Algorithms for Gaussian random field generation

Géraldine Pichot

informatics mathematics

Algorithms for Gaussian random field generation

Géraldine Pichot

TECHNICAL REPORT

N° 484

December 13, 2017

Project-Team SERENA

ISSN 0249-0803 ISRN INRIA/RT--484--FR+ENG

Algorithms for Gaussian random field generation

Géraldine Pichot

Project-Team SERENA

Technical Report n° 484 — December 13, 2017 — 13 pages

Abstract: Natural permeability fields are classically modeled by a second-order stationary field which is a lognormal distribution, with an isotropic exponential correlation function. In this technical report, we expose the algorithms to generate Gaussian random fields. In particular, the algorithms based on the Circulant Embedding methods are given.

Key-words: Gaussian Random Fields, Circulant Embedding method

RESEARCH CENTRE
PARIS – ROCQUENCOURT

Domaine de Voluceau, - Rocquencourt
B.P. 105 - 78153 Le Chesnay Cedex

Algorithmes pour la génération de champs aléatoires gaussiens

Résumé : Dans les milieux souterrains, les champs de perméabilité sont classiquement modélisés par des champs aléatoires. Ces champs ont classiquement une distribution log-normale de fonction de corrélation exponentielle. Dans ce rapport technique, nous exposons les algorithmes pour générer de tels champs. En particulier, nous exposons les algorithmes basés sur la méthode de "Circulant Embedding".

Mots-clés : Champs aléatoires gaussiens, méthode de "Circulant Embedding"

1 Basics

Let Ω be a domain of $\mathbb{R}^d$.

1.1 Definitions

Definition 1 **A random field** *is a collection of random variables* $\{Y(\mathbf{x})\}_{\mathbf{x}\in\Omega}$ *defined on a multidimensional domain* $\Omega \in \mathbb{R}^d$.

Definition 2 $\{Y(\mathbf{x})\}_{\mathbf{x}\in\Omega}$ *is called* **a (real) Gaussian random field** *if*

$\forall n \in \mathbb{N}\backslash\{0\}, \forall \mathbf{x}_1, \dots, \mathbf{x}_N \in \Omega,$ *the random vector* $(Y(\mathbf{x}_1), \dots, Y(\mathbf{x}_n))$ *is Gaussian.*

Remark 3 $\forall \mathbf{x} \in \Omega$, *the random variable* $Y(\mathbf{x})$ *is Gaussian with mean*

$$m(\mathbf{x}) := \mathbb{E}[Y(\mathbf{x})]$$

and with autocovariance function

$$Cov[Y(\mathbf{x}), Y(\mathbf{x}')] := \mathbb{E}[(Y(\mathbf{x}) - m(\mathbf{x}))(Y(\mathbf{x}') - m(\mathbf{x}')], \textit{ for } \mathbf{x}, \mathbf{x}' \in \Omega$$

Properties 4

1st order stationarity: $\exists \mu \in \mathbb{R}, \forall \mathbf{x} \in \Omega, m(\mathbf{x}) = \mu$

2nd order stationarity: *1st order stationarity + the autocovariance function* $Cov[Y(\mathbf{x}), Y(\mathbf{x}')]$ *is a function of only the difference* $\mathbf{h} = \mathbf{x} - \mathbf{x}'$:

$$Cov[Y(\mathbf{x}), Y(\mathbf{x}')] = C(\mathbf{h})$$

Remark 5 *If* $\{Y(\mathbf{x})\}_{\mathbf{x}\in\Omega}$ *is a 2nd order stationary Gaussian field with mean* 0 *and autocovariance function* $C(\mathbf{h})$, $m + \sigma Y(\mathbf{x})$ *is a 2nd order stationary Gaussian field with mean* m *and autocovariance function* $\sigma * C(\mathbf{h})$.

1.2 Examples of autocovariance functions

1. **Exponential covariance (separable):** $C_E(\mathbf{h}) = e^{-\sum_{k=1}^{d} \frac{|h_k|}{\lambda_k}}$

2. **Exponential covariance (non separable):** $C_{Ens}(\mathbf{h}) = e^{-\sqrt{\sum_{k=1}^{d} \frac{h_k^2}{\lambda_k^2}}}$

3. **Gaussian covariance:** $C_G(\mathbf{h}) = e^{-\sum_{k=1}^{d} \frac{h_k^2}{\lambda_k^2}}$

$\boldsymbol{\lambda} = (\lambda_k)_k$ is the correlation length vector. Remark that

$$Cov[Y(\mathbf{x}), Y(\mathbf{x})] = Var[Y(\mathbf{x})] = \mathbb{E}[Y(\mathbf{x})^2] = C(0) = 1.$$

1.3 Covariance matrix

We discretize Ω over a regular grid composed of $N_\Omega + 1$ equally spaced points. Let us considered the discrete representation of $\{Y(\mathbf{x})\}_{\mathbf{x}\in\Omega}$ as $\mathbf{Y} = \{Y_i\}_{i=0,\dots,N_\Omega}$ with $Y_i = Y(\mathbf{x}_i)$, $\mathbf{x}_i \in \Omega$. The random variables Y_i are a gaussian with covariance matrix $\mathbf{R} = (R_{jk})_{0\le j,k\le N}$ such as:

$$R_{jk} := Cov[Y_j, Y_k].$$

For a 2nd order stationary Gaussian field $\{Y(\mathbf{x})\}_{\mathbf{x}\in\Omega}$ with mean 0 and autocovariance function $C(\mathbf{h})$:

$$R_{jk} = C(|\mathbf{x}_j - \mathbf{x}_k|) = \mathbb{E}[Y_j\, Y_k].$$

The sampled autocovariance function over the grid is defined as:

$$c_i := Cov[Y_0, Y_i] = \mathbb{E}[Y_0\, Y_i] = C(|x_i - x_0|)$$

with $i = 0, 1, \dots, N_\Omega$.

