

Gaussian Random Field Generation for Stochastic PDEs

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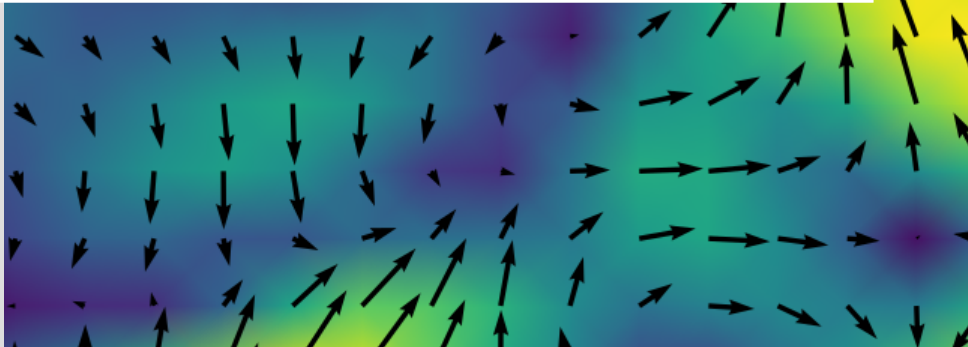
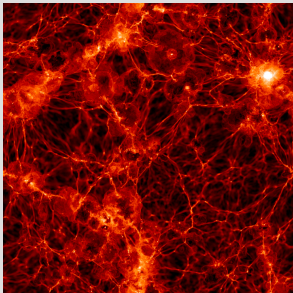


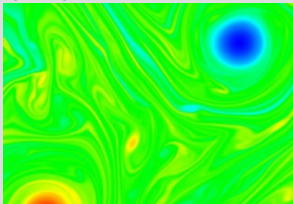
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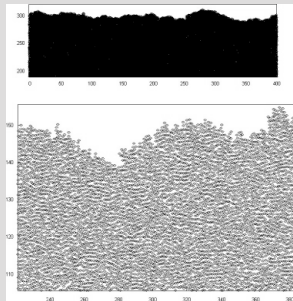
Motivation: Exemplary applications



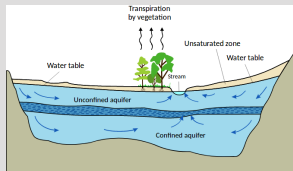
Vogelsberger et al. 2014, Illustris simulation



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, approximation, 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

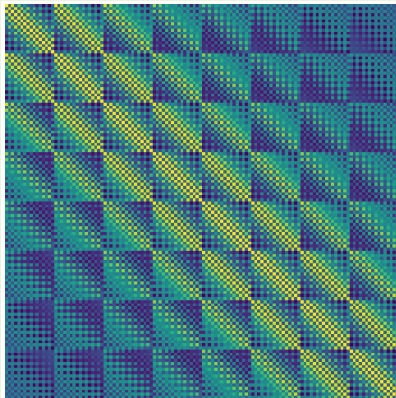
Decomposing this matrix becomes prohibitively expensive really fast!

Theory:

How to generate stationary GRFs

Example 10

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



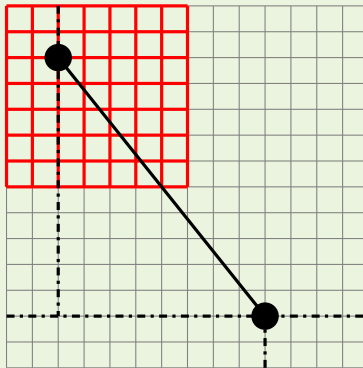
Block Toeplitz matrix (BTM)

Theory:

How to generate stationary GRFs

Example 10 (continued, 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 11 (circulant embedding)

- The extended covariance matrix need not be positive (semi)definite!
⇒ 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

Theory:

How to generate stationary GRFs

Theorem 12 (Spectral method, continuous FT)

Let ξ be a stationary GRF on \mathbb{R}^d with correlation matrix χ . Denote by \mathbf{W} the d -dimensional white noise $\langle \mathbf{W}(\mathbf{x}') \mathbf{W}(\mathbf{x})^T \rangle = I_d \delta(\mathbf{x}' - \mathbf{x})$, and by \mathcal{F} the Fourier transform (FT) on \mathbb{R}^d . Decompose the correlation in Fourier space as $\hat{\chi}(\mathbf{k}) := \mathcal{F}\chi(\mathbf{k}) = \Lambda(\mathbf{k})\Lambda^\dagger(\mathbf{k})$. Then, the following statements hold:

- 1 $\psi := (\mathcal{F}^{-1}\Lambda\mathcal{F}) \mathbf{W} \stackrel{\mathcal{D}}{=} \xi$.
- 2 $\hat{\mathbf{W}}$ has covariance $\langle \hat{\mathbf{W}}(\mathbf{k}') \hat{\mathbf{W}}(\mathbf{k})^\dagger \rangle = (2\pi)^d I_d \delta(\mathbf{k}' - \mathbf{k})$ and pseudo-covariance $\langle \hat{\mathbf{W}}(\mathbf{k}') \hat{\mathbf{W}}(\mathbf{k})^T \rangle = (2\pi)^d I_d \delta(\mathbf{k}' + \mathbf{k})$.
- 3 $\hat{\xi}$ has covariance $\langle \hat{\xi}(\mathbf{k}') \hat{\xi}(\mathbf{k})^\dagger \rangle = (2\pi)^d \hat{\chi}(\mathbf{k}) \delta(\mathbf{k}' - \mathbf{k})$ and pseudo-covariance $\langle \hat{\xi}(\mathbf{k}') \hat{\xi}(\mathbf{k})^T \rangle = (2\pi)^d \hat{\chi}(\mathbf{k}) \delta(\mathbf{k}' + \mathbf{k})$.

Theory:

How to generate stationary GRFs

Proof: (1) Standard computation

$$\begin{aligned}
 \langle \psi(\mathbf{x}') \psi(\mathbf{x})^\dagger \rangle &= \left\langle \frac{1}{(2\pi)^d} \int d^d k' e^{i\mathbf{k}' \cdot \mathbf{x}'} \Lambda(\mathbf{k}') \int d^d y' e^{-i\mathbf{k}' \cdot \mathbf{y}'} \mathbf{W}(\mathbf{y}') \right. \\
 &\quad \cdot \left. \frac{1}{(2\pi)^d} \int d^d y \mathbf{W}(\mathbf{y})^T e^{i\mathbf{k} \cdot \mathbf{y}} \int d^d k \Lambda(\mathbf{k})^\dagger e^{-i\mathbf{k} \cdot \mathbf{x}} \right\rangle \\
 &= \frac{1}{(2\pi)^{2d}} \int d^d k' \int d^d k \int d^d y' \int d^d y e^{i\mathbf{k}' \cdot (\mathbf{x}' - \mathbf{y}') + i\mathbf{k} \cdot (\mathbf{y} - \mathbf{x})} \\
 &\quad \cdot \Lambda(\mathbf{k}') \underbrace{\langle \mathbf{W}(\mathbf{y}') \mathbf{W}(\mathbf{y})^T \rangle}_{=I_d \delta(\mathbf{y}' - \mathbf{y})} \Lambda(\mathbf{k})^\dagger \\
 &= \frac{1}{(2\pi)^d} \int d^d k' \int d^d k \underbrace{\frac{1}{(2\pi)^d} \int d^d y' e^{i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{y}'}}_{=\delta(\mathbf{k} - \mathbf{k}')} e^{i\mathbf{k}' \cdot \mathbf{x}' - i\mathbf{k} \cdot \mathbf{x}} \Lambda(\mathbf{k}') \Lambda(\mathbf{k})^\dagger \\
 &= \frac{1}{(2\pi)^d} \int d^d k e^{i\mathbf{k} \cdot (\mathbf{x}' - \mathbf{x})} \underbrace{\Lambda(\mathbf{k}) \Lambda(\mathbf{k})^\dagger}_{=\hat{\chi}(\mathbf{k})} = \chi(\mathbf{x}' - \mathbf{x})
 \end{aligned}$$

Theory:

How to generate stationary GRFs

Proof: (2) (and (3) analogously)

$$\langle \hat{\mathbf{W}}(\mathbf{k}') \hat{\mathbf{W}}(\mathbf{k})^\dagger \rangle = \int d^d x' \int d^d x e^{-i\mathbf{k}' \cdot \mathbf{x}'} e^{i\mathbf{k} \cdot \mathbf{x}} \langle \mathbf{W}(\mathbf{x}') \mathbf{W}(\mathbf{x})^T \rangle = (2\pi)^d I_d \delta(\mathbf{k}' - \mathbf{k})$$

$$\mathbf{W} \text{ is real} \implies \langle \hat{\mathbf{W}}(\mathbf{k}') \hat{\mathbf{W}}(\mathbf{k})^T \rangle = (2\pi)^d I_d \delta(\mathbf{k}' + \mathbf{k})$$

Remark 13

Theorem 11 shows that the Fourier modes of a stationary GRF are "decoupled" (modulo symmetry, due to ξ being real). Thus, instead of decomposing a $(N_1 \cdots N_d d) \times (N_1 \cdots N_d d)$ matrix, we need to decompose (analytically, so far) a single $d \times d$ matrix.

Theory:

How to generate stationary GRFs

Example 14

Homogeneous, isotropic, solenoidal correlation tensor

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

with $f(r) := \chi_0 e^{-r^2/2\lambda^2}$ for $d = 2$:

$$\begin{aligned} \chi(\mathbf{r}) &= \frac{\chi_0}{\lambda^2} e^{-\frac{r^2}{2\lambda^2}} \begin{pmatrix} \lambda^2 - y^2 & xy \\ xy & \lambda^2 - x^2 \end{pmatrix} \\ \implies \hat{\chi}(\mathbf{k}) &= 2\pi\chi_0\lambda^4 e^{-\frac{1}{2}k^2\lambda^2} \begin{pmatrix} k_y^2 & -k_x k_y \\ -k_x k_y & k_x^2 \end{pmatrix} \end{aligned}$$

Numerical implementation

What happens/changes if we want to apply the spectral method to generate GRF realizations on a grid in a bounded domain numerically, using the discrete fast Fourier transform (FFT)?

- 1 Sample discretized white noise:

$$\langle \mathbf{w}_i \mathbf{w}_j^T \rangle = \frac{1}{\Delta_d} I_d \delta_{ij} ; \Delta_d := \frac{L_1 \dots L_d}{N_1 \dots N_d}$$

- 2 Apply FFT to obtain discretized version of $\hat{\mathbf{W}}$ (alternatively: start in Fourier space, need to make sure though that symmetry is fulfilled!)
- 3 Multiply by $(2\pi)^{d/2} \Lambda(\mathbf{k})$ which was calculated analytically via continuous FT on \mathbb{R}^d (!)
- 4 Apply inverse FFT/ $(2\pi)^{d/2}$

⇒ Conceptually, we start in Fourier space and impose the correlation $\hat{\chi}$ there! What kind of correlation do we obtain in real space if we use the discrete FT?

Numerical implementation

For simplicity: Consider $d = 1$ and let

$$\varphi(x) = \sum_{m=-\infty}^{\infty} \chi(x + mL)$$

be the L -periodic summation of the initial correlation function χ .
Formally computing the Fourier transform yields

$$\hat{\varphi}(k) = \hat{\chi}(k) \sum_{m=-\infty}^{\infty} e^{\mathrm{i} k m L} = \frac{2\pi}{L} \hat{\chi}(k) \sum_{m=-\infty}^{\infty} \delta\left(k - m \frac{2\pi}{L}\right)$$

Applying the inverse FT:

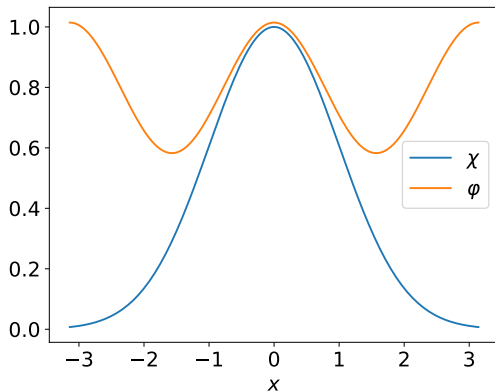
$$\varphi(x) = \frac{1}{L} \sum_{m=-\infty}^{\infty} \hat{\chi}\left(m \frac{2\pi}{L}\right) e^{2\pi \mathrm{i} \frac{m}{L} x}$$

