SPARTAN RANDOM FIELDS FOR GEOSTATISTICAL APPLICATIONS: NON-CONSTRAINED SIMULATIONS OF GAUSSIAN PROBABILITY DENSITIES ON SQUARE LATTICES AND IRREGULAR SUPPORTS

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Spartan random fields are special cases of Gibbs random fields. Their joint probability density function is defined by means of an energy functional determined from a small set of model parameters. The terms in the energy functional represent physically motivated “interactions” instead of data-oriented covariance measures. Spartan random fields provide computationally fast stochastic models for the variability of spatially distributed processes. Their potential applications include interpolation, gridding, and simulation of environmental, health, and geophysical data sets, as well image analysis. Here we develop methods for simulating Spartan fields without constraints on regular (e.g., the square lattice) and irregular supports in two spatial dimensions. We focus on the FGC Spartan model that includes fluctuations of a scalar field, its gradient and its curvature, according to a Gaussian energy
functional. The methods described here for the nearest-neighbor FGC model, can be extended to more general classes of Gaussian random fields.

1. Introduction

A random field is a set of inter-dependent, spatially distributed random variables [2,3,11]. Hence, a random field involves an ensemble of different realizations (states), each manifested with a probability determined from the joint probability density function of the field. Spartan random fields have recently been introduced [8] as a model for spatially distributed processes. Potential applications include the estimation at non-sampled locations (interpolation) and the simulation of various environmental and geophysical variables characterized by variability and measurement uncertainty (e.g., subsurface fluid permeability, concentration of atmospheric pollutants, temperature variations) and mineral resources concentrations. Other applications involve models of structural, mechanical and transport properties of industrial non-homogeneous materials (e.g., porous composites, paper products), and compression of information (e.g., images acquired by remote sensing satellites, morphological variations of paper surface).

Spartan random fields have a joint probability density function that is motivated by physical interactions, and it is determined from a small set of model parameters. The term “Spartan”, hinting at the frugal lifestyle of the ancient Spartans, is thus appropriate. In classical geostatistical analysis, the parameters of spatial dependence are determined from the statistical analysis of the data, e.g., [6]. Spartan random fields employ an “energy functional” that permits incorporating physical principles such as knowledge of the origin of fluctuations and the most favorable configurations for the system under consideration. A practical implication of Spartan random fields
is that the calculation of two-point functions (e.g., correlation function, variogram) from the data is avoided. The calculation of these functions is a computationally intensive inverse problem with numerical complexity $O(N^2)$, where $N$ is the sample size. The computations for the inference of the Spartan field parameters are considerably faster. In addition, for general distributions (e.g., irregular distribution of sampling points, anisotropic spatial dependence with unknown a priori principal directions) the calculation of two-point functions involves various empirical assumptions related to the choice of lag classes, number of pairs per class, lag and angle tolerance, etc. [6].

2. Spartan Random Field Models

Spartan random fields are special cases of Gibbs random fields, which have a joint probability density function given by $f_{\lambda}[X] = Z^{-1} \exp\{-H[X]\}$, where $Z$ is a normalization factor (partition function), and $H[X]$ is an “energy functional” of the random field “states” (also known as realizations, samples, configurations) $X(s)$. In the case of Spartan random fields, the energy functional involves states $X_{\lambda}(s)$ with limited resolution (the subscript “$\lambda$” is a length scale defining the resolution). In practical situations, $\lambda$ is determined from the support scale of the measurements. In the case of simulations, $\lambda$ is determined from the lattice spacing. In contrast with random field models typically used in geostatistics that represent point-like variations, Spartan random fields incorporate an intrinsic notion of scale, which explicitly restricts the observable scales of spatial variability. This is a physically meaningful property, since a finite resolution characterizes every investigation of variability.
Spartan random fields have the following general properties: (i) The energy functional couples the values of the field within specified local neighborhoods. (ii) The field couplings (interactions) are motivated by physical or geometric constraints. (iii) For a model with specified interactions, the energy functional is completely determined from a small set of parameters. (iv) The model parameters must be estimated from the available experimental information, which in most geostatistical investigations consists of a single sample of the process. In this case, the ergodic hypothesis needs to be invoked in order to estimate the model parameters, since an ensemble of states is not available. In other cases (e.g., in the analysis of material surface structure) many samples may be available, thus allowing an improved approximation of the ensemble average.

Spartan models are defined in either continuum or discrete spaces. The latter involve both regular lattices and irregular (off-lattice) distributions of measurement points. Continuum models are most useful for theoretical investigations, while discrete models are more suitable for numerical simulations. Regular lattices are appropriate if the measured process can be systematically scanned and monitored. This occurs for remote-sensing images and for industrial materials that are easily accessible to scanning by various methods. Irregular distributions are more suitable for ground measurements of environmental distributions, for which financial cost and other considerations limit the number of sampling locations.