Let us give the expression of the matrix $\mathbf{R}$ for a 2nd order stationary Gaussian field with mean 0 and autocovariance function $C(\mathbf{h})$ in dimension 1, 2 and 3.

In one dimension:

Let Ω be discretized over a regular grid composed of $N + 1$ equally spaced points $x_0, x_1, \dots, x_N$.

The covariance matrix in 1D of order $(N + 1)^2$, $\mathbf{R}_1$, writes:

$$\mathbf{R}_1 = \begin{pmatrix} c_0 & c_1 & . & . & . & c_{N-1} & c_N \\ c_1 & c_0 & c_1 & . & . & . & c_{N-1} \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ c_{N-1} & . & . & . & c_1 & c_0 & c_1 \\ c_N & c_{N-1} & . & . & . & c_1 & c_0 \end{pmatrix}$$

In two dimension:

Let Ω be discretized over a regular grid composed of $(N+1)*(M+1)$ equally spaced points $\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_{(N+1)(M+1)-1}$.

The covariance matrix in 2D of order $((N + 1) * (M + 1))^2$, $\mathbf{R}_2$, writes:

$$\mathbf{R}_2 = \begin{pmatrix} [\mathbf{R}_1]_{00} & \dots & [\mathbf{R}_1^*]_{0M} \\ \vdots & \ddots & \vdots \\ [\mathbf{R}_1^*]_{M0} & \dots & [\mathbf{R}_1]_{MM} \end{pmatrix}$$

with $[\mathbf{R}_1]_{ii}$ the autocovariance matrix of size $(N + 1)^2$ of the variables over the line i of the grid (same matrix as in 1D) and $[\mathbf{R}_1^*]_{ij}$ the covariance matrix of size $(N + 1)^2$ of the variables between the line i and the line j of the grid.

In three dimension:

Let Ω be discretized over a regular grid composed of $(N+1)*(M+1)*(K+1))$ equally spaced points $\mathbf{x}_0, \mathbf{x}_1, \ldots, \mathbf{x}_{(N+1)(M+1)(K+1)-1}$.

The covariance matrix in 3D of order $((N+1)(M+1)(K+1))^2$, $\mathbf{R}_3$, writes:

$$\mathbf{R}_3 = \begin{pmatrix} [\mathbf{R}_2]_{00} & \ldots & [\mathbf{R}_2^*]_{0K} \\ \vdots & \ddots & \vdots \\ [\mathbf{R}_2^*]_{K0} & \ldots & [\mathbf{R}_2]_{KK} \end{pmatrix}$$

with $[\mathbf{R}_2]_{ii}$ the autocovariance matrix of size $((N+1)*(M+1))^2$ of the variables over the plane i of the grid (same matrix as in 2D) and $[\mathbf{R}_2^*]_{ij}$ the covariance matrix of size $((N+1)*(M+1))^2$ of the variables between the plane i and the plane j of the grid.

Remark 6 *A Gaussian field* $\mathbf{Y}$ *is entirely determined by its mean and its autocovariance function* $\mathbf{C}(\mathbf{h})$ *or equivalently by its mean and its covariance matrix* $\mathbf{R}$.

2 General algorithm for random field generation

If $\mathbf{C}(\mathbf{h})$ is a valid autocovariance function , $\mathbf{R}$ is a symmetric positive definite Toeplitz (diagonal-constant) matrix.

To generate a realization of the random vector $\mathbf{Y}$ of normal variables with zero mean and autocovariance matrix $\mathbf{R}$, algorithm 1 is used.

Algorithm 1 General algorithm

1: Factorize $\mathbf{R} = \mathbf{B}\mathbf{B}^T$
2: Generate a vector $\boldsymbol{\theta} = (\theta_0, \theta_1 \ldots \theta_N)^T$ of realizations of random normal variables with zero mean $\boldsymbol{\mu_\theta} = (0, 0, \ldots, 0)^T$ and uncorrelated: $\mathbf{R}_\theta = \mathbb{E}[\boldsymbol{\theta}\boldsymbol{\theta}^T] = \mathbf{Id}_N$
3: One realization is obtained by computing $\mathbf{Y} = \mathbf{B}\boldsymbol{\theta}$

Using Algorithm 1, $\mathbf{Y}$ has $\mathbf{R}$ as autocovariance matrix:

$$\mathbb{E}[\mathbf{Y}\mathbf{Y}^T] = \mathbb{E}[(\mathbf{B}\boldsymbol{\theta})(\mathbf{B}\boldsymbol{\theta})^T] = \mathbf{B}\mathbb{E}[\boldsymbol{\theta}\boldsymbol{\theta}^T]\mathbf{B}^T = \mathbf{B}\mathbf{B}^T = \mathbf{R}.$$

Algorithm 1 requires the generation of $N+1$ random normal variates.

From the first step of Algorithm 1, we must find a factorization of the covariance matrix $\mathbf{R}$. Cholesky factorization $\mathbf{R} = \mathbf{L}\mathbf{L}^T$ or eigenvalue decomposition $\mathbf{R} = \mathbf{V}\boldsymbol{\Delta}\mathbf{V}^T = (\mathbf{V}\sqrt{\boldsymbol{\Delta}})(\mathbf{V}\sqrt{\boldsymbol{\Delta}})^T$ are quite expensive for large N. Moreover the matrix $\mathbf{R}$ can be ill-conditioned, implying numerical difficulties. An alternative is to use the circulant embedding approach.

3 Circulant embedding method

For the sake of simplicity, we restrict the presentation to the dimension one.

