RUHR-UNIVERSITÄT BOCHUM

Gaussian Random Field Generation for stochastic PDEs

March 3, 2019

Timo Schorlepp

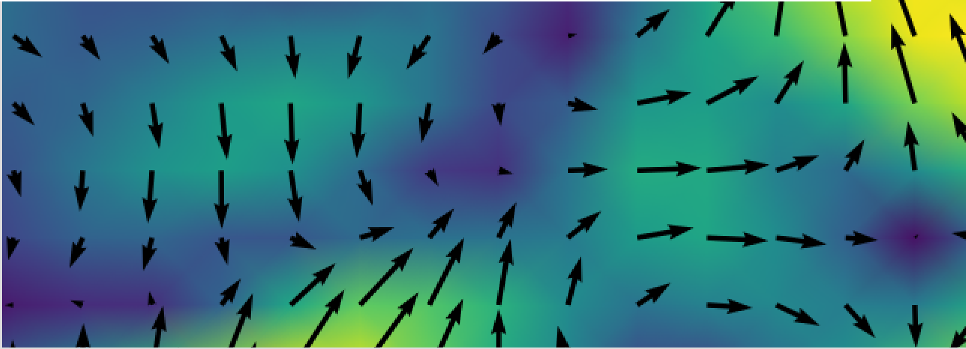
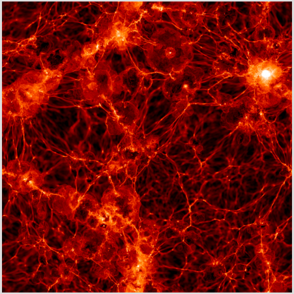
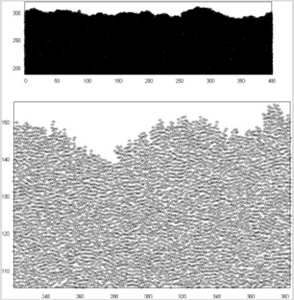


Table of contents

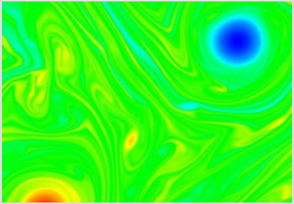
Motivation: Exemplary applications



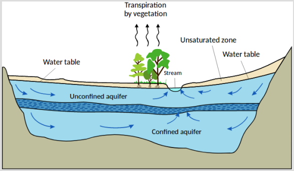
Vogelsberger et al. 2014, Illustris simulation



Kuennen, Wang 2008, KPZ surface growth



Murray 2017, 2D stochastic NSE vorticity



Wikimedia, aquifer sketch

Motivation: Mathematical examples

Deterministic incompressible NSE for $\boldsymbol{u} : \mathbb{T}^d \times \mathbb{R}_+ \to \mathbb{R}^d$:

$$\partial_t \boldsymbol{u} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} + \nabla p = \nu \Delta \boldsymbol{u} \ , \ \nabla \cdot \boldsymbol{u} = 0$$

Without forcing:

$$\frac{\mathrm{d}}{\mathrm{d}t} \int \mathrm{d}V \ \frac{1}{2} |\boldsymbol{u}|^2 = -2\nu \int \mathrm{d}V \ \mathrm{tr}((\nabla \otimes \boldsymbol{u})^T (\nabla \otimes \boldsymbol{u})) \leq -2C\nu \int \mathrm{d}V \ |\boldsymbol{u}|^2$$

Gronwall: Energy decays exponentially, need forcing for interesting long-term behavior, e.g. Gaussian forcing with homogeneous, isotropic correlation matrix!

