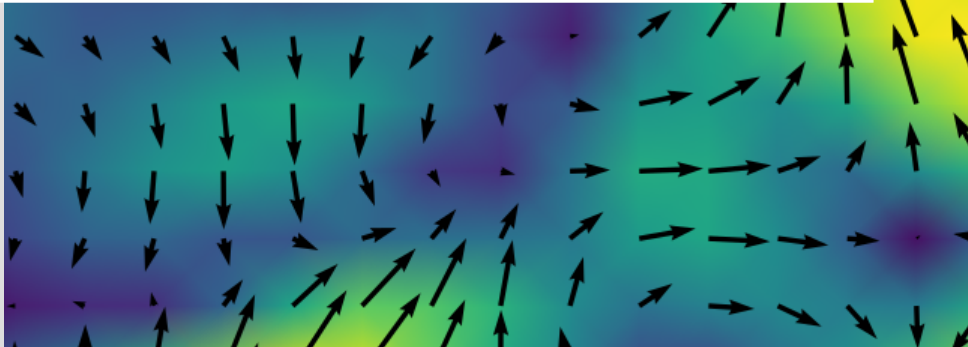


Gaussian Random Field Generation for stochastic PDEs

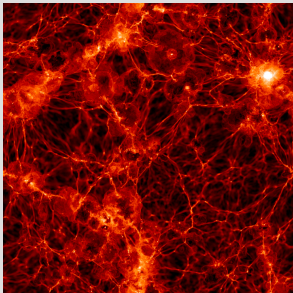
March 3, 2019

Timo Schorlepp

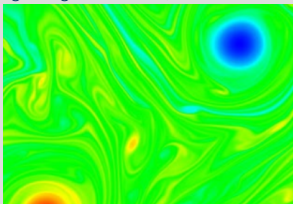


- 1 Motivation
- 2 Theory
 - Basic Definitions
 - How to generate stationary GRFs
- 3 Numerical implementation
- 4 Results
- 5 Conclusion
- 6 Literature

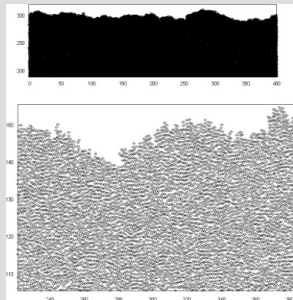
Motivation: Exemplary applications



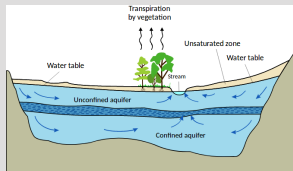
Vogelsberger et al. 2014, Illustris simulation



Murray 2017, 2D stochastic NSE vorticity



Kuennen, Wang 2008, KPZ surface growth



Wikimedia, aquifer sketch

Motivation: Mathematical examples

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

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

Without forcing:

$$\frac{d}{dt} \int dV \frac{1}{2} |\mathbf{u}|^2 = -2\nu \int dV \operatorname{tr}((\nabla \otimes \mathbf{u})^T (\nabla \otimes \mathbf{u})) \leq -2C\nu \int dV |\mathbf{u}|^2$$

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

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

Remark 2

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

Theory:

Basic Definitions

Definition 3

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

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

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

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

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 $\mu(\mathbf{x})$ and $\chi(\mathbf{x}', \mathbf{x}) \implies$ easy!
- We will assume $\mu(\mathbf{x}) \equiv 0$ wlog in the following (also necessary for isotropy) as well as $d = m$
- Σ needs to be positive semidefinite for all $\mathbf{x}^{(0)}, \dots, \mathbf{x}^{(k-1)}$ since $\sum_{i,j} \mathbf{a}_i^T \chi(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) \mathbf{a}_j = \text{Var}(\sum_i \mathbf{a}_i^T \xi^{(i)}) \geq 0$

Theory:

Basic Definitions

Example/Definition 5

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

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

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

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

Example 7

Assuming we can generate independent $\mathcal{N}(0, 1)$ samples, how do we generate vectors $\xi \sim \mathcal{N}(0, C)$ 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

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

Theory:

How to generate stationary GRFs

Theorem 8 (Direct method)

Let

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

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

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

Remark 9

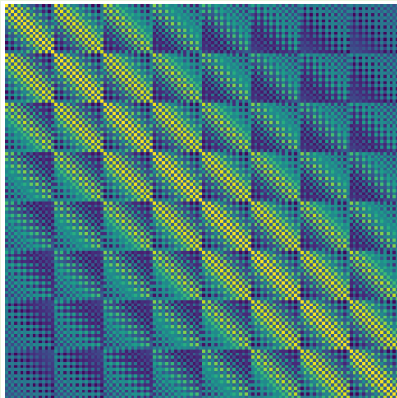
Decomposing this matrix becomes prohibitively expensive really fast!

Theory:

How to generate stationary GRFs

Example 10

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



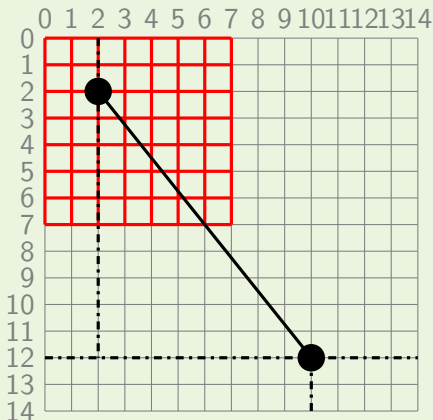
Block Toeplitz matrix (BTM)

Theory:

How to generate stationary GRFs

Example 10 (continued)

Idea: Embed the BTM into a block *circulant* matrix (BCM) by extending the grid with periodic boundary conditions!



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.