Research Article

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Simulation of Gaussian random field in a ball

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Abstract: We address the problem of statistical simulation of a scalar real Gaussian random field inside the unit 3D ball. Two different methods are studied: (i) the method based on the known homogeneous isotropic power spectrum developed by Meschede and Romanowicz [M. Meschede and B. Romanowicz, Non-stationary spherical random media and their effect on long-period mantle waves, *Geophys. J. Int.* **203** (2015), 1605–1625] and (ii) the method based on known radial and angular covariance functions suggested in this work. The first approach allows the extension of the simulation technique to the inhomogeneous or anisotropic case. However, the disadvantage of this approach is the lack of accurate statistical characterization of the results. The accuracy of considered methods is illustrated by numerical tests, including a comparison of the estimated and analytical covariance functions. These methods can be used in many applications in geophysics, geodynamics, or planetary science where the objective is to construct spatial realizations of 3D random fields based on a statistical analysis of observations collected on the sphere or within a spherical region.

Keywords: Random fields, spherical harmonics

MSC 2010: 65C05, 65C20, 86-08

1 Introduction

This paper is devoted to the modeling of spatially inhomogeneous objects with the shape of a ball. For example, this work can be used in planetary sciences or studies focusing on the 3D thermochemical structure of the Earth’s mantle. The geophysical and geochemical data suggest that the Earth’s mantle contains heterogeneities on a broad range of scales: from thousands of km down to the grain size [19]. The stochastic mantle heterogeneity can be attributed to thermal and chemical variations due to mantle convection and melting processes [3, 4]. As a rule, due to the complex nature of physical processes and the lack of measurement data, a fully deterministic description of the problem is impossible. Therefore, efficient statistical modeling methods are required for a better understanding of the formation and preservation of the 3D planetary heterogeneity. This approach involves generating a statistical ensemble of realizations instead of a single deterministic solution. This allows, for example, to estimate the confidence intervals of the desired characteristics, as well as to perform uncertainty quantification and sensitivity analyzes [11, 21].

Over the past decade, a wide range of mathematical techniques based on the Schoenberg representation of the covariance function has been developed for modeling homogeneous isotropic random fields on a spherical surface (e.g., [5, 6]). For example, the correlation structure of the Laplace equation solution in a ball with boundary conditions defined by the isotropic random field on the sphere was studied in [15]. Nevertheless, volumetric modeling in a ball (full-sphere) is not well covered. To the best of our knowledge in the scientific literature, this subject is mostly restricted by the isotropic homogeneous case [10, 22].

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Meschede and Romanowicz [12] extended the random field simulation technique to the non-homogeneous distribution along the radius using the Karhunen–Loève expansion. However, in our opinion, the disadvantage of this approach is the difficulty of a rigorous mathematical description of the simulated random field. In the presented work, we develop an alternative method for modeling a random field in a ball [7]. Below, we describe in detail the methods of statistical modeling, their testing, and qualitative comparison.

2 Statistical modeling

2.1 Modeling Gaussian random fields in Cartesian coordinates

Gaussian random fields are fully determined by the mean values and covariance function, which in the real case has form

\[ C(x, y) = E[(f(x) - E[f(x)])(f(y) - E[f(y)])], \quad x, y \in \mathbb{R}^3. \]

Here and below in this work, we use bold font for vectors and matrices. Moreover, \( E \) denotes the mathematical expectation, \( f(x) \) and \( f(y) \) are values of random field realization at the coordinates defined by the vectors \( x \) and \( y \), respectively. Further in this work, we deal with zero mean random fields.

In the homogeneous case, the covariance function depends only on the distance between the considered points:

\[ C(x, y) = C(|x - y|) = C(d). \]

The covariance of the isotropic random field does not depend on the orientation of the vector \( d \):

\[ C(d) = C(d), \quad d = |d|. \]

In the homogeneous case, an important characteristic of a random field is the power spectrum \( S(k) \), which is related to the covariance function through the Fourier transform [1, 12]:

\[ S(k) = \int_{\mathbb{R}^3} C(d) e^{-i k \cdot d} d d, \]

where \( k \) is a wave vector and \( k \cdot d \) indicates the scalar product.

