Gaussian Random Field Generation for stochastic PDEs

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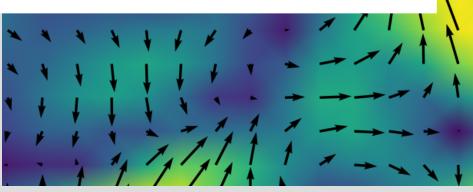
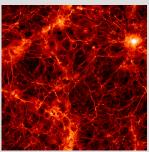


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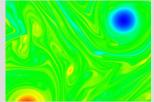
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RUB

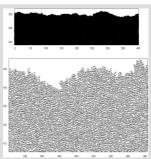
Motivation: Exemplary applications



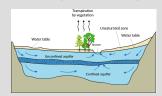
Vogelsberger et al. 2014, Illustris simulation



Murray 2017, 2D stochastic NSE vorticity



Kuennen, Wang 2008, KPZ surface growth



Wikimedia, aquifer sketch

Motivation: Mathematical examples

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

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

Without forcing:

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

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

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

Remark 2

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

Theory: Basic Definitions

Definition 3

A random field $\boldsymbol{\xi}$ is called Gaussian iff $\forall k \in \mathbb{N} : \forall \{\boldsymbol{x}^{(0)}, \cdots, \boldsymbol{x}^{(k-1)}\} \subseteq \mathcal{T} : \boldsymbol{\xi}(\boldsymbol{x}^{(0)}) =: \boldsymbol{\xi}^{(0)}, \cdots \boldsymbol{\xi}(\boldsymbol{x}^{(k-1)}) =: \boldsymbol{\xi}^{(k-1)}$ 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

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

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

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:

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

lacksquare Stationary diagonal correlation $\chi_{ij}(m{x}',m{x})=\chi_0\exp\Bigl(-rac{|m{x}'-m{x}|}{\lambda}\Bigr)\delta_{ij}$

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 $\boldsymbol{\xi} \sim \mathcal{N}(0,C)$ for a given covariance $d \times d$ -matrix C?

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

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

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

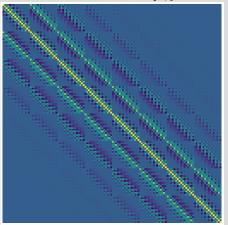
Decomposing this matrix becomes prohibitively expensive really fast!

Theory:

RUB

How to generate stationary GRFs

Grid covariance matrix for stationary χ on 2D 8 \times 8 grid:



(Block Toeplitz matrix)

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Α

bla

R

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.