{11}	\dot{Q}_{22}	\dot{Q}_{12}	N _{eff,11}	N _{eff,22}	N _{eff,12}
0.1	15.237	28.232	-0.109	424	420	359
0.2	1.508	0.584	0.002	380	385	298
0.3	0.703	0.442	-0.005	355	368	265
0.4	0.653	0.336	-0.033	323	334	216
0.5	0.466	0.229	-0.039	295	309	180
0.6	0.303	0.218	-0.056	263	282	141
0.7	0.298	0.193	-0.052	241	255	110
0.8	0.281	0.175	-0.060	192	202	69
0.9	0.172	0.139	-0.034	169	171	55
1.0	0.161	0.132	-0.005	156	154	40
1.1	0.150	0.121	-0.041	137	129	31
1.2	0.152	0.084	0.008	125	99	17
1.3	0.143	0.084	-0.002	99	84	12
1.4	0.141	0.074	0.009	84	68	8
1.5	0.151	0.078	-0.020	74	52	6

Table I

	Q_{11}	Q_{22}	Q_{12}	<i>R</i> ₂₍₁₎	θ
$\xi_1 = 4.5, \ \xi_2 = 3$					
Estimated	0.1132	0.1250	-0.0441	1.48	41.18
Theoretical	0.1605	0.1605	-0.0617	1.50	45
$\xi_1 = 7.5, \ \xi_2 = 5$					
Estimated	0.0475	0.0486	-0.0193	1.53	44.17
Theoretical	0.0578	0.0578	-0.022	1.50	45
$\xi_1 = 15, \ \xi_2 = 10$					
Estimated	0.0130	0.0147	-0.0037	1.32	38.46
Theoretical	0.0144	0.0144	-0.0056	1.50	45

Table II