Similarly: Stochastic heat equation
Why Gaussian? CLT, easy, algorithms exist

Theory: Basic Definitions

Definition 1

A random field ξ is an indexed family of random variables

$$\boldsymbol{\xi} = \left\{ \boldsymbol{\xi}(\boldsymbol{x}) : \Omega \to \mathbb{R}^m \, ; \, \boldsymbol{x} \in T \subseteq \mathbb{R}^d \right\}.$$

Remark 2

- Generalization of stochastic processes
- No details on Kolmogorov Existence Theorem etc. here

Theory: Basic Definitions

RUB

Definition 3

A random field $\boldsymbol{\xi}$ is called Gaussian iff $\forall k \in \mathbb{N} : \forall \{\boldsymbol{x}^{(0)}, \cdots, \boldsymbol{x}^{(k-1)}\} \subseteq T : \boldsymbol{\xi}(\boldsymbol{x}^{(0)}) =: \boldsymbol{\xi}^{(0)}, \cdots \boldsymbol{\xi}(\boldsymbol{x}^{(k-1)}) =: \boldsymbol{\xi}^{(k-1)}$ are jointly normally distributed, i.e.

$$p_{\boldsymbol{\xi}^{(0)},\cdots,\boldsymbol{\xi}^{(k-1)}}(\boldsymbol{y}^{(0)}, \cdots \boldsymbol{y}^{(k-1)}) = \det(2\pi\Sigma)^{-\frac{1}{2}} \cdot \cdot \exp\left(-\frac{1}{2}(\boldsymbol{y}-\boldsymbol{\mu})^T \Sigma^{-1} (\boldsymbol{y}-\boldsymbol{\mu})\right)$$

where Σ is the $km \times km$ covariance matrix

$$\Sigma_{mr+i,ms+j} = \mathrm{Cov}\left(\xi_i^{(r)}, \xi_j^{(s)}\right) =: \chi_{ij}\left(\boldsymbol{x}^{(r)}, \boldsymbol{x}^{(s)}\right)$$

and $\boldsymbol{\mu}$ is the km-dim. mean vector $\mu_{mr+i} = \left\langle \xi_i^{(r)} \right\rangle$.

Theory: Basic Definitions

Remark 4

- Gaussian random fields (GRF) are completely specified by $\boldsymbol{\mu}(\boldsymbol{x})$ and $\chi\left(\boldsymbol{x}', \boldsymbol{x}\right) \Longrightarrow$ easy!
- We will assume $\boldsymbol{\mu}(\boldsymbol{x}) \equiv 0$ wlog in the following (also necessary for isotropy) as well as $d = m$
- Σ needs to be positive semidefinite for all $\boldsymbol{x}^{(0)}, \cdots, \boldsymbol{x}^{(k-1)}$ since $\sum_{i,j} \boldsymbol{a}_i^T \chi\left(\boldsymbol{x}^{(i)}, \boldsymbol{x}^{(j)}\right) \boldsymbol{a}_j = \mathrm{Var}\left(\sum_i \boldsymbol{a}_i^T \boldsymbol{\xi}^{(i)}\right) \geq 0$

Theory: Basic Definitions

Example/Definition 5

- White noise $\chi_{ij}(\boldsymbol{x}', \boldsymbol{x}) = \delta(\boldsymbol{x}' - \boldsymbol{x})\delta_{ij}$
- Homogeneous (translation-invariant, stationary), isotropic ($O(n)$-invariant) and solenoidal correlation tensor:

$$\chi_{ij}(\boldsymbol{x}', \boldsymbol{x}) = \chi_{ij}(\boldsymbol{x}' - \boldsymbol{x}) = \chi_{ij}(\boldsymbol{r}) = f(r)\delta_{ij} + \frac{rf'(r)}{d-1}\left(\delta_{ij} - \frac{r_i r_j}{r^2}\right)$$

- Stationary diagonal correlation $\chi_{ij}(\boldsymbol{x}', \boldsymbol{x}) = \chi_0 \exp\left(-\frac{|\boldsymbol{x}' - \boldsymbol{x}|}{\lambda}\right)\delta_{ij}$

Remark 6

We do not distinguish between correlation and covariance matrices here (they differ by a constant factor in the stationary case)

Theory: How to generate stationary GRFs

RUB

Example 7

Assuming we can generate independent $\mathcal{N}(0,1)$ samples, how do we generate vectors $\boldsymbol{\xi} \sim \mathcal{N}(0, C)$ for a given covariance $d \times d$-matrix C?

