RUHR-UNIVERSITÄT BOCHUM

Gaussian Random Field Generation for Stochastic PDEs

April 29, 2019

Timo Schorlepp

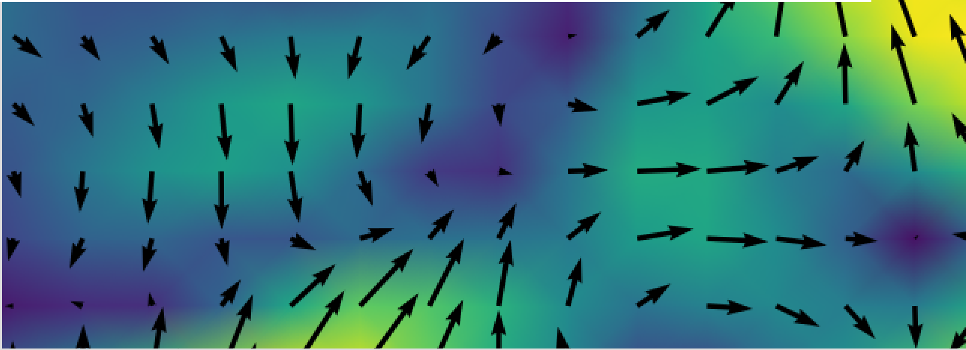
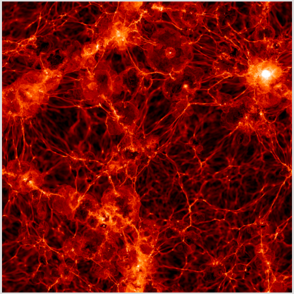
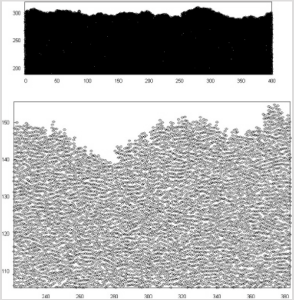


Table of contents

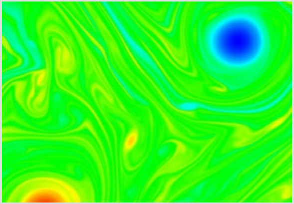
Motivation: Exemplary applications



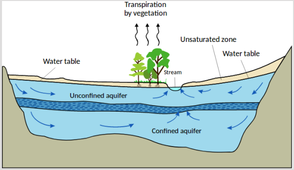
Vogelsberger et al. 2014, Illustris simulation



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, approximation, 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

- Stochastic process with index set in $\mathbb{R}^d$
- No details on Kolmogorov Existence Theorem etc. here

Theory: Basic Definitions

Definition 3

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

RUB

Remark 4

- Gaussian random fields (GRF) are completely specified by $\boldsymbol{\mu}(\boldsymbol{x})$ and $\chi(\boldsymbol{x}', \boldsymbol{x}) \Longrightarrow$ 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 (semi)definite 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

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 (semi)definite, 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

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

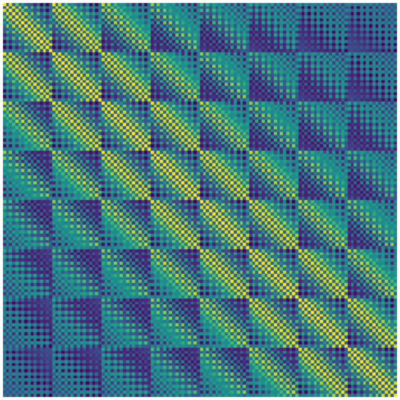
Remark 9

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:

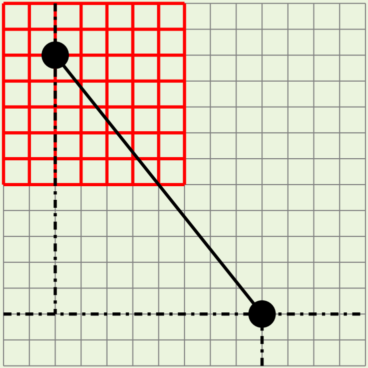


Block Toeplitz matrix (BTM)

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 11 (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

Theory: How to generate stationary GRFs

RUB

Theorem 12 (Spectral method, continuous FT)

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

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

Theory: How to generate stationary GRFs

Proof: (1) Standard computation

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

Theory: How to generate stationary GRFs

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

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

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

Remark 13

Theorem 12 shows that the Fourier modes of a stationary GRF are "decoupled" (modulo symmetry, due to $\boldsymbol{\xi}$ 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

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

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

$$\chi(\boldsymbol{r}) = \frac{\chi_0}{2\pi\lambda^4} e^{-\frac{r^2}{2\lambda^2}} \begin{pmatrix} \lambda^2 - y^2 & xy \\ xy & \lambda^2 - x^2 \end{pmatrix}$$

$$\Longrightarrow \hat{\chi}(\boldsymbol{k}) = \chi_0 \lambda^2 e^{-\frac{1}{2}k^2\lambda^2} \begin{pmatrix} k_y^2 & -k_x k_y \\ -k_x k_y & k_x^2 \end{pmatrix}$$

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:
   $\left\langle \boldsymbol{W}_i \boldsymbol{W}_j^T \right\rangle = \frac{1}{\Delta_d} I_d \delta_{ij}$; $\Delta_d := \frac{L_1 \cdots L_d}{N_1 \cdots N_d}$
2. Apply FFT to obtain discretized version of $\hat{\boldsymbol{W}}$ (alternatively: start in Fourier space, need to make sure though that symmetry is fulfilled!)
3. Multiply by $(2\pi)^{d/2}\Lambda(\boldsymbol{k})$ which was calculated analytically via continuous FT on $\mathbb{R}^d$ (!)
4. Apply inverse FFT$/(2\pi)^{d/2}$