2.1. The FGC Spartan Model in Two Dimensions

Let us consider a square lattice with \( L \) nodes per side (below we assume that \( L \) is an even integer) and a total of \( N \) sites, \( s_n, n = 1, \ldots, N \). The nearest neighbors of each
The site are given by the vectors \( s_n \pm a \hat{e}_i \), \( i = x, y, \) where \( a \) is the lattice step and \( \hat{e}_i \) the unit vector in the respective direction. We then define the following field-gradient-curvature (FGC) discrete energy functional [8]

\[
H[X] = \frac{1}{2 \eta_0 \xi^2} \sum_{n=1}^{N} \mathcal{H}_n(\eta_1, \xi; X_n),
\]

(1)

\[
\mathcal{H}_n(\eta_1, \xi; X_n) = [X_n(s_n) - m_X]^2 + \eta_1 \xi^2 \sum_{i=x,y} \frac{[X_n(s_n + a \hat{e}_i) - X_n(s_n)]^2}{a^2} + \\
+ \xi^4 \sum_{i=x,y} \frac{[X_n(s_n + a \hat{e}_i) - 2X_n(s_n) + X_n(s_n - a \hat{e}_i)]^2}{a^2}.
\]

(2)

In the above, \( \mathcal{H}_n(\eta_1, \xi; X_n) \) is the energy associated with field values at the site \( s_n \) and interactions with the nearest neighbors. The terms in \( \mathcal{H}_n(\eta_1, \xi; X_n) \) have a physical motivation: The first term denotes the deviation of the local field value from the ensemble mean, the second term is proportional to the square of the local gradient of the field, and the third term is proportional to the square of the local curvature. If the values of the field represent a surface in \( d \)-dimensional space, the above geometric parameters characterize the shape of the surface.

The model parameters are the ensemble mean \( m_X \), the scale coefficient \( \eta_0 \), the shape coefficient \( \eta_1 \), and the correlation length \( \xi \). The parameter \( m_X \) is determined from the spatial mean of the sample. The other parameters are determined by minimizing a metric that represents the “distance” between sample constraints (i.e., spatial moments obtained from the sample) and stochastic constraints (i.e., moments obtained by integrating the joint probability density function). We present the
definition of the constraints and the optimization procedure used to estimate the coefficients from the sample in [8]. In the following, we concentrate on the simulation of Spartan fields with known parameters. More specifically, we focus on non-constrained simulation, i.e., the generation of states from the ensemble that do not require the field to obey “experimental” constraints at certain locations.

Ensemble averages will be denoted by the expectation $E[\cdot]$. The joint probability density function derived from Eqs. (1) and (2) is Gaussian, because the energy is a quadratic functional of the field. The Spartan field is statistically homogeneous [2,11] because the mean value and the coefficients $\eta_0$, $\eta_1$ and $\xi$ in Eq. (2) are uniform in space. The scale coefficient $\eta_0$ determines the total variability (i.e., the fluctuation variance), $\xi$ determines the range of the spatial dependence, and $\eta_1$ affects the shape of the covariance function. The field is “quasi-isotropic” because there is no distinction between the two orthogonal lattice directions (the structure of the square lattice prevents full isotropy). Anisotropic distributions are obtained by introducing coefficients with directional dependence.

2.2. The Covariance Spectral Density

The covariance function of the random field, defined by means of

$$G_{\lambda,\lambda}(r) \equiv E[X_\lambda(s)X_\lambda(s + r)] - E[X_\lambda(s)]E[X_\lambda(s + r)],$$

is the most important measure of spatial dependence. For Gaussian random fields, the covariance function fully determines the spatial dependence.

The covariance spectral density, i.e., the Fourier transform of the covariance function, is defined by means of the following Fourier integral

$$F_{\lambda,\lambda}(k) = \int G_{\lambda,\lambda}(r) e^{-2\pi i k \cdot r} dr.$$
\[ \tilde{G}_{x,\lambda}(k) = \int d\mathbf{r} e^{-ik \cdot \mathbf{r}} G_{x,\lambda}(\mathbf{r}). \]  

(3)

The spectral density is well approximated by its continuum counterpart, which is expressed in terms of the coefficients \( \eta_0, \eta_1, \xi \) as follows [8]

\[ \tilde{G}_{x,\lambda}(k) = |\tilde{Q}_x(k)|^2 g_s(k), \quad g_s(k) = \frac{\eta_0 \xi^d}{1 + \eta_1 (k \xi)^2 + (k \xi)^4}. \]  

(4)

In the above, \( \mathbf{k} \) is the spatial frequency vector (wave-vector). The coarse-graining kernel \( |\tilde{Q}_x(k)|^2 \) cuts off fluctuations at length scales smaller than the resolution \( \lambda \). For square lattices with step \( a \), we approximate the kernel with a sharp cutoff at \( k_{max} = 2\pi/a \), which leads to band-limited covariance functions.

For Gaussian random fields, the existence of the first-order derivatives in the mean-square sense [2,11] is guaranteed if the second-order derivative of the covariance function exists at zero distance \( \mathbf{r} \) [2,11]. This condition is satisfied if the integral \( \int d\mathbf{k} k^2 \tilde{G}_{x,\lambda}(k) \) is finite. If \( \lambda \to 0 \), integration extends over all frequencies leading to a divergent integral for the Spartan spectral density (4) in \( d \geq 2 \). However, if the spectral density is band-limited, the integral is defined, and so are the derivatives of the Spartan random fields.

The parameters of Spartan models are not completely free, since Bochner’s theorem e.g., [3,11] requires the spectral density to be non-negative and integrable. This leads to the conditions (i) \( \eta_0 > 0, \xi > 0 \) and \( \eta_1 \geq 0 \), or (ii) \( \eta_0 > 0, \xi > 0 \) and \( \eta_1 < 0, \eta_1^2 < 4 \) [8]. For positive \( \eta_1 \) the spectral density declines monotonically with
frequency. In contrast, for negative values of $\eta$, the spectral density peaks at some finite frequency; as $\eta \to -2$ the spectral density tends to develop a singular peak as shown in Figure 1. The physical significance of the peak is the existence of a negative hole in the real-space covariance function.