3.1 General principle

Let $\mathbf{a} = (c_0, \ldots, c_N, c_{N-1}, \ldots, c_1) \in \mathbb{R}^{2N}$. Based on cyclic permutations of the vector $\mathbf{a}$, we define the circulant matrix $\mathbf{A} = \mathrm{circ}(\mathbf{a})$ as a circulant embedding of the covariance matrix $\mathbf{R}_1$. The matrix $\mathbf{A}$ is real symmetric of size $2N$ and is spd if N is large enough.

Example with $N = 4$:

$$\mathbf{A} = \begin{pmatrix} c_0 & c_1 & c_2 & c_3 & c_4 & c_3 & c_2 & c_1 \\ c_1 & c_0 & c_1 & c_2 & c_3 & c_4 & c_3 & c_2 \\ c_2 & c_1 & c_0 & c_1 & c_2 & c_3 & c_4 & c_3 \\ c_3 & c_2 & c_1 & c_0 & c_1 & c_2 & c_3 & c_4 \\ c_4 & c_3 & c_2 & c_1 & c_0 & c_1 & c_2 & c_3 \\ c_3 & c_4 & c_3 & c_2 & c_1 & c_0 & c_1 & c_2 \\ c_2 & c_3 & c_4 & c_3 & c_2 & c_1 & c_0 & c_1 \\ c_1 & c_2 & c_3 & c_4 & c_3 & c_2 & c_1 & c_0 \end{pmatrix}$$

Circulant matrices are diagonalized by a discrete Fourier transform.

The Discrete Fourier Transform for vector of size $2N$ is given by the $(2N)^2$ matrix $\mathbf{F}$ defined as $\mathbf{F} = (\beta^{kj})_{0 \le j,k \le 2N-1}, \beta = e^{-2i\pi/2N} = e^{-i\pi/N}$:

$$\mathbf{F} = \begin{pmatrix} 1 & 1 & 1 & \ldots & 1 \\ 1 & \beta & \beta^2 & \ldots & \beta^{(2N-1)} \\ \ldots & \ldots & \ldots & \ldots & \\ 1 & \beta^{2N-1} & \beta^{2(2N-1)} & \ldots & \beta^{(2N-1)^2} \end{pmatrix}$$

Properties:

- $\mathbf{F}$ is a unitary matrix multiplied by a factor $2N$: $\mathbf{F}\mathbf{F}^* = 2N\,\mathbf{Id}_{2N}$
- $\mathbf{F}$ is symmetric: $\mathbf{F}^* = \overline{\mathbf{F}}^T = \overline{\mathbf{F^T}} = \overline{\mathbf{F}}$
- Inverse Discrete Fourier Transform: $\mathbf{F}^{-1} = \frac{1}{2N}\mathbf{F}^* = \frac{1}{2N}\overline{\mathbf{F}}$

We denote $\mathbf{F}_1$ and $\mathbf{F}_2$ the real and imaginary matrices of $\mathbf{F}$ so that: $\mathbf{F} = \mathbf{F}_1 + i\mathbf{F}_2$. As $\mathbf{F}$ is symmetric so are $\mathbf{F}_1$ and $\mathbf{F}_2$.

The Fourier matrix contains the eigenvectors of circulant matrices. Then

$$\mathbf{A} = \mathbf{F}^{-1}\mathbf{D}\mathbf{F} = \frac{1}{2N}\overline{\mathbf{F}}\mathbf{D}\mathbf{F}.$$

The matrix $\mathbf{D}$ is a diagonal matrix whose elements on the diagonal are the eigenvalues s_i of $\mathbf{A}$. If we multiply the previous expression by $\mathbf{F}$, we obtain:

$$\mathbf{F}\mathbf{A} = \mathbf{D}\mathbf{F}.$$

The first row of $\mathbf{F}$ is a vector full of one of size $2N$ and the first row of $\mathbf{A}$ is the vector $\mathbf{a}$, then the eigenvalues $\mathbf{s} = (s_j)_{0 \le j \le 2N}$ are given by:

$$s = \mathbf{F}\mathbf{a}.$$

This computation can be done quickly with a FFT algorithm.

The eigenvalue s_j is expressed as:

$$\begin{aligned} s_j &= \sum_{k=0}^{2N-1} c_k\, e^{-\frac{j\, i\pi\, k}{N}} \\ &= c_0 + \sum_{k=1}^{N-1} c_k\, e^{-\frac{j\, i\pi\, k}{N}} + c_N\, e^{-j\, i\pi} + \sum_{k=N+1}^{2N-1} c_k\, e^{-\frac{j\, i\pi\, k}{N}} \\ &= c_0 + \sum_{k=1}^{N-1} c_k\, e^{-\frac{j\, i\pi\, k}{N}} + c_N\, e^{-j\, i\pi} + \sum_{k=1}^{N-1} c_{2N-k}\, e^{-\frac{j\, i\pi\, (2N-k)}{N}} \end{aligned}$$

As $e^{-\frac{j\, i\pi\, (2N-k)}{N}} = e^{\frac{j\, i\pi\, k}{N}}$ and $c_{2N-k} = c_k,\ k = 1, \ldots, N-1$,

$$s_j = c_0 + 2 \sum_{k=1}^{N-1} c_k\, cos(\frac{j\, \pi\, k}{N}) + c_N\, (-1)^j$$

Then the eigenvalues $s_j, 0 \leq j \leq 2N$ are real. Moreover $s_{2N-k} = s_k,\ k = 1, \ldots, N-1$.