Answer: C is positive semidefinite, allowing for a Cholesky or eigenvalue/-vectors decomposition $C = B^T B$, so if we sample ϕ with independent $\mathcal{N}(0,1)$ entries, we get

$$\left\langle B^T \phi \left(B^T \phi\right)^T \right\rangle = B^T \underbrace{\left\langle \phi \phi^T \right\rangle}_{= I_d} B = B^T B = C$$

Theory: How to generate stationary GRFs

Theorem 8 (Direct method)

Let

$$G = \left\{ \left(j_1 \frac{L_1}{N_1}, \cdots, j_d \frac{L_d}{N_d} \right) ; j_s \in \{0, 1, 2, \cdots, N_s - 1\} \right\}$$

be a uniformly spaced grid in $[0, L_1] \times \cdots \times [0, L_d]$. Decomposing the overall $(N_1 \cdots N_d d) \times (N_1 \cdots N_d d)$ grid covariance matrix $\Sigma = \Lambda^T \Lambda$ of the grid and sampling $\phi \sim \mathcal{N}(0, I_{N_1 \cdots N_d d})$ yields

$$\Lambda^T \phi \sim \mathcal{N}(0, \chi)$$

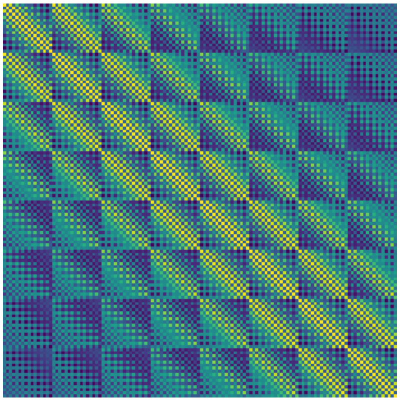
Remark 9

Decomposing this matrix becomes prohibitively expensive really fast!

Theory: How to generate stationary GRFs

Example 10

Grid covariance matrix for stationary χ on $2D$ 8×8 grid:

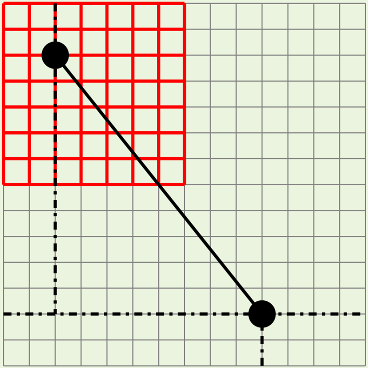


Block Toeplitz matrix (BTM)

Theory: How to generate stationary GRFs

Example 10 (continued, circulant embedding)

Idea: Embed the BTM into a block *circulant* matrix (BCM) by extending the grid with periodic boundary conditions. Goal: Use properties of BCMs (eigenvalues may be found via FFT of the individual $d \times d$ blocks)



Theory: How to generate stationary GRFs

Remark 10 (circulant embedding)

- The extended covariance matrix need not be positive (semi)definite! $\Longrightarrow$ Grid may need to be very large
- No further details here, check the literature list on last slide if you are interested in circulant embedding methods

Title

.

Title

.

Title

A

bla

B

bla

C

bla

Literature: Recommendations for further reading

- A. Yaglom, Correlation Theory of Stationary and Related Random Functions, Springer Series in Statistics, 1987.
- P. Abrahamsen, A Review of Gaussian Random Fields and Correlation Functions, Norsk Regnesentral/Norwegian Computing Center, 1997.
- G. Chan, A. T. A. Wood, Simulation of stationary Gaussian vector fields, Statistics and Computing, 1999.
- A. Lang, J. Potthoff, Fast simulation of Gaussian random fields, Monte Carlo Methods and Applications, 2011.