The variance $\sigma_{x,x}^2 = G_{x,x}(0)$ is the integral of the covariance spectral density, i.e.,

$$\sigma_{x,x}^2 = (2\pi)^{-1} \int_0^{k_{\text{max}}} dk \, k \, g_x(k).$$

Using the transformation $(k\xi)^2 \to \kappa$ and assuming that the resolution scale is negligibly small compared to the correlation scale, i.e., $k_{\text{max}}\xi > 1$, the variance $\sigma_x^2$ can be evaluated explicitly using integral tables [1, p.12] as follows

$$\sigma_x^2 = \int_0^\infty d\kappa \frac{\eta_0/4\pi}{1 + \eta_1 \kappa + \kappa^2} = \begin{cases} \frac{\eta_0/2\pi}{(4 - \eta_1^2)^{3/2}} \left( \frac{\pi}{2} - \tan^{-1} \left[ \frac{\eta_1}{(4 - \eta_1^2)^{3/2}} \right] \right), & \eta_1 < 4 \\ \frac{\eta_0/4\pi}{(\eta_1^2 - 4)^{1/2}} \ln \left[ \frac{\eta_1 + (\eta_1^2 - 4)^{1/2}}{\eta_1 - (\eta_1^2 - 4)^{1/2}} \right], & \eta_1 > 2 \\ \frac{\eta_0}{4\pi}, & \eta_1 = 2 \end{cases}.$$  

The above expressions show that the variance is independent of the correlation length $\xi$. We show the dependence of the variance on the shape coefficient in Figure 2. If the parameters $\eta_0$ and $\xi$ are fixed, the variance decreases with increasing $\eta_1$.

The covariance for non-zero separation distance follows from the inverse Fourier transform of the spectral density [8], i.e.,

$$G_{x,x}(r) = \frac{1}{(2\pi)^3} \int dk \, \tilde{G}_{x,x}(k) e^{ikr}. \quad (6)$$
For isotropic spectral densities, \( \tilde{G}_{x,\lambda}(k) = \tilde{G}_{x,\lambda}(k) \) where \( k = \|k\| \) is the magnitude of the frequency vector, evaluation of the integral in Eq. (6) requires (in most cases), one numerical integration over \( k \). The direct transform is given by the integral

\[
\tilde{G}_{x,\lambda}(k) = \int d\mathbf{r} G_{x,\lambda}(\mathbf{r}) e^{-ik\mathbf{r}}. \tag{7}
\]

We have identified the parameter \( \xi \) with the correlation length of the fluctuations without justification. If we define the correlation length by means of

\[
r_{\text{cor}}^2 = \int d\mathbf{r} G_{x,\lambda}(\mathbf{r})/G_{x,\lambda}(0),
\]

this is equivalent to \( r_{\text{cor}}^2 = \tilde{G}_{x,\lambda}(k = 0)/G_{x,\lambda}(0) \). Hence, it follows from Eq. (4) that \( r_{\text{cor}} = \xi \).

### 2.3. Inference of Model Parameters from Samples

We investigated this issue in detail in [8], where we calculated the optimal Spartan model parameters from synthetic samples simulating experimental distributions. More specifically, Gaussian random fields in two dimensions with (i) exponential (ii) Gaussian and (iii) hole-type covariance functions were used to simulate the samples on square lattices and at a random distribution of sites. We present the method used in [8] for the simulation of irregular distributions in Section 4 below.

We found that the best match between the synthetic samples and the FGC Spartan model is obtained for the samples with exponential covariance dependence. This observation is supported by the Markov character of the FGC Spartan model defined by Eq. (2), which involves only short-range, nearest-neighbor coupling. In the cases
of Gaussian and hole-type dependence, the optimal Spartan field showed a negative shape coefficient, which implies a negative hole in the covariance function. This feature is absent from the samples with Gaussian covariance. We believe that this effect results from the effort to match the relatively smooth Gaussian dependence with the FGC Spartan model that involves only nearest-neighbor interactions. Incorporating terms with longer-range dependence in the energy functional should help to reduce this discrepancy. On the other had, we should point out that the comparisons carried out in [8] assume that the experimental information permits reliable estimation of the covariance function even at long range. However, this is not always possible in practical situations, especially if the number of available measurements is small. In these cases, the Spartan models seem like a more natural choice.

3. Fast-Fourier-Transform Simulation Method

Simulations of Spartan random fields on a lattice can take advantage of the geometric symmetries and the efficiency of the Fast Fourier Transform (FFT). The method of Fourier filtering [9] is easily implemented for jointly Gaussian distributions. The main idea is to generate a set of Gaussian random numbers, and pass them through a frequency filter that enforces correlations by a suitable truncation of the high frequencies. These operations are linear in the size $N$ of the lattice ($N = L^2$ for a square lattice with $L$ nodes per side). The random field in real space follows from the inverse Fast Fourier Transform of the filtered set of Gaussian numbers, which is an $O(N \log N)$ operation. This accounts for the very fast performance of the algorithm compared with methods based on the covariance matrix decomposition [3], which are
\(O(N^2)\) in time and memory intensive. The FFT method generates the fluctuation field, to which any trends should be added.