In terms of $\mathbf{F}_1$ and $\mathbf{F}_2$ the matrix $\mathbf{A}$ writes:

$$\begin{aligned} \mathbf{A} &= \frac{1}{2N}(\mathbf{F}_1 - i\mathbf{F}_2)\mathbf{D}(\mathbf{F}_1 + i\mathbf{F}_2) \\ &= \frac{1}{2N}(\mathbf{F}_1\, \mathbf{D}\mathbf{F}_1 + \mathbf{F}_2\, \mathbf{D}\mathbf{F}_2 + i(\mathbf{F}_1\, \mathbf{D}\mathbf{F}_2 - \mathbf{F}_2\, \mathbf{D}\mathbf{F}_1)) \end{aligned}$$

The matrix $\mathbf{A}$ is real, then:

$$\mathbf{F}_1\, \mathbf{D}\mathbf{F}_2 - \mathbf{F}_2\, \mathbf{D}\mathbf{F}_1 = 0 \tag{1}$$

$$\mathbf{A} = \frac{1}{2N}(\mathbf{F}_1\, \mathbf{D}\mathbf{F}_1 + \mathbf{F}_2\, \mathbf{D}\mathbf{F}_2) \tag{2}$$

and

The component (kl) of the matrix $\mathbf{A}$ is then:

$$\begin{aligned} (\mathbf{A})_{kl} &= \frac{1}{2N}(\sum_{j=0}^{2N-1} cos(\frac{k\, \pi\, j}{N})\, s_j\, cos(\frac{l\, \pi\, j}{N}) + \sum_{j=0}^{2N-1} sin(\frac{k\, \pi\, j}{N})\, s_j\, sin(\frac{l\, \pi\, j}{N})) \\ &= \frac{1}{2N}(s_0 + cos(k\, \pi)\, cos(l\, \pi)\, s_N + 2\sum_{j=1}^{N-1} cos(\frac{k\, \pi\, j}{N})\, s_j\, cos(\frac{l\, \pi\, j}{N})) \\ &\quad + \frac{1}{2N}(2\sum_{j=1}^{N-1} sin(\frac{k\, \pi\, j}{N})\, s_j\, sin(\frac{l\, \pi\, j}{N})) \\ &= \frac{1}{2N}(s_0 + cos(k\, \pi)\, cos(l\, \pi)\, s_N + 2\sum_{j=1}^{N-1} cos(\frac{(k-l)\, \pi\, j}{N})\, s_j). \end{aligned} \tag{3}$$

Proposition 7 *If* $\mathbf{A}$ *is spd then* $\mathbf{A} = \mathbf{C}^*\mathbf{C}$ *with* $\mathbf{C} = \frac{1}{\sqrt{2N}}\mathbf{D}^{\frac{1}{2}}\mathbf{F}$. *If* $\mathbf{A}$ *is not spd,* $\mathbf{a}$ *can be completed by a padding or* N *can be increased.*

3.2 Standard algorithm of the circulant embedding method

From Algorithm 1, we can take $\mathbf{B} = \mathbf{C}^* = \frac{1}{\sqrt{2N}}\mathbf{F}^*\mathbf{D}^{\frac{1}{2}}$ together with a restriction over $0, \ldots, N$. Algorithm 2 is a standard algorithm of the circulant embedding method to generate two independent realizations $\mathbf{Y}_1$ and $\mathbf{Y}_2$ of Gaussian random discrete fields of size $N+1$ with zero mean and covariance matrix $\mathbf{R}$. This algorithm uses $4N$ standard normal random variates.The computation of $\mathbf{C}^*\boldsymbol{\theta}$ can be done quickly with a iFFT algorithm. This algorithm is presented in details for example in [1, 2].

Algorithm 2 Generation of two independent realizations $\mathbf{Y}_1$ and $\mathbf{Y}_2$ of Gaussian random fields of size $N+1$ with $4N$ standard normal random variates

1: Sample the autocovariance function: vector $\mathbf{c}$ and circulant vector $\mathbf{a}$
2: Compute $\mathbf{s} = \mathbf{Fa}$
3: Generate two realizations of standard normal random vectors of size $2N$ $\boldsymbol{\theta}^{re}$ and $\boldsymbol{\theta}^{im}$:
$$\boldsymbol{\theta} = \boldsymbol{\theta}^{re} + i\boldsymbol{\theta}^{im}$$
4: Apply iFFT to compute $\mathbf{C}^*\boldsymbol{\theta}$ with $\mathbf{C}^* = \frac{1}{\sqrt{2N}}\mathbf{F}^*\mathbf{D}^{\frac{1}{2}}$
5: Take
$$\mathbf{Y}_1 = (\mathbf{C}^*\boldsymbol{\theta})^{re}(0:N) \text{ and } \mathbf{Y}_2 = (\mathbf{C}^*\boldsymbol{\theta})^{im}(0:N)$$

Let us now check that we obtain the desired fields that is:

(C1) **Y1** and **Y2** are of zero mean: $\mathbb{E}[\mathbf{Y}_1] = \mathbf{0}$ and $\mathbb{E}[\mathbf{Y}_2] = \mathbf{0}$

(C2) The two random vectors $\mathbf{Y}_1$ and $\mathbf{Y}_2$ are independent i.e. the covariance matrix between $\mathbf{Y}_1$ and $\mathbf{Y}_2$ is zero: $Cov[\mathbf{Y}_1, \mathbf{Y}_2] = \mathbf{0}$

(C3) The covariance matrix of $\mathbf{Y}_1$ is $\mathbf{R}$ and the covariance matrix of $\mathbf{Y}_2$ is also $\mathbf{R}$.