Spectral methods using \( S(k) \) are among the most popular for homogeneous random fields simulation in Cartesian coordinates (e.g., [13]) and on a spherical surface [10].

In the case when the values of the random field \( f(x) \) should be generated in the finite number of fixed spatial points, the traditional approach to simulate the realizations is based on the Cholesky decomposition of the covariance matrix \( C \) (see [14]):

\[ C = LL^T, \quad f = L \xi, \quad (2.1) \]

where \( \xi \) is a vector of mutually independent random numbers with zero mean and unit variance, and \( L^T \) is the transpose of the lower triangular matrix \( L \).

Another approach to statistical modeling uses the Karhunen–Loève expansion [9]:

\[ C = V^T D V, \quad f = V^T \sqrt{D} \xi, \quad (2.2) \]

where \( D \) and \( V \) are a diagonal matrix of eigenvalues and a matrix whose columns are the corresponding eigenvectors of the covariance matrix, respectively. In the truncated Karhunen–Loève expansion, only the eigenvectors corresponding to significant eigenvalues are considered.

Equations (2.1) and (2.2) can also be applied to simulate inhomogeneous random fields. However, in practice, the size of the matrix \( C \) is often too large, and decomposition in these equations is computationally consuming due to the need to perform the Cholesky decomposition or to solve the eigenvalues problem in a high dimension. In application to simulation of the 3D random field in a ball, Meschede and Romanowicz [12] suggested to apply the Karhunen–Loève expansion only in the radial direction to avoid this numerical problem.
2.2 2D random fields on the sphere

This subsection is devoted to the modeling of isotropic random fields on the surface of a sphere. Consider the unit sphere \( S^2 = \{ \mathbf{x} \in \mathbb{R}^3 : |\mathbf{x}| = 1 \} \). A basis formed by spherical harmonic functions (see [8])

\[
Y_n^k(\phi, \theta) = \frac{2n + 1}{4\pi} \frac{(n - k)!}{(n + k)!} P_n^k(\cos(\theta)) e^{ik\phi}
\]

is used to describe such random fields. Here \( P_n^k \) are associated Legendre functions, where \( n \) and \( k \) are the degree and order of spherical harmonics, respectively, such as \( n \geq 0, -n \leq k \leq n, 0 \leq \phi < 2\pi \) is the longitude, and \( 0 \leq \theta \leq \pi \) is the colatitude. The \( S^2 \) metric is the geodesic distance which defines the distance between points \( \mathbf{x} \) and \( \mathbf{y} \) as the angle

\[
\alpha = \arccos(\mathbf{x} \cdot \mathbf{y}),
\]

where

\[
\mathbf{x} = (\cos(\phi_x) \sin(\theta_x), \sin(\phi_x) \sin(\theta_x), \cos(\theta_x)), \\
\mathbf{y} = (\cos(\phi_y) \sin(\theta_y), \sin(\phi_y) \sin(\theta_y), \cos(\theta_y)).
\]

Then any complex function \( f \in L^2(S^2) \) can be presented as

\[
f(\mathbf{x}) = f(\phi, \theta) = \sum_{n=0}^{\infty} \sum_{k=-n}^{n} f_n^k Y_n^k(\phi, \theta),
\]

where, due to the orthonormality of the basis of spherical harmonics coefficients, \( f_n^k \) has the form

\[
f_n^k = \frac{2\pi}{4\pi} \int_0^\pi \int_0^{2\pi} f(\phi, \theta) Y_n^k(\phi, \theta) \, d\theta \, d\phi.
\]

Here and below, the bar denotes the complex conjugate.

The spherical harmonics satisfy the important property for two arbitrary points on the spherical surface defined by the vectors \( \mathbf{x} \) and \( \mathbf{y} \):

\[
\frac{4\pi}{2n + 1} \sum_{k=-n}^{n} Y_n^k(\mathbf{x}) \overline{Y_n^k(\mathbf{y})} = P_n(\mathbf{x} \cdot \mathbf{y}), \quad \mathbf{x}, \mathbf{y} \in S^2,
\]

where \( P_n = P_n^0 \) is a Legendre polynomial.