For a real-valued, continuum random field the Fourier transform of a single state (realization) is given by \(\tilde{X}(\mathbf{k}) = u(\mathbf{k})\left[\tilde{G}_{\lambda,\lambda}(\mathbf{k})\right]^{1/2}\), where \(u(\mathbf{k})\) is a complex, zero-mean Gaussian process with localized correlations \(E[u^*(\mathbf{k}')]u(\mathbf{k})] = (2\pi)^2 \delta(\mathbf{k} - \mathbf{k}')\). This implies the following integral equation
\[
\int d\mathbf{k}' E[u^*(\mathbf{k}')]u(\mathbf{k})] = (2\pi)^2. \tag{8}
\]
This construction ensures that the field \(X(\mathbf{s}) = \text{IFFT}[\tilde{X}(\mathbf{k})]\) has a covariance function with spectral density \(\tilde{G}_{\lambda,\lambda}(\mathbf{k})\). In addition, since the field \(X(\mathbf{s})\) is real, it is required that \(u^*(-\mathbf{k}) = u(\mathbf{k})\).

3.1. **Lattice Simulations**

We present an implementation of Spartan random field simulations in the Matlab\textsuperscript{®} programming environment, based on the FFT approach discussed above. This requires adapting the continuum models for use with discrete Fourier transforms (DFT). The direct and inverse DFT on a square lattice with unit spacing are given by the following Fourier series [10]
\[
\tilde{X}_{j,l} = \sum_{n=1}^{L} \sum_{m=1}^{L} X_{m,n} \exp\left[-\frac{2\pi i[(m-1)(l-1)+(n-1)(j-1)]}{L}\right], \quad j,l = 1,\ldots,L. \tag{9}
\]
\[ X_{m,n} = \frac{1}{N} \sum_{n=1}^{L} \sum_{m=1}^{L} \tilde{X}_{j,l} \exp \left[ \frac{2\pi i [(m-1)(l-1)+(n-1)(j-1)]}{L} \right], \quad m, n = 1, \ldots, L. \] (10)

The lattice is represented by a position matrix \( s_{nm} = (n, m), \) where the integers \( m, n \) are the row and column indices; the integers \( j, l \) are respectively the row and column indices of the spatial frequency matrix \( k'_{jl} = \frac{2\pi}{L} (l, j). \) The variable \( X_{m,n} \) is the value of the field at \( s_{nm} \) and \( \tilde{X}_{j,l} \) is the Fourier transform at the frequency \( k'_{jl}. \)

A frequency index equal to one corresponds to the physical frequency component being equal to zero, i.e., \( k'_{jl} \) means that \( k_j = 0; \) indices from 2 to \( L/2 + 1 \) correspond to positive frequencies, while the indices from \( L/2 + 2 \) to \( L \) represent negative frequencies. Hence, the elements \( k'_{jl} \) of the frequency matrix correspond to physical frequencies \( k_{jl} = \frac{2\pi}{L} [\zeta(l), \zeta(j)], l, j = 1, \ldots, L, \) where \( \zeta(l) = l - 1 \) if \( L/2 + 1 \geq l \geq 1 \) and \( \zeta(l) = L/2 + 1 - l \) if \( L \geq l \geq L/2 + 2. \) To obtain the discrete spectral density, the continuum spectral density \( \tilde{G}_{k,\lambda}(k) \) is evaluated at the discrete frequencies. The resulting function, \( \tilde{G}_{k,\lambda}(k_{jl}), \) is symmetric around the zero frequency, as shown for the one-dimensional example of Figure 3 (top). However, if we use the DFT frequency counting scheme, the spectrum \( \tilde{G}_{k,\lambda}(k'_{jl}) \) is transformed as shown schematically in Figure 3 (bottom). The number of frequencies in the positive band (P) exceeds those in the negative band (N) by one, thus leading to a slight asymmetry between the two frequency bands. Note that in the top figure the frequency axis is labeled in descending order, implying that the symmetric spectral density be stored in a one-dimensional array with the high-frequency components to the left of low-frequency components. This ordering allows using the Matlab function “fftshift” to
re-organize the spectrum (Figure 3, bottom) in the form required for the DFT calculations. Extension of the procedure in two dimensions is straightforward.

The DFT normalization ensures that the discrete series for the covariance function converges to the Fourier transform integrals. This is because in the direct Fourier transform \( \sum_{n=1}^{L} \rightarrow \int dy \) (if the lattice spacing is \( \delta y \neq 1 \) the DFT should be multiplied by \( \delta y \)) and for the inverse Fourier transform \( \sum_{m=1}^{L} \rightarrow \frac{1}{2\pi} \int dk_y \) or \( \frac{1}{\pi} \sum_{m=1}^{L} \rightarrow \frac{1}{2\pi} \int dk_y \) (if \( \delta y \neq 1 \) the DFT should be divided by \( \delta y \)).

The field components in frequency space are given by \( \tilde{X}(k) = u_y \sqrt{G_{\delta y}}(k) \), where \( u_y \) are the elements of a matrix of random coefficients from the normal distribution. The matrix \( u \) should satisfy certain symmetry properties to guarantee that the inverse Fourier transform of \( \tilde{X}_{j,d} \) is real. This happens if \( u \) has the following block-matrix structure

\[
\begin{bmatrix}
  u_{1,1} & \mathbf{b}_{1,R}^T & u_{1,L/2+1} & U_{180}^\prime (\mathbf{b}_{1,R}^T)^\ast \\
  \mathbf{b}_{C,1}^T & [C] & \mathbf{b}_{C,L/2+1}^T & U_{180}^\prime (\mathbf{D}^\ast) \\
  u_{L/2+1,1} & \mathbf{b}_{L/2+1,R}^T & u_{L/2+1,L/2+1} & U_{180}^\prime (\mathbf{b}_{L/2+1,R}^T)^\ast \\
  U_{180}^\prime (\mathbf{b}_{C,1}^T) & [D] & U_{180}^\prime (\mathbf{b}_{C,L/2+1}^T) & U_{180}^\prime (\mathbf{C}^\ast) 
\end{bmatrix}.
\] (11)