First let us give the expressions of $\mathbf{C}^*\,\boldsymbol{\theta}$:

$$\begin{aligned}\mathbf{C}^*\,\boldsymbol{\theta} &= \frac{1}{\sqrt{2N}}(\mathbf{F_1} - i\mathbf{F_2})\mathbf{D}^{\frac{1}{2}}\,(\boldsymbol{\theta}^{re} + i\boldsymbol{\theta}^{im}) \\ &= \frac{1}{\sqrt{2N}}[(\mathbf{F_1}\mathbf{D}^{\frac{1}{2}}\boldsymbol{\theta}^{re} + \mathbf{F_2}\mathbf{D}^{\frac{1}{2}}\boldsymbol{\theta}^{im}) + i(\mathbf{F_1}\mathbf{D}^{\frac{1}{2}}\boldsymbol{\theta}^{im} - \mathbf{F_2}\mathbf{D}^{\frac{1}{2}}\boldsymbol{\theta}^{re})]\end{aligned}$$

Then:

$$\begin{aligned}\mathbf{Y}_1^f &= \frac{1}{\sqrt{2N}}(\mathbf{F_1}\mathbf{D}^{\frac{1}{2}}\boldsymbol{\theta}^{re} + \mathbf{F_2}\mathbf{D}^{\frac{1}{2}}\boldsymbol{\theta}^{im}) \\ \mathbf{Y}_2^f &= \frac{1}{\sqrt{2N}}(\mathbf{F_1}\mathbf{D}^{\frac{1}{2}}\boldsymbol{\theta}^{im} - \mathbf{F_2}\mathbf{D}^{\frac{1}{2}}\boldsymbol{\theta}^{re})\end{aligned}$$

We keep the first $N+1$ components to obtain the desired random vectors: $\mathbf{Y}_1 = \mathbf{Y}_1^f(0:N)$ and $\mathbf{Y}_2 = \mathbf{Y}_2^f(0:N)$.

The random variable k of $\mathbf{Y}_1$, for $k = 0, \ldots, N$, is:

$$
\begin{aligned}
(\mathbf{Y}_1)_k &= \frac{1}{\sqrt{2N}}[\sum_{j=0}^{2N-1} cos(\frac{jk\pi}{N})\sqrt{s_j}\,\theta_j^{re} + \sum_{j=0}^{2N-1} sin(\frac{jk\pi}{N})\sqrt{s_j}\,\theta_j^{im}] \\
&= \frac{1}{\sqrt{2N}}[\sqrt{s_0}\theta_0^{re} + \sum_{j=1}^{N-1} cos(\frac{jk\pi}{N})\sqrt{s_j}\,\theta_j^{re} + \sum_{j=N+1}^{2N-1} cos(\frac{jk\pi}{N})\sqrt{s_j}\,\theta_j^{re} + (-1)^k\sqrt{s_N}\theta_N^{re}] \\
&\quad + \frac{1}{\sqrt{2N}}[\sum_{j=1}^{N-1} sin(\frac{jk\pi}{N})\sqrt{s_j}\,\theta_j^{im} + \sum_{j=N+1}^{2N-1} sin(\frac{jk\pi}{N})\sqrt{s_j}\,\theta_j^{im}] \\
&= \frac{1}{\sqrt{2N}}[\sqrt{s_0}\theta_0^{re} + \sum_{j=1}^{N-1} cos(\frac{jk\pi}{N})\sqrt{s_j}\,\theta_j^{re} + \sum_{j=1}^{N-1} cos(\frac{jk\pi}{N})\sqrt{s_{2N-j}}\,\theta_{2N-j}^{re} + (-1)^k\sqrt{s_N}\theta_N^{re}] \\
&\quad + \frac{1}{\sqrt{2N}}[\sum_{j=1}^{N-1} sin(\frac{jk\pi}{N})\sqrt{s_j}\,\theta_j^{im} - \sum_{j=1}^{N-1} sin(\frac{jk\pi}{N})\sqrt{s_{2N-j}}\,\theta_{2N-j}^{im}]
\end{aligned}
$$

Since $s_{2N-j} = s_j$, $j = 1, \ldots, N-1$, we have:

$$
\begin{aligned}
(\mathbf{Y}_1)_k &= \frac{1}{\sqrt{2N}}[\sqrt{s_0}\theta_0^{re} + \sum_{j=1}^{N-1} cos(\frac{jk\pi}{N})\sqrt{s_j}\,(\theta_j^{re} + \theta_{2N-j}^{re}) + (-1)^k\sqrt{s_N}\theta_N^{re}] \\
&\quad + \frac{1}{\sqrt{2N}}[\sum_{j=1}^{N-1} sin(\frac{jk\pi}{N})\sqrt{s_j}\,(\theta_j^{im} - \theta_{2N-j}^{im})]
\end{aligned} \tag{4}
$$

Similarly, we derive the random variable k of $\mathbf{Y}_2$, for $k = 0, \ldots, N$, is:

$$
\begin{aligned}
(\mathbf{Y}_2)_k &= \frac{1}{\sqrt{2N}}[\sqrt{s_0}\theta_0^{im} + \sum_{j=1}^{N-1} cos(\frac{jk\pi}{N})\sqrt{s_j}\,(\theta_j^{im} + \theta_{2N-j}^{im}) + (-1)^k\sqrt{s_N}\theta_N^{im}] \\
&\quad - \frac{1}{\sqrt{2N}}[\sum_{j=1}^{N-1} sin(\frac{jk\pi}{N})\sqrt{s_j}\,(\theta_j^{re} - \theta_{2N-j}^{re})]
\end{aligned} \tag{5}
$$

Check of (C1) $\mathbb{E}[\mathbf{Y}_1] = \mathbf{0}$ and $\mathbb{E}[\mathbf{Y}_2] = \mathbf{0}$

From the linearity of the expectation operator and as θ_j^{re} and θ_j^{im} for $j = 0, \ldots, 2N-1$ are standard normal random variables, we have, for $k = 0, \ldots, N$:

$$
\begin{aligned}
\mathbb{E}[(\mathbf{Y_1})_k] &= \frac{1}{\sqrt{2N}}[\sqrt{s_0}\,\mathbb{E}[\theta_0^{re}] + \sum_{j=1}^{N-1} cos(\frac{jk\pi}{N})\sqrt{s_j}\,(\mathbb{E}[\theta_j^{re}] + \mathbb{E}[\theta_{2N-j}^{re}]) + (-1)^k\sqrt{s_N}\,\mathbb{E}[\theta_N^{re}]]. \\
&\quad + \frac{1}{\sqrt{2N}}[\sum_{j=1}^{N-1} sin(\frac{jk\pi}{N})\sqrt{s_j}\,(\mathbb{E}[\theta_j^{im}] - \mathbb{E}[\theta_{2N-j}^{im}])] = 0.
\end{aligned}
$$

Similarly, $\mathbb{E}[(\mathbf{Y_2})_k] = 0$.