We consider \( f(\mathbf{x}) \) as a real isotropic random field with zero mean on \( S^2 \). Then \( f(\mathbf{x}) \) is isotropic if the covariance at two points \( \mathbf{x} \) and \( \mathbf{y} \), i.e.

\[
\text{Cov}(f(\mathbf{x}), f(\mathbf{y})) = C_\alpha(a(\mathbf{x}, \mathbf{y})), \quad \mathbf{x}, \mathbf{y} \in S^2,
\]

is finite and depends only on the geodesic distance between them. Here \( a \) is an angle between points \( \mathbf{x}, \mathbf{y} \) on a sphere, i.e. \( \cos(a) = \mathbf{x} \cdot \mathbf{y} \).

According to the Schoenberg theorem [17], \( C_\alpha \) can be a covariance function of an isotropic random field on the sphere if and only if

\[
C_\alpha(a) = \sum_{n=0}^{\infty} a_n P_n \cos(a), \quad a \in [0, \pi], \tag{2.3}
\]

for some summable series of non-negative coefficients \( \{a_n\} \) (see [8]). A detailed survey of known functions and corresponding decompositions can be found, for example, in [8, 20]. In practice, the summation from 0 to a finite spherical harmonic degree number \( n_{max} \) is used in (2.3). The numerical realizations of the random field on the sphere can be obtained using the mathematical apparatus described in, e.g., [5, 6, 8].
2.3 Modeling a random field in a ball based on the known spectrum of an isotropic homogeneous random field

The isotropic random fields whose covariance function $C(d)$ is fully determined by the absolute value of the separation vector $d = |d|$ have a special place in geophysical applications. In the three-dimensional case, the positive definite covariance function of the isotropic homogeneous random field has the form (see [16, 22])

$$C(d) = \int_{0}^{\infty} f_{1/2}(kd) (kd)^{1/2} \Phi(k) \, dk,$$

where $k = |k|$, $f_{1/2}$ is the Bessel function of order $\frac{1}{2}$ (see [2]), and $\Phi(k)$ is any non-negative function.

To simulate a random field corresponding to the first modeling approach, we use the method described in [12]. The 3D spherical random field in a spherical coordinate system is represented in terms of spherical harmonics:

$$f(r, \phi, \theta) = \sum_{n=0}^{\infty} \sum_{k=-n}^{n} f_{n}^{k}(r) Y_{n}^{k} \phi(\phi, \theta).$$

(2.4)

The main idea of this approach is to find the coefficients $f_{n}^{k}(r)$, which allow for generating in spherical coordinates the isotropic homogeneous random field with spectrum $S(k)$ which corresponds to some covariance function $C(d)$ given in Cartesian coordinates.

The method developed by Meschede and Romanowicz [12] is based on the computation of the covariance matrix $C_n$ of spherical harmonic coefficients in (2.4). In the numerical implementation of this method, the summation in (2.4) is up to $n_{\text{max}}$. In this work, the medium is parameterized using $M$ spherical layers with constant thickness. The matrix $C_n$ is defined for radius values $r_i, i = 1, \ldots, M$. The elements of the matrix $C_n$ are determined for all pairs of spherical layers using a 3D spectrum $S(k)$ in Cartesian coordinates:

$$C_n(r_i, r_j) = \sum_{k=-n}^{n} \overline{f_n^{k}(r_i)} f_n^{k}(r_j) = \frac{4\pi}{(2n)!} \int_{0}^{\infty} S(k) j_n(kr_i) j_n(kr_j) k^2 \, dk,$$

(2.5)

where the $j_n$ are the spherical Bessel functions [2, 12].

Then the coefficients $f_{n}^{k}(r_i)$ for radius value $r_i$ have the form

$$f_{n}^{k}(r_i) = 2\sqrt{\pi} \sum_{j=1}^{M} D_{n}^{j} V_{n}^{j} s_{n,k}^{j},$$

where $D_{n}$ and $V_{n}$ are eigenvalues and eigenvectors, respectively, of the covariance matrix $C_n$ and $s_{n,k}^{j}$ are the mutually independent random numbers with zero mean and unit variance. Finally, (2.4) is used to generate random field realizations.