The elements \( u_{1,1}, u_{1,L/2+1}, u_{L/2+1,1} \) and \( u_{L/2+1,L/2+1} \) are the only purely real numbers. This ensures that for the frequencies \( k_y = (0,0), (0,\pi), (\pi,0), (\pi,\pi) \) the transform \( \tilde{X}(k) \) is a real number, in agreement with the definition (9). The blocks \( \mathbf{b}_{1,R}^T = [u_{1,2} \ldots u_{1,L/2}] \) and \( \mathbf{b}_{L/2+1,R}^T = [u_{L/2+1,2} \ldots u_{L/2+1,L/2}] \) are complex-valued row vectors with \( L/2 - 1 \) columns. In general, there is no correlation between the real and the imaginary parts.
The blocks $\mathbf{b}_{c,i} = [u_{2,i} \ldots u_{L/2,i}]^T$, $\mathbf{b}_{c,i/2+1} = [u_{2,i/2+1} \ldots u_{L/2,i/2+1}]^T$ represent column vectors with $L/2-1$ rows. The size of the square matrices of complex coefficients $\mathbf{C}$ and $\mathbf{D}$ is $L/2-1$. The operation $U_{180}^\circ [\mathbf{M}]$ denotes rotation of the matrix $\mathbf{M}$ by $180^\circ$ (reflection) and the star ($\mathbf{M}^*$) indicates the complex conjugate of all the elements of matrix $\mathbf{M}$.

The elements $u_{j,l}$ can be expressed as $u_{j,l} = c_0 w_{j,l}$, where $c_0$ is a real normalization constant and the random numbers $w_{j,l}$ have real and imaginary parts drawn from the $N(0, 2^{-1/2})$ normal distribution. The standard deviation $2^{-1/2}$ accounts for the existence of uncorrelated real and imaginary parts and guarantees that the elements $w_{j,l}$ have correlation equal to one, $E[w_{j,l}^* w_{j',l'}] = \delta_{j,j'} \delta_{l,l'}$. To determine the constant $c_0$, we obtain the discrete equivalent of the integral (8). Using $dk_x \to \frac{2\pi}{T} \sum_{j=1}^{L} dx$ and $dk_y \to \frac{2\pi}{T} \sum_{j=1}^{L} dy$, the integral is replaced by a sum as follows

$$\sum_{i=1}^{L} \sum_{j=1}^{L} E[u_{j,l}^* u_{j',l'}] = L^2. \quad (12)$$

This equation is satisfied by the numbers $u_{j,l}$ if $c_0 = L$. At this point, the Fourier transform of Spartan field states $\tilde{X}_{j,l}$ is fully determined by $\tilde{X}_{j,l} = [\tilde{G}_{x,l}]^{1/2} u_{j,l}$. The Spartan state in real space follows from the inverse Fourier transform, which can be numerically evaluated by means of the Matlab function “ifft”.
3.2. Numerical Experiments

We show two examples of Spartan random field states, obtained with the method described in section 3, in Figure 4 and Figure 5. The field shown in Figure 4 is ergodic, but the field shown in Figure 5 is not, because the main geometrical features are of similar scale as the entire domain. In the first case, the sample standard deviation is equal to the theoretical (ensemble) variance predicted by Eq. (5), i.e., $\sigma_{x,t} = 0.34$. In the second case, the sample standard deviation differs from the ensemble value $\sigma_{x,t} = 0.63$.

In Figure 6 we compare the ensemble covariance, which is obtained by the numerical inversion of the Spartan spectral density of Eq. (4), with two sample-based covariance functions obtained from simulated Spartan states. The sample covariance function is evaluated as follows: We first obtain a set of $L$ one-dimensional covariance functions along one of the lattice directions, and then calculate the ensemble average over the one-dimensional functions. We observe good agreement between the sample-based and the ensemble covariance functions.

4. Mode Superposition Method

The FFT method is not suitable for simulating Spartan random fields at positions that are not on a regular lattice. In this case a mode superposition method [1,7] is more appropriate

$$X_{\lambda}(s) \equiv m_{x} + \sigma_{x,t} \sqrt{\frac{2}{N_{M}}} \sum_{p=1}^{N_{M}} \cos(k_{p} \cdot s + \phi_{p}).$$

(13)
Each mode is characterized by a frequency $k_p$ and a phase $\phi_p$. The phases $\phi_p$ are random numbers distributed uniformly in $[0, 2\pi]$. The mode frequencies $k_p$ are also random numbers that follow the probability density function specified by the normalized covariance spectral density as follows

$$f_k(k) = \frac{\tilde{G}_{\lambda}(k)}{(2\pi)^d \sigma_{\lambda}^2}. \tag{14}$$

In the above, $\tilde{G}_{\lambda}(k)$ is the spectral density given explicitly by Eq. (4). Note that since the variance of the field is given by the integral $\sigma_{\lambda}^2 = (2\pi)^{-d} \int dk \tilde{G}_{\lambda}(k)$, the function $f_k(k)$ is properly normalized, i.e., $\int dk f_k(k) = 1$.

