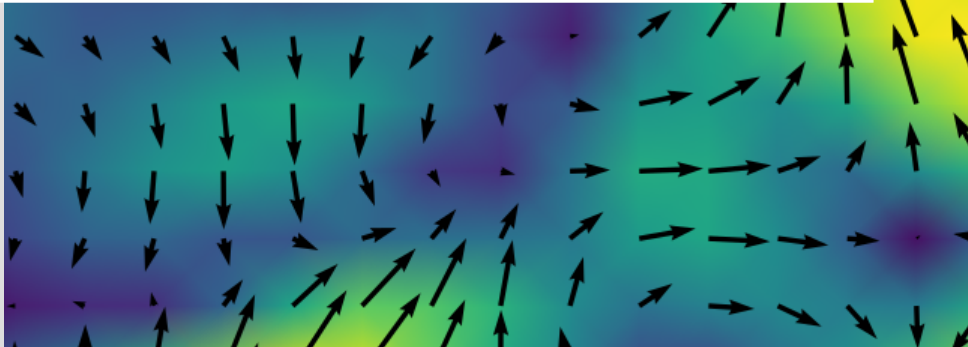


# Gaussian Random Field Generation for Stochastic PDEs

March 12, 2019

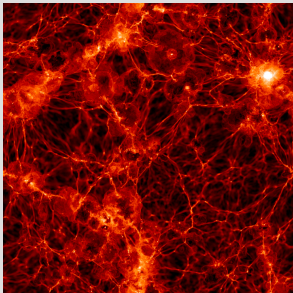
Timo Schorlepp



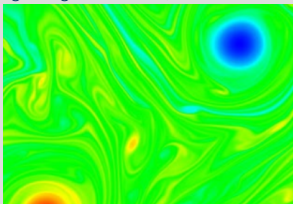
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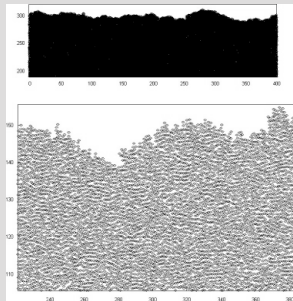
# Motivation: Exemplary applications



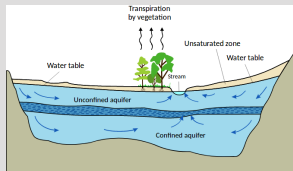
Vogelsberger et al. 2014, Illustris simulation



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  $\xi$  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  $\xi$  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  $\Sigma$  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  $d = m$
- $\Sigma$  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  $\phi$  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

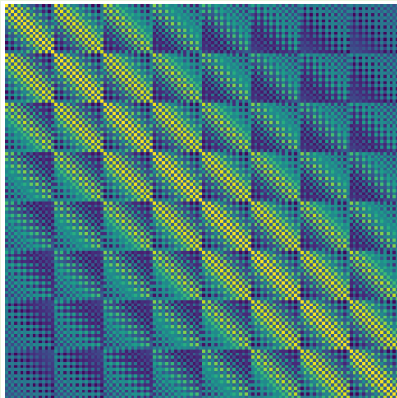
Decomposing this matrix becomes prohibitively expensive really fast!

# Theory:

## How to generate stationary GRFs

### Example 10

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



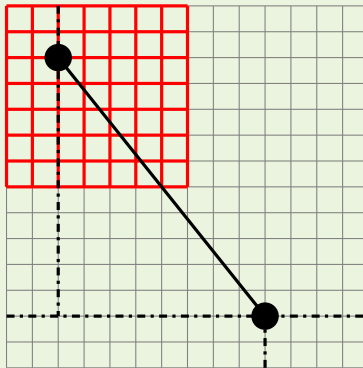
Block Toeplitz matrix (BTM)

# 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  $\xi$  be a stationary GRF on  $\mathbb{R}^d$  with correlation matrix  $\chi$ . 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

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

# 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  $\xi$  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

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

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  $\chi$ .  
Formally computing the Fourier transform yields

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

Applying the inverse FT:

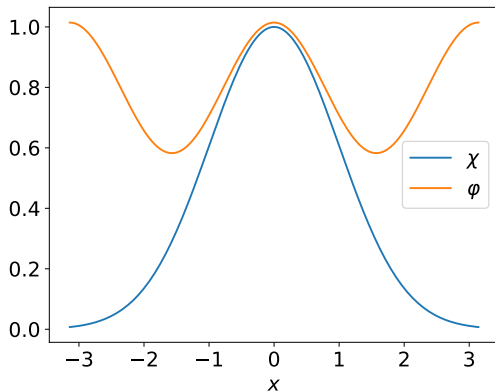
$$\varphi(x) = \frac{1}{L} \sum_{m=-\infty}^{\infty} \hat{\chi}\left(m \frac{2\pi}{L}\right) e^{2\pi \mathrm{i} \frac{m}{L} x}$$

# 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: Setup

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

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

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

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

Discretization using Heun scheme

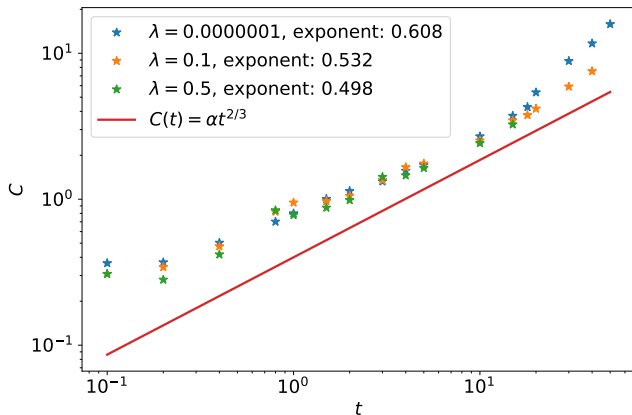
$$h_n^{(1)} = h_n(t_i) + \frac{\nu \Delta t}{(\Delta x)^2} [h_{n+1}(t_i) - 2h_n(t_i) + h_{n-