The computation of the covariance matrix $C_n$ in the radial direction (see (2.5)) is the key point of the presented statistical method. It allows to construct the spherical statistically homogeneous and isotropic random field. This matrix can be modified to introduce radial inhomogeneity and anisotropy of generated random fields [12]. Meschede and Romanowicz [12] suggested to extend this method to the anisotropic case by using the transformation

$$C_n^{\text{aniso}}(r, r') = C_n(r_i, r_j),$$

(2.6)

where

$$r_i = (1 + q) \frac{r}{2} + (1 - q) \frac{r'}{2},$$

$$r_j = (1 - q) \frac{r}{2} + (1 + q) \frac{r'}{2},$$

where $q > 1$ defines the layered and $q < 1$ the vertical structures of the model. This approach also allows the use of an inhomogeneous correlation matrix $C_n$ which should satisfy the condition of positive definiteness.
In addition, the matrix may change in different sub-regions. The disadvantage of this approach is that for such transformation it becomes difficult to estimate the angular distribution of the generated random field. Note that $C_n$ in (2.5) is not a covariance matrix $C$ of the simulated random field $f(x)$. Therefore, in the inhomogeneous or anisotropic case, the modeling of the random field with the given required positive definite $C$ is complicated.

2.4 Modeling a random field in a ball based on the known radial and angular covariance functions

In this subsection, we consider Gaussian random fields distributed in a 3D filled sphere (ball). The modeling approach is based on using the covariance function assumed proportional to the product of the radial and isotropic angular covariance functions (see [7])

$$C(x, y) = E\{f(x)f(y)\} \sim C_r(r_x, r_y)C_\alpha(\alpha).$$ (2.7)

Here $x$ and $y$ are a pair of points in spherical coordinates

$$x = (r_x \cos(\phi_x) \sin(\theta_x), r_x \sin(\phi_x) \sin(\theta_x), r_x \cos(\theta_x)),$$

$$y = (r_y \cos(\phi_y) \sin(\theta_y), r_y \sin(\phi_y) \sin(\theta_y), r_y \cos(\theta_y)),$$

$C_r$ is a covariance function in Cartesian coordinates, and $C_\alpha$ is a covariance function on a sphere that has the form (2.7) and

$$\alpha = \arccos\left(\frac{x \cdot y}{r_x r_y}\right).$$

This representation of the 3D covariance function with (2.7) allows a rigorous mathematical description of a radially inhomogeneous volumetric random field in a full sphere. In contrast to the statistical method developed by Meschede and Romanowicz [12], the angular distribution for the second method is explicitly described by the covariance function $C_\alpha$. Moreover, both the angular and radial covariance functions can be estimated based on regional or global geophysical observations.

The random field realizations $f(x)$ on a sphere can be generated using the spectral method developed in [8]. The simulation formula has the form

$$f(x) = \frac{1}{\sqrt{N}} \sum_{l=1}^{N} f_l(x).$$ (2.8)

The central limit theorem ensures that for a large number of realizations $N$ and independent identically distributed $f_l$, equation (2.8) generates a Gaussian random field.

Each realization of $f_l$ is generated according to the following algorithm:

- Generate an integer random number according to the distribution $a_n$ in (2.3):
  $$n_l \sim a_n.$$

- Generate an integer random number uniformly distributed in the interval $[-n_l, n_l]$:
  $$k_l \sim U[-n_l, n_l].$$

- The resulting formula for modeling $f_l$ is
  $$f_l(x) = 2\sqrt{\pi A} (\xi \text{Re}(Y^{k_l}_{n_l}(x)) + \eta \text{Im}(Y^{k_l}_{n_l}(x))),$$

where $\xi$ and $\eta$ are the mutually independent random numbers with zero mean and unit variance and

$$A = \sum_{0}^{n_{\max}} a_n.$$
For generalization to the three-dimensional case with covariance function defined by (2.7), we suggest a method based on the Cholesky decomposition of the radial covariance matrix $C_r = L_r L_t^T$ using (2.1) or the Karhunen–Loève expansion $C_r = V_t^T D_r V_r$ using (2.2). The matrix $C_r$ is defined by the values of the function $C_r$ in (2.7) for all pairs of radius values $r_i, i = 1, \ldots, M$.