$\Longrightarrow$ 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

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

Applying the inverse FT:

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

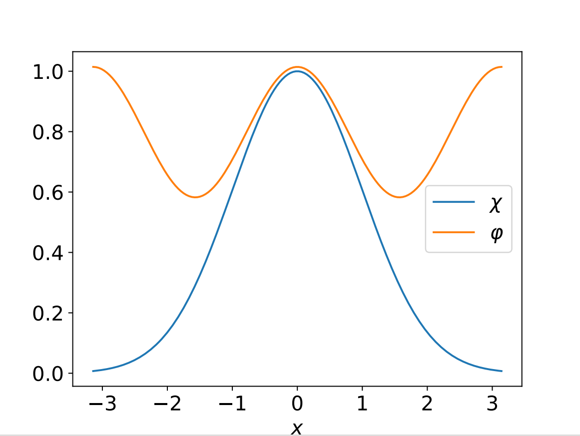
Numerical implementation

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

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

Numerical implementation

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



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

Numerical implementation

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: Setup

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

$$\partial_t h = \nu \Delta h + \frac{\lambda}{2} |\nabla h|^2 + \xi$$
$$\left\langle \xi(x', t') \xi(x, t) \right\rangle = D\, \chi(x' - x) \delta(t' - t)$$

where $\chi(x' - x) = \delta(x' - x)$ in the classical KPZ equation.
In this case, for $d = 1$ with a two-sided Wiener process as initial height profile, the stationary two-point correlation scales as

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

and in particular

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

(Prähofer, Spohn 2004)

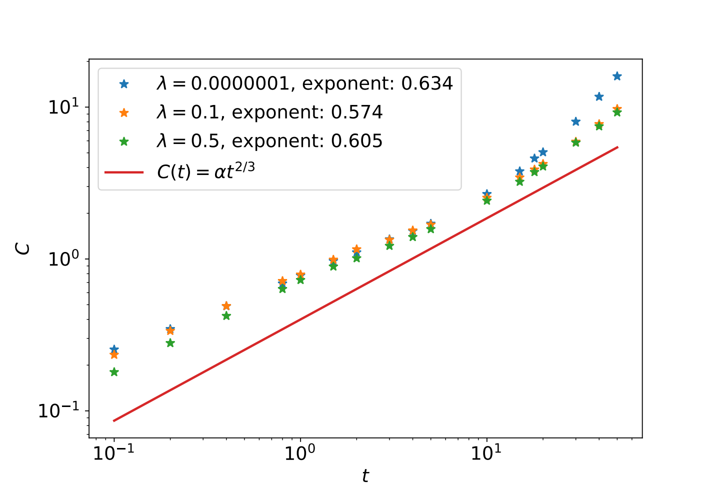
Application to 1d KPZ equation: Discretization

Discretization using Heun scheme

$$
\begin{aligned}
h_n^{(1)} &= h_n(t_i) + \frac{\nu \Delta t}{(\Delta x)^2}\left[h_{n+1}(t_i) - 2h_n(t_i) + h_{n-1}(t_i)\right] \\
&\quad + \frac{\lambda \Delta t}{8(\Delta x)^2}\left[h_{n+1}(t_i) - h_{n-1}(t_i)\right]^2 + \sqrt{\Delta t}\,\xi_{ni} \\
h_n(t_{i+1}) &= h_n(t_i) + \frac{\nu \Delta t}{2(\Delta x)^2}\Big[h_{n+1}(t_i) - 2h_n(t_i) + h_{n-1}(t_i) \\
&\quad + h_{n+1}^{(1)} - 2h_n^{(1)} + h_{n-1}^{(1)}\Big] \\
&\quad + \frac{\lambda \Delta t}{16(\Delta x)^2}\left[\left(h_{n+1}(t_i) - h_{n-1}(t_i)\right)^2 + \left(h_{n+1} - h_{n-1}\right)^2\right] \\
&\quad + \sqrt{\Delta t}\,\xi_{ni}
\end{aligned}
$$

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

Application to 1d KPZ equation: Results



Conclusion

- Successfully sampled GRF realizations with stationary, isotropic and solenoidal correlation matrix
- Used the FFT to avoid dealing with large grid covariance matrices, imposes periodic boundary conditions
- Implemented a simple application for the $1d$ KPZ equation, could investigate further
- Other follow-ups: Implement and compare to circulant embedding, try different correlation matrices, application to stochastic NSE

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.
- J. Carron, M. Wolk, I. Szapudi, On fast generation of cosmological random fields, MNRAS, 2014.

Literature: Recommendations for further reading

- M. Kardar, G. Parisi, Y. Zhang, Dynamic Scaling of Growing Interfaces, Phys. Rev. Lett. , 1986
- M. Prähofer, H. Spohn, Exact Scaling Functions for One-Dimensional Stationary KPZ Growth, Journal of Statistical Physics, 2004
- S. Mathey et. al., KPZ equation with short-range correlated noise: emergent symmetries and non-universal observables, Phys. Rev. E, 2016
- R. Toral, P. Colet, Stochastic Numerical Methods: An Introduction for Students and Scientists, John Wiley & Sons, 2014