Check of (C2) $Cov[\mathbf{Y1}, \mathbf{Y2}] = \mathbf{0}$

$$
\begin{aligned}
Cov[\mathbf{Y}_1^f, \mathbf{Y}_2^f] &= \mathbb{E}[\mathbf{Y}_1^f \mathbf{Y}_2^{f,T}] \\
&= \frac{1}{\sqrt{2N}} \mathbb{E}[(\mathbf{F_1} \mathbf{D}^{\frac{1}{2}} \boldsymbol{\theta}^{re} + \mathbf{F_2} \mathbf{D}^{\frac{1}{2}} \boldsymbol{\theta}^{im})(\mathbf{F_1} \mathbf{D}^{\frac{1}{2}} \boldsymbol{\theta}^{im} - \mathbf{F_2} \mathbf{D}^{\frac{1}{2}} \boldsymbol{\theta}^{re})^T] \\
&= \frac{1}{\sqrt{2N}} \mathbb{E}[\mathbf{F_1} \mathbf{D}^{\frac{1}{2}} \boldsymbol{\theta}^{re} \boldsymbol{\theta}^{im,T} \mathbf{D}^{\frac{1}{2}} \mathbf{F_1}] - \frac{1}{\sqrt{2N}} \mathbb{E}[\mathbf{F_1} \mathbf{D}^{\frac{1}{2}} \boldsymbol{\theta}^{re} \boldsymbol{\theta}^{re,T} \mathbf{D}^{\frac{1}{2}} \mathbf{F_2}] \\
&\quad + \tfrac{1}{\sqrt{2N}} \mathbb{E}[\mathbf{F_2} \mathbf{D}^{\frac{1}{2}} \boldsymbol{\theta}^{im} \boldsymbol{\theta}^{im,T} \mathbf{D}^{\frac{1}{2}} \mathbf{F_1}] - \tfrac{1}{\sqrt{2N}} \mathbb{E}[\mathbf{F_2} \mathbf{D}^{\frac{1}{2}} \boldsymbol{\theta}^{im} \boldsymbol{\theta}^{re,T} \mathbf{D}^{\frac{1}{2}} \mathbf{F_2}].
\end{aligned}
$$

By definition θ^{re} and θ^{im} are independent standard normal random vectors, then $\mathbb{E}[\theta^{re}\, \theta^{im,T}] = \mathbf{0}$ and $\mathbb{E}[\theta^{re}\, \theta^{re,T}] = \mathbf{Id}_{2N}$ and $\mathbb{E}[\theta^{im}\, \theta^{im,T}] = \mathbf{Id}_{2N}$, therefore using (1):

$$
Cov[\mathbf{Y}_1^f, \mathbf{Y}_2^f] = \frac{1}{\sqrt{2N}}[-\mathbf{F_1} \mathbf{D} \mathbf{F_2} + \mathbf{F_2} \mathbf{D} \mathbf{F_1}] = \mathbf{0}.
$$

Then it is also true for the restricted covariance matrix of order $N+1$: $Cov[\mathbf{Y1}, \mathbf{Y2}] = \mathbf{0}$.

Check of (C3) $Cov[\mathbf{Y}_1, \mathbf{Y}_1] = \mathbb{E}[\mathbf{Y}_1 \mathbf{Y}_1^T] = \mathbf{R}$ **and** $Cov[\mathbf{Y}_2, \mathbf{Y}_2] = \mathbb{E}[\mathbf{Y}_2 \mathbf{Y}_2^T] =$ **R.**

$$
\begin{aligned}
Cov[\mathbf{Y}_1^f, \mathbf{Y}_1^f] &= \mathbb{E}[\mathbf{Y}_1^f \mathbf{Y}_1^{f,T}] \\
&= \frac{1}{\sqrt{2N}}[(\mathbf{F_1} \mathbf{D}^{\frac{1}{2}} \boldsymbol{\theta}^{re} + \mathbf{F_2} \mathbf{D}^{\frac{1}{2}} \boldsymbol{\theta}^{im})(\mathbf{F_1} \mathbf{D}^{\frac{1}{2}} \boldsymbol{\theta}^{re} + \mathbf{F_2} \mathbf{D}^{\frac{1}{2}} \boldsymbol{\theta}^{im})^T] \\
&= \frac{1}{\sqrt{2N}} \mathbb{E}[\mathbf{F_1} \mathbf{D}^{\frac{1}{2}} \boldsymbol{\theta}^{re} \boldsymbol{\theta}^{re,T} \mathbf{D}^{\frac{1}{2}} \mathbf{F_1}] - \frac{1}{\sqrt{2N}} \mathbb{E}[\mathbf{F_1} \mathbf{D}^{\frac{1}{2}} \boldsymbol{\theta}^{re} \boldsymbol{\theta}^{im,T} \mathbf{D}^{\frac{1}{2}} \mathbf{F_2}] \\
&\quad + \tfrac{1}{\sqrt{2N}} \mathbb{E}[\mathbf{F_2} \mathbf{D}^{\frac{1}{2}} \boldsymbol{\theta}^{im} \boldsymbol{\theta}^{re,T} \mathbf{D}^{\frac{1}{2}} \mathbf{F_1}] - \tfrac{1}{\sqrt{2N}} \mathbb{E}[\mathbf{F_2} \mathbf{D}^{\frac{1}{2}} \boldsymbol{\theta}^{im} \boldsymbol{\theta}^{im,T} \mathbf{D}^{\frac{1}{2}} \mathbf{F_2}]. \\
&= \frac{1}{\sqrt{2N}}[\mathbf{F_1} \mathbf{D} \mathbf{F_1} + \mathbf{F_2} \mathbf{D} \mathbf{F_2}] = \mathbf{A} \text{ from (2)}
\end{aligned}
$$