The resulting simulation formula [7] is

$$f(r_i, \phi, \theta) = 2\sqrt{\pi A} \sqrt{N} \sum_{l=1}^{N} \left( \xi((r_i) \Re(Y_{nk}^l(\phi, \theta)) + \eta(r_i) \Im(Y_{nk}^l(\phi, \theta))) \right),$$

(2.9)

where

$$\xi = L_r \xi_0, \quad \eta = L_r \eta_0,$$

(2.10)

or

$$\xi = V_t^T \sqrt{D_r} \xi_0, \quad \eta = V_t^T \sqrt{D_r} \eta_0.$$

(2.11)

Here, $\xi_0, \eta_0$ are the vectors of mutually independent Gaussian random numbers with zero mean and unit variance. According to the central limit theorem, the summation over sufficiently large $N$ in (2.9) provides the Gaussian distribution of the simulated random field. The algorithm described above ensures the reproducing of the covariance function $C(x, y)$, which proves the positive definiteness of the product in (2.7).

### 3 Numerical results

In this section, we present the results of statistical modeling performed by the method described above.

#### 3.1 Statistical modeling based on a spectrum of random field

The first approach is based on the representation of the homogeneous isotropic random field in spherical coordinates [12, 22]. In this case, the main input is the spectrum $S(k)$ which should be proportional to the function $\Phi(k)/k^3$. In this subsection, we use the spectrum

$$\Phi(k) = \left( \frac{1}{2\pi} \right)^{\frac{3}{2}} \frac{\sigma^2 k^2 I^3}{(1 + k^2 I^2)^2}, \quad S(k) = \frac{8\pi \sigma^2 I^3}{(1 + k^2 I^2)^2},$$

(3.1)

related to the exponential covariance function

$$C_r(d) = C_r(r_x, r_y) = \sigma^2 \exp\left( -\frac{|r_x - r_y|}{I} \right),$$

(3.2)

where $\sigma$ is a standard deviation and $I$ is a correlation length of the random field.

To test the technique described in Section 2.3, we use the relation between the spherical covariance and the corresponding angular power spectrum

$$C(|x - x'|) = \sum_{n=0}^{n_{max}} C_n(r, r') P_n(\cos(\alpha))(n + 1)$$

(3.3)

based on the numerical estimation of $C_n$ by (2.5).

In Figure 1, we compare the covariance function $C$ calculated on the segment between points

$$\left( r_x = 0.5, \phi_x = \frac{\pi}{6}, \theta_x = \frac{\pi}{6} \right) \quad \text{and} \quad \left( r_y = 1, \phi_y = \frac{\pi}{2}, \theta_y = \frac{\pi}{2} \right).$$

In Figure 1, we compare the covariance function $C$ calculated by (3.3) and the analytical radial covariance function (3.2). We can see that curves presented in this figure for two different correlation lengths $I = 0.05$ and $I = 0.25$ practically coincide indicating the numerical accuracy of the method described above.
Further in this subsection, we restrict the numerical study to the case of radially homogeneous random fields. We first focus on the isotropic case for the first modeling approach. Later the anisotropy is introduced by stretching or squeezing the wavenumbers. In Section 2.3, we described a generalization of this technique to anisotropic and inhomogeneous cases [12]. The disadvantage of this approach is the difficulty of accurate statistical characterization of the resulting anisotropic and inhomogeneous random field.

In Figure 2, we present 3D realizations of a random field related to the spectrum (3.1) for two different correlation lengths $I$ of 0.05 and 0.25, respectively, and $\sigma = 1$. Figure 2 shows the effect of the parameter $I$ in (3.2). The colors are the values of the generated function $f$ normalized by one standard deviation. The average size of spatial inhomogeneities, characterized by the correlation length $I$, is obviously higher for the right plots.