The mode superposition converges to $X_\lambda(s)$ as the number of modes $N_M$ tends to infinity. Finite $N_M$ approximations with a few thousand modes can accurately reproduce the statistics of $X_\lambda(s)$. The numerical complexity of this method is $O(N_M N)$. Hence, it is computationally more intensive than the FFT method for the same number of points. However, the mode superposition is applicable to any type of spatial distributions, since it does not rely on lattice symmetries. The method requires calculation of the cosine function for all mode and site combinations. Since the calculation can not be expressed as a matrix operation to completely avoid numerical loops, it does not take full advantage of Matlab’s efficiency for matrix calculations.

Random numbers following a specific probability distribution are simulated using nonlinear transformations of uniform variates and the conservation of probability under the transformation, e.g. [10]. We derive in section 4.1 below the
transformations for generating the distribution of mode frequencies for the three types of spatial dependence used in the simulation of synthetic sample fields with specified covariance function (i.e., Gaussian, exponential, and hole-type covariance functions).

4.1. Mode Probability Distribution for Various Covariance Structures

In this section, we present methods for simulating various covariance structures using transformations of the frequency vector into random variables that follow the Gaussian or the uniform distribution. For isotropic spectral densities, it is useful to define the probability density of the mode amplitude, \( k = \| \mathbf{k} \| \) via

\[
p_k(k) \equiv k^{d-1} \int d\hat{\mathbf{k}} f_k(\mathbf{k}), \quad (15)
\]

so that \( \int_0^\infty dk \ p_k(k) = 1 \). The frequency components in the orthogonal directions follow from random magnitudes drawn from \( p_k(k) \), and random vectors \( \hat{\mathbf{k}} \) obtained from uniform angle distribution. For example, in two dimensions \( k_x = k \cos \phi \) and \( k_y = k \sin \phi \), where the angle \( \phi = U(0, 2\pi) \) is uniformly distributed.

Below, we show how to simulate the mode probability distribution for specific covariance spectral density functions. The first three cases apply to Gaussian, exponential and hole-type covariance functions, which were used in [8] to generate synthetic samples. The fourth case determines the mode distribution for a Spartan random field with an FGC covariance structure given by Eq. (4).
**Gaussian Covariance:** For the anisotropic Gaussian covariance

\[ G_x(r) = \sigma_x^2 \exp\left(-\sum_{i=1}^{d} r_i^2 / \ell_i^2 \right) \]

the mode probability density function in \( d \) spatial dimensions is given by

\[ f_k(k) = \prod_{i=1}^{d} \left( \frac{\ell_i}{2\sqrt{\pi}} \right) \exp\left(-\sum_{i=1}^{d} k_i^2 \ell_i^2 / 4 \right). \]  

(16)

The distribution of the frequency component in each direction is zero-mean Gaussian with variance \( 2/\ell_i^2 \), and hence it is possible to simulate it with a Gaussian random number generator (e.g., the Matlab function “randn”).

**Exponential Covariance:** For the anisotropic exponential covariance

\[ G_x(r) = \sigma_x^2 \exp\left(-\sum_{i=1}^{d} r_i^2 / \ell_i^2 \right) \]

the \( f_k(k) \) in \( d \) dimensions is given by

\[ f_k(k) = \frac{\ell^d \Gamma(d)/\Gamma(0.5d)}{2^{d-1} \pi^{d/2} \left[1 + (k\ell)^2\right]^{(d+1)/2}}. \]  

(17)

For an isotropic exponential covariance in two spatial dimensions,

\[ f_k(k) = \frac{\ell^2}{2\pi(1+k^2\ell^2)^{3/2}}, \]  

and thus based on (15) we obtain \( p_k(k) = \frac{\ell^2 k}{(1+k^2\ell^2)^{1/2}} \) for the mode amplitude distribution. We can simulate the frequency modes from a uniform random variable \( x \) with \( p(x) = U(0,1) \) and the probability conservation relation

\[ |p_k(k)dx| = |p_k(k)dk| \]  

[10; p.277], which for \( U(0,1) \) becomes \( |dx/dk| = p_k(k) \). The
nonlinear relation \( x = V(k) \) between the variables \( x \) and \( k \) is thus \( x = \int_0^k dk' \, p_k(k') \).

The solution of this equation, i.e., \( k = V^{-1}(x) \), for the mode amplitude \( k \) is given by

\[
k = \frac{\sqrt{1 - (1 - x)^2}}{\xi(1 - x)}.
\] (18)

**Hole-Type Covariance:** For the anisotropic hole-type covariance, \( G(x) = \sigma^2_x \prod_{i=1}^d \text{sinc}(r_i/\ell_i) \), where \( \text{sinc}(y) = \sin(y)/y \), the mode probability density \( f_k(k) \) is given by the uniform density

\[
f_k(k) = \begin{cases} 
1/\left(\prod_{i=1}^d 2\ell_i\right), & |k| < \ell_i^{-1}, \forall i = 1, \ldots, d \\
0 & \text{otherwise}
\end{cases}
\] (19)

The mode distribution can thus be simulated from \( d \) uniform random numbers \( x_i = U(0,1) \) and the equation

\[
k_i = -\frac{1}{\ell_i} + 2 \frac{x_i}{\ell_i}.
\] (20)

**FGC Spartan Covariance:** We now focus on the mode amplitude distribution for the Spartan spectral density given by Eq. (4). Ignoring the cutoff, the mode probability density is given by
\[ f_k(k) = \frac{\eta_0 \xi^d}{(2\pi)^d \sigma_{x,d}^2 \left[ 1 + \eta_i (k \xi)^2 + (k \xi)^4 \right]} . \]  

(21)