The restricted matrix of order $N+1$ of $\mathbf{A}$ from 0 to N is exactly $\mathbf{R}$, then $Cov[\mathbf{Y}_1, \mathbf{Y}_1] = \mathbf{R}$. Simarly we show that $Cov[\mathbf{Y}_2, \mathbf{Y}_2] = \mathbf{R}$.

3.3 Two alternative algorithms to generate one real field

From the expression $(\mathbf{Y}_2)_k$ given by (5), we see that a a symmetry in the random vector $\boldsymbol{\theta}^{re}$ such as $\theta^{re}_{2N-j} = \theta^{re}_j$, $j = 1, \dots, N-1$ and the particular choices of $\theta^{im}_0 = 0$, $\theta^{im}_N = 0$ and $\theta^{im}_{2N-j} = -\theta^{im}_j$, $j = 1, \dots, N-1$ yields $\mathbf{Y}_2 = \mathbf{0}$. Then an algorithm can be derived to generate one realization of the real field $\mathbf{Y} = \mathbf{Y}_1$.

With these choices, the expression of $(\mathbf{Y}_1)_k$, for $k = 0, \dots, N$, is now:

$$
\begin{aligned}
(\mathbf{Y}_1)_k &= \frac{1}{\sqrt{2N}}[\sqrt{s_0}\theta_0^{re} + 2\sum_{j=1}^{N-1} cos(\frac{jk\pi}{N})\,\sqrt{s_j}\,\theta_j^{re} + (-1)^k \sqrt{s_N}\theta_N^{re}] \\
&\quad + \frac{1}{\sqrt{2N}}[2\sum_{j=1}^{N-1} sin(\frac{jk\pi}{N})\,\sqrt{s_j}\,\theta_j^{im}]
\end{aligned}
\tag{6}
$$

We still have $\mathbb{E}[\mathbf{Y}_1] = \mathbf{0}$ and as $\mathbb{E}[\theta_j^{re}\theta_k^{re}] = \mathbb{1}_{jk}$ and $\mathbb{E}[\theta_j^{re}\theta_k^{im}] = 0$ for all $j,k = 1,\dots N-1$:

$$\begin{aligned}
& Cov[(\mathbf{Y}_1)_k, (\mathbf{Y}_1)_l] = \mathbb{E}[(\mathbf{Y}_1)_k\,(\mathbf{Y}_1)_l] \\
= \; & \frac{1}{2N}\mathbb{E}[(\sqrt{s_0}\theta_0^{re} + 2\sum_{j=1}^{N-1} cos(\frac{jk\pi}{N})\,\sqrt{s_j}\,\theta_j^{re} + cos(k\,\pi)\sqrt{s_N}\theta_N^{re} + 2\sum_{j=1}^{N-1} sin(\frac{jk\pi}{N})\,\sqrt{s_j}\,\theta_j^{im}) \\
& *(\sqrt{s_0}\theta_0^{re} + 2\sum_{m=1}^{N-1} cos(\frac{ml\pi}{N})\,\sqrt{s_m}\,\theta_m^{re} + cos(l\,\pi)\sqrt{s_N}\theta_N^{re} + 2\sum_{m=1}^{N-1} sin(\frac{ml\pi}{N})\,\sqrt{s_m}\,\theta_m^{im})] \\
= \; & \frac{1}{2N}(s_0\mathbb{E}[(\theta_0^{re})^2] + s_N\mathbb{E}[(\theta_N^{re})^2]\,cos(k\pi)cos(l\,\pi)) \\
& +\frac{1}{2N}(4\sum_{j=1}^{N-1} cos(\frac{jk\pi}{N})\,cos(\frac{jl\pi}{N})\,s_j\,\mathbb{E}[(\theta_j^{re})^2]) \\
& +\frac{1}{2N}(4\sum_{j=1}^{N-1} sin(\frac{jk\pi}{N})\,sin(\frac{jl\pi}{N})\,s_j\,\mathbb{E}[(\theta_j^{im})^2])
\end{aligned}$$

By identification with $(\mathbf{A})_{kl}$ given by (3), the random vectors $\boldsymbol{\theta}^{re}$ and $\boldsymbol{\theta}^{im}$ must satisfy:

$$\mathbb{E}[(\theta_0^{re})^2] = 1,\; \mathbb{E}[(\theta_N^{re})^2] = 1,\; \mathbb{E}[(\theta_j^{re})^2] = \mathbb{E}[(\theta_j^{im})^2] = \frac{1}{2} \text{ for } j = 1,\dots,N-1$$

Then, one can simulate one realization of the Gaussian random field $\mathbf{Y}$ of size $N+1$ with $2N$ with standard normal random variates as proposed in Algorithm 3.