In Figure 3, we present the realizations of an anisotropic random field (using covariance of spherical harmonic coefficients (2.6)) for the anisotropy parameter $q$ equal to 0.25 and 3, respectively (spectrum (3.1)). That figure demonstrates that varying the parameter $q$ makes it possible to simulate anisotropic random fields in the range from radial to angular distribution of inhomogeneities.
3.2 Statistical modeling based on radial and angular covariance functions

In this work, we consider the covariance function (2.7) employed in the second statistical method in the form

$$C(x, y) = \sigma^2 \frac{C_r(0)}{C_a(0)} C_a(a),$$

which ensures that the variance $\sigma^2$ is consistent with the first statistical method. We use the homogeneous radial exponential covariance function $C_r(d)$ (see (3.2)) and the angular covariance $C_a(a)$ which has the form (see [20])

$$C_a(a) = \sum_{n=0}^{\infty} \rho^n P_n(\cos(a)) = \frac{1}{\sqrt{1 - 2\rho \cos(a) + \rho^2}}, \quad a_n = \rho^n, \quad \rho \in (0, 1).$$

(3.4)

Here the coefficients $a_n$ define the spectrum [a_n] in (2.3).

To assess the accuracy of the method described in Section 2.4, we compare the covariance function $C$ obtained using (2.9)–(2.11), where $C_r$ and $C_a$ have the forms (3.2) and (3.4), respectively. Figure 4 shows a good agreement between the estimated and analytic curves for two different combinations of the parameters $I$ and $\rho$. The testing geometry is the same as specified for the first modeling method in Figure 1. The covariance function estimated based on spatial realizations coincides with the analytical curve. It confirms that the numerical realizations accurately reproduce the assumed statistical model. These results confirm the numerical accuracy of the method described in Section 2.4.

In Figure 5, we illustrate 3D realizations of a random field for $I = 0.2, \rho = 0.8$ and $\rho = 0.98$. In Figure 6, we present 3D realizations of a random field for $I = 0.05, \rho = 0.8$ and $\rho = 0.98$. Comparison of Figures 5 and 6 demonstrates the radial influence of the parameter $I$. Comparison of left and right plots in Figures 5 and 6 demonstrate the angular influence of the parameter $\rho$. In particular, it can be seen that an increase in the value of $I$ and a decrease in $\rho$ leads to an increase in the characteristic spatial dimensions of the inhomogeneity in the radial and angular directions, respectively. Figures 5 and 6 show that the tuning of the parameters of the second modeling method also allows for generating anisotropic random fields.

Figures 5 and 6 were generated using (2.9) and (2.11). The summation in (2.11) was carried out for the eigenvectors $v_i$ corresponding to the largest eigenvalues $\lambda_i$ of $M_1$ consisting up to 95% of the trace of the covariance matrix $C_r$:$$\xi = \sum_{i=1}^{M_1} \sqrt{\lambda_i} v_i \xi_i.$$
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Figure 4: 2D cross-sections for $l = 0.25$ and $\rho = 0.9$ (left plot) and $l = 0.05$ and $\rho = 0.6$ (right plot).

Figure 5: The realizations of random field related to the second modeling method for $l = 0.2$ and $\rho = 0.98$ (left plot) and $\rho = 0.8$ (right plot). The color scale is in the values of the standard deviation (std).

where $\{v_i\}$ are the eigenvectors corresponding to $\{\lambda_i\}$ and $\{\xi_i\}$ are independent standard Gaussian random values.

The visual comparison shows the qualitatively different behavior of the two considered modeling approaches. On the other hand, both approaches allow generating a rather wide family of statistical models for the distribution of the required parameters in the ball.

### 4 Conclusion

We propose a new method for statistical modeling of a 3D scalar real Gaussian inhomogeneous random field in a unit ball. A numerical method for generating realizations of the corresponding random fields has been developed and tested. This approach is compared to the statistical model suggested by Meschede and Romanowicz [12]. In the present work, we do not conclude which approach is better to describe real data and focus more on theoretical development and numerical examples. A comparison of random fields’ realizations is performed in Section 3. The results presented in Figures 2, 3, 5 and 6 show that two considered statistical techniques generate qualitatively different spatial realizations.
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The new statistical modeling method imposes strict conditions on the form of the covariance function (see (2.7)). On the other hand, this approach allows a rigorous mathematical description of the simulated random field in an angular direction even in the inhomogeneous case. Both methods have shown high computational accuracy when testing based on reproducing specified covariance functions. The first modeling method is more computationally difficult for a high-resolution model because of the need to evaluate numerically the integral equation (2.5) a large number of times. In turn, the second method requires much fewer computation resources.

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