In light of Eq. (15), and using the integral over the directional degrees of freedom, i.e., \[ \int d\hat{k} = S_d = 2\pi^{d/2}/\Gamma(d/2), \] we obtain the following distribution for the mode amplitude

\[ p_k(k) = \frac{A_d}{\sigma_{x,d}^2} \frac{\eta_0 \xi^d k^{d-1}}{\left[ 1 + \eta_i (k \xi)^2 + (k \xi)^4 \right]} , \]  

(22)

where

\[ A_d = \frac{1}{2^{d-1} \pi^{d/2} \Gamma(d/2)} . \]  

(23)

The equation \( x = V(k) \) is thus expressed as follows in terms of the dimensionless frequency variable \( \kappa = k' \xi \)

\[ x = \frac{\eta_0 A_d}{\sigma_{x,d}^2} \int_{0}^{\kappa \xi} d\kappa' \frac{\kappa'^{d-1}}{\left[ 1 + \eta_i \kappa'^2 + \kappa'^4 \right]} . \]  

(24)

Next, we focus on \( d = 2 \), so that the integral in (24) is expressed as

\[ x = \frac{\eta_0}{4\pi \sigma_{x,d}^2} \int_{0}^{(k \xi)^2} d\omega \frac{1}{1 + \eta_i \omega + \omega^2} . \]  

(25)
We evaluate explicitly the integral in Eq.(25), by distinguishing between three cases depending on the value of $\eta$, as follows:

(A) For $\eta = 2$ we obtain $x = \left\{ \eta_0 (k \xi)^2 / 4 \pi \sigma^{2}_{x,\lambda} \left[ 1 + (k \xi)^2 \right] \right\}$; using Eq. (5) for the variance this leads to $x = (k \xi)^2 / \left[ 1 + (k \xi)^2 \right]$. The mode amplitude then follows from

$$ (k \xi)^2 = \frac{x}{1 - x}, \quad (26) $$

(B) For $\eta \neq 2$ we obtain

$$ x = \frac{\eta_0}{4 \pi \sigma^{2}_{x,\lambda} \sqrt{\eta^2 - 4}} \int_{0}^{(k \xi)^2} \frac{dy}{(1 + \eta y + y^2)} = $$

$$ = \frac{\eta_0}{2 \pi \sigma^{2}_{x,\lambda} \sqrt{\eta^2 - 4}} \left[ \tanh^{-1} \left( \frac{\eta}{\sqrt{\eta^2 - 4}} \right) - \tanh^{-1} \left( \frac{2(k \xi)^2 + \eta}{\sqrt{\eta^2 - 4}} \right) \right]. \quad (27) $$

We further elaborate this result for two separate cases, depending on the discriminant $\Delta = \sqrt{\eta^2 - 4}$.

(B.1) If $\Delta$ is real, i.e., for $\eta > 2$,

we use the identity $\tanh^{-1}(z) = \frac{1}{2} \ln \left( \frac{1+z}{1-z} \right)$, which allows expressing the Eq. (27) in the form
\[ x = \frac{\eta_i}{4\pi \sigma^2_{\omega,d}\Delta} \ln \left[ \frac{\Delta + \eta_i}{\Delta - \eta_i} \right] \left[ \frac{\Delta - \eta_i - 2(k\xi)^2}{\Delta + \eta_i + 2(k\xi)^2} \right]. \]  

(28)

Next, using Eq. (5) for the variance this leads to the following relation between the random variate \( x \) and the mode amplitude

\[ x = \ln \left[ \frac{\eta_i + \Delta}{\eta_i - \Delta} \right] \left[ \frac{\eta_i + 2(k\xi)^2 - \Delta}{\eta_i + 2(k\xi)^2 + \Delta} \right] \left[ \ln \left( \frac{\eta_i + \Delta}{\eta_i - \Delta} \right) \right]^{-1}. \]  

(29)

The right hand side of Eq. (29) must be between zero and one, as required by the equality with the random variate. The arguments of both logarithms are bigger than one; this is obvious for the logarithm in the denominator. The argument of the logarithm in the numerator is expressed as

\[ \frac{\eta_i - \Delta^2 + 2(k\xi)^2}{\eta_i - \Delta^2 + 2(k\xi)^2} > 1. \]  

Hence, both logarithms are positive. In addition, the argument of the logarithm in the denominator exceeds that of the logarithm in the numerator. This follows by examining the ratio of the logarithmic arguments, i.e.,

\[ \frac{\eta_i + \Delta}{\eta_i - \Delta} > \frac{4(\eta_i - \Delta) + 8(k\xi)^2}{4(\eta_i + \Delta) + 8(k\xi)^2}. \]  

We then invert the Eq. (28) as follows

\[ \frac{2 + (\eta_i + \Delta)(k\xi)^2}{2 + (\eta_i - \Delta)(k\xi)^2} = \left( \frac{\eta_i + \Delta}{\eta_i - \Delta} \right)^{1-x}. \]  

(30)
Next, we define the random function $\varphi(x) = \left[ (\eta + \Delta)/(\eta - \Delta) \right]^{1-x}$, by means of which we obtain the dimensionless mode amplitude in terms of the random variable $x$ as follows

\[
(k_\xi)^2 = 2 \frac{\varphi(x) - 1}{[\varphi(x) + 1][\Delta - \eta][\varphi(x) - 1]}.
\] (31)

Since $\varphi(x) \geq 1$ and $\eta \geq \Delta$ it follows from the above that $(k_\xi)^2 \geq 0$ is non-negative, as it should.