Numerical implementation

Using our algorithm (and notation $k_p = \frac{2\pi}{L}p$):

$$\begin{aligned}
 \langle \xi_r \xi_s^\dagger \rangle &= \frac{1}{N^2} \sum_{j,j',p,p'=0}^{N-1} e^{-\frac{2\pi i}{N}(lj-p'j'+rp-sp')} \Lambda(k_p) \underbrace{\langle W_p W_{p'}^T \rangle}_{=N/L \delta_{jj'}} \Lambda(k_{p'})^\dagger \\
 &= \frac{1}{NL} \sum_{j,p,p'=0}^{N-1} e^{-\frac{2\pi i}{N}j(p-p')} e^{\frac{2\pi i}{N}(sp'-rp)} \Lambda(k_p) \Lambda(k_{p'})^\dagger \\
 &= \frac{1}{L} \sum_{p,p'=0}^{N-1} \delta_{pp'} e^{\frac{2\pi i}{N}(sp'-rp)} \Lambda(k_p) \Lambda(k_{p'})^\dagger \\
 &= \frac{1}{L} \sum_{p=0}^{N-1} \hat{\chi}(k_p) e^{\frac{2\pi i}{N}p(s-r)} \approx \varphi\left((s-r)\frac{L}{N}\right) = \varphi(x_s - x_r)
 \end{aligned}$$

Example: $d = 1$ and $\chi(r) = \chi_0 e^{-r^2/2\lambda^2}$



⇒ Method only applicable if we use periodic boundary conditions in real space OR correlation length small + boundaries unimportant!

Now: Switch to source code!

We will see a concrete implementation of the algorithm and a demonstration of convergence of the covariance for increasing number of samples.

Application to 1d KPZ equation

The evolution of the height h of a growing interface may be modelled by the Kardar-Parisi-Zhang equation (1986):

$$\partial_t h = \nu \Delta h + \frac{\lambda}{2} |\nabla h|^2 + \xi$$

$$\langle \xi(x', t') \xi(x, t) \rangle = D \chi(x' - x) \delta(t' - t)$$

where $\chi(x' - x) = \delta(x' - x)$ in the classical KPZ equation.

In this case, for $d = 1$ with initial height profile ... the stationary two-point correlation scales as

$$C(x, t) = \langle (h(x, t) - h(0, 0) - t \langle \partial_t h \rangle)^2 \rangle \propto t^{2/3} g \left(x t^{-2/3} \right)$$

and in particular

$$C(0, t) \propto t^{2/3}.$$

(Prähofer, Spohn 2004)

Application to 1d KPZ equation

Discretization using Heun scheme

$$h_n^{(1)} = h_n(t_i) + \frac{\nu \Delta t}{(\Delta x)^2} [h_{n+1}(t_i) - 2h_n(t_i) + h_{n-1}(t_i)] \\ + \frac{\lambda \Delta t}{8(\Delta x)^2} [h_{n+1}(t_i) - h_{n-1}(t_i)]^2 + \sqrt{\Delta t} \xi_{ni}$$

$$h_n(t_{i+1}) = h_n(t_i) + \frac{\nu \Delta t}{2(\Delta x)^2} [h_{n+1}(t_i) - 2h_n(t_i) + h_{n-1}(t_i) \\ + h_{n+1}^{(1)} - 2h_n^{(1)} + h_{n-1}^{(1)}] \\ + \frac{\lambda \Delta t}{16(\Delta x)^2} [(h_{n+1}(t_i) - h_{n-1}(t_i))^2 + (h_{n+1}^{(1)} - h_{n-1}^{(1)})^2] \\ + \sqrt{\Delta t} \xi_{ni}$$

CFL: At least deterministic condition $\Delta t \leq (\Delta x)^2 / (2\nu)$ necessary!

Literature:

Recommendations for further reading

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Literature:

Recommendations for further reading

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- S. Mathey et. al. , KPZ equation with short-range correlated noise: emergent symmetries and non-universal observables, Phys. Rev. E, 201
- R. Toral, P. Colet, Stochastic Numerical Methods: An Introduction for Students and Scientists, John Wiley & Sons, 2014