Algorithm 3 Generation of one realization of the Gaussian random field $\mathbf{Y}$ of size $N+1$ with $2N$ with standard normal random variates

---

1: Sample the autocovariance function: vector $\mathbf{c}$ and circulant vector $\mathbf{a}$
2: Compute $\mathbf{s} = \mathbf{Fa}$ by FFT
3: Generate two realizations of random standard normal uncorrelated vectors of size $N+1$: $\boldsymbol{\theta}^{re}$ and $\boldsymbol{\theta}^{im}$ such that

$$\boldsymbol{\theta} = \boldsymbol{\theta}^{re} + i\boldsymbol{\theta}^{im},$$

satisfying:

$$E[(\theta_j^{re})^2] = E[(\theta_j^{im})^2] = 1/2, j = 1,\dots,N-1,$$

$$E[(\theta_0^{re})^2] = E[(\theta_N^{re})^2] = 1,\; \theta_{2N-j}^{re} = \theta_j^{re},\; j = 1,\dots,N-1,$$

$$\theta_0^{im} = 0, \theta_N^{im} = 0,\; \theta_{2N-j}^{im} = -\theta_j^{im},\; j = 1,\dots,N-1$$

4: Apply iFFT to compute $\mathbf{C}^*\boldsymbol{\theta}$ with $\mathbf{C}^* = \frac{1}{\sqrt{2N}}\mathbf{F}^*\mathbf{D}^{\frac{1}{2}}$
5: Take

$$\mathbf{Y} = (\mathbf{C}^*\boldsymbol{\theta})(0:N)$$

Another possibility is to uniform random vector $\boldsymbol{\phi}$ of size $N+1$ over $[0, 2\pi]$ instead of standard normal random vectors. This alternative is presented in [3], except that some corrections on the random vector are needed to recover the covariance matrix.

We choose

$$\theta_j^{re} = cos(\phi_j), j = 1, \ldots, N-1,$$
$$\theta_j^{im} = sin(\phi_j), j = 1, \ldots, N-1$$

and

$$\theta_{2N-j}^{re} = \theta_j^{re},\ j = 1, \ldots, N-1,$$
$$\theta_0^{im} = 0, \theta_N^{im} = 0,$$
$$\theta_{2N-j}^{im} = -\theta_j^{im},\ j = 1, \ldots, N-1.$$

Those conditions allow to get $\mathbf{Y}_2 = 0$.

From the expression (6) of $(\mathbf{Y}_1)_k$, it is a sum of random variables, so by the Central Limit Theorem, $(\mathbf{Y}_1)_k$ converges in distribution to Gaussian law as N tends to infinity.

We also have to satisfy

$$\mathbb{E}[(\theta_0^{re})^2] = 1,\ \mathbb{E}[(\theta_N^{re})^2] = 1,\ \mathbb{E}[(\theta_j^{re})^2] = \mathbb{E}[(\theta_j^{im})^2] = \frac{1}{2} \text{ for } j = 1, \ldots, N-1$$

to recover the covariance matrix.

As $\mathbb{E}[cos(\phi_0)^2] = \dfrac{1}{2\,\pi}\displaystyle\int_0^{2\pi} cos^2(x)dx = \dfrac{1}{2}$, we choose

$$\theta_0^{re} = \sqrt{2}cos(\phi_0), \theta_N^{re} = \sqrt{2}cos(\phi_N).$$

Notice that in [3], the $\sqrt{2}$ factor is missing.

Then we obtain the algorithm 4

References

[1] Xuan Hung Dang. *Identification de la variabilité spatiale des champs de contraintes dans les agrégats polycristallins et application à l'approche locale de la rupture.* Theses, Université Blaise Pascal - Clermont-Ferrand II, October 2012.

[2] C. R. Dietrich and G. N. Newsam. A fast and exact method for multidimensional gaussian stochastic simulations. *Water Resources Research*, 29(8):2861–2869, 1993.

[3] E. Pardo-Igúzquiza and M. Chica-Olmo. The fourier integral method: An efficient spectral method for simulation of random fields. *Mathematical Geology*, 25(2):177–217, 1993.

Algorithm 4 Generation of one realization of a Gaussian random field $\mathbf{Y}$ with of size $N+1$ with $N+1$ uniform random variates

1: Sample the autocovariance function: vector $\mathbf{c}$ and circulant vector $\mathbf{a}$
2: Compute $\mathbf{s} = \mathbf{Fa}$ by FFT
3: Generate a realization of the random vector $\boldsymbol{\phi} = (\phi_0, \ldots, \phi_N)$ such that $\phi_k \in [0, 2\pi[$ is a random variable of uniform law
4: Compute $\boldsymbol{\theta}^{re}$ and $\boldsymbol{\theta}^{im}$ such that

$$\boldsymbol{\theta} = \boldsymbol{\theta}^{re} + i\boldsymbol{\theta}^{im},$$

satisfying:

$$\theta_j^{re} = cos(\phi_j), j = 1, \ldots, N-1,$$

$$\theta_j^{im} = sin(\phi_j), j = 1, \ldots, N-1$$

and

$$\theta_{2N-j}^{re} = \theta_j^{re},\ j = 1, \ldots, N-1,$$

$$\theta_0^{im} = 0, \theta_N^{im} = 0,$$

$$\theta_{2N-j}^{im} = -\theta_j^{im},\ j = 1, \ldots, N-1.$$

$$\theta_0^{re} = \sqrt{2}cos(\phi_0), \theta_N^{re} = \sqrt{2}cos(\phi_N).$$

5: Apply iFFT to compute $\mathbf{C}^*\boldsymbol{\theta}$ with $\mathbf{C}^* = \frac{1}{\sqrt{2N}}\mathbf{F}^*\mathbf{D}^{\frac{1}{2}}$
6: Take

$$\mathbf{Y} = (\mathbf{C}^*\boldsymbol{\theta})(0:N)$$

RESEARCH CENTRE
PARIS – ROCQUENCOURT

Domaine de Voluceau, - Rocquencourt
B.P. 105 - 78153 Le Chesnay Cedex

Publisher
Inria
Domaine de Voluceau - Rocquencourt
BP 105 - 78153 Le Chesnay Cedex
inria.fr

ISSN 0249-0803