(B.2) If $\Delta$ is imaginary, i.e., $-2 < \eta < 0$,

we define $\Delta = i \Delta'$ where $\Delta' = \sqrt{4 - \eta^2}$ is the imaginary part. Using the identity $\tanh^{-1}(z) = -i \tan^{-1}(iz)$, it follows from Eq. (27) that

\[
x = \frac{\eta_0}{2\pi \sigma_{x,i}^2} i \Delta' \left[ -i \tan^{-1} \left( \frac{\eta}{\Delta'} \right) + i \tan^{-1} \left( \frac{2(k_\xi)^2 + \eta}{\Delta'} \right) \right] = \\
= \frac{\eta_0}{2\pi \sigma_{x,i}^2 \Delta'} \tan^{-1} \left( \frac{2(k_\xi)^2 + \eta}{\Delta'} \right) - \tan^{-1} \left( \frac{\eta}{\Delta'} \right) \right].
\] (32)

Furthermore, using the identity $\tan^{-1}(z_1) - \tan^{-1}(z_2) = \tan^{-1} \left( \frac{z_1 - z_2}{1 + z_1 z_2} \right)$ we obtain

\[
\frac{\sigma_{x,i}^2 \Delta'}{\eta_0 \Delta} \left[ x = \tan^{-1} \left\{ \frac{2(k_\xi)^2 \Delta'}{\Delta^2 + \eta \left[ 2(k_\xi)^2 + \eta \right]} \right\} = \tan^{-1} \left\{ \frac{2(k_\xi)^2 \Delta'}{4 + 2(k_\xi)^2 \eta} \right\}. \right.
\] (33)
In light of Eq. (5) for the variance this identity is expressed as

\[
\left[ \frac{\pi}{2} - \tan^{-1}\left(\frac{\eta}{\Delta'}\right) \right]_x = \tan^{-1}\left[ \frac{2(k\xi)^2\Delta'}{4 + 2(k\xi)^2\eta_i} \right] \Rightarrow \\
\frac{2(k\xi)^2\Delta'}{4 + 2(k\xi)^2\eta_i} = \tan\psi(x), \quad \psi(x) = \left[ \frac{\pi}{2} - \tan^{-1}\left(\frac{\eta_i/\Delta'}{\eta_i}\right) \right]_x.
\] (34)

The above equation leads to an explicit expression for the mode amplitude in terms of the random variate \(x\), i.e.,

\[
(k\xi)^2 = \frac{2\tan\psi(x)}{\Delta' - \eta_i\tan\psi(x)}.
\] (35)

5. Conclusions and Discussion

Spartan random fields, introduced in [8], provide compact and computationally fast models of spatial dependence with potential applications in environmental and geophysical processes, mining exploration, image analysis, and materials structure characterization. In [8] we have shown how to determine the parameters of Spartan fields from the available sample using synthetic data. We show here how to simulate Spartan random fields with a Gaussian energy functional on the square lattice and for irregular distributions of field locations in two dimensions. For the lattice calculations, we use a very fast algorithm based on the Fast Fourier Transform. For irregular distributions, we present a method based on the superposition of harmonic modes with frequencies distributed according to the covariance spectral density. This
may not be the most efficient numerical choice, as fast methods, e.g., based on the Radon space transform [3,4] can also be implemented. However, in this case one has to trade computational speed for numerical artifacts (e.g., spurious linear features). The methods presented here can be extended to higher dimensions and different lattice structures. Anisotropic spatial distributions can be handled by introducing directional coefficients for the gradient and curvature terms. Alternatively, it is possible, at least in principle, to transform the initial distribution into an isotropic one. For differentiable random fields, one can use the method proposed in [7] to determine the parameters of the transformation.

Further research is required to establish whether the parameter inference procedure is stable if the data are contaminated with random (uncorrelated) noise, and to validate the Spartan models with real data sets. Estimation of the field values at non-sampled locations, briefly discussed in [8], also requires further investigation. Another issue of practical importance is the development of methods for constrained simulation. Spartan random fields provide explicit and numerically efficient expressions for the energy functional, and they are thus ideal for constrained simulations based on simulated annealing techniques. Finally, extensions to non-Gaussian Spartan random fields are also possible and will be necessary for modeling data with heavy tails.
6. References


7. **Figure Captions**

Figure 1: Plot of the covariance spectral density for negative values of the shape coefficient.

Figure 2: Plot of the standard deviation as a function of the shape coefficient for \( \eta_0 = 1 \) using the Eq. (5).

Figure 3: Plot of a spectral density symmetric around zero (top). The same spectral density is plotted using the DFT frequency counting scheme (bottom). The horizontal axis (frequency) is in multiples of the frequency increment \( \pi/10 \).

Figure 4: Simulation of a Spartan random field with coefficients \( \eta_0 = 1 \), \( \eta_1 = 0.2 \) and \( \xi = 5 \) on a square lattice with \( L = 800 \).

Figure 5: Simulation of a Spartan random field with coefficients \( \eta_0 = 3 \), \( \eta_1 = -0.2 \) and \( \xi = 50 \) on a square lattice with \( L = 800 \).

Figure 6: Plot of the covariance function of a Spartan random field with parameters \( \eta_1 = 0.2 \) and \( \xi = 5 \). The theoretical covariance (solid line) and two sample covariance functions obtained from a square lattice with \( L = 500 \) (+) and \( L = 800 \) (*) are shown.
Figure 1
Figure 2
Figure 3
Figure 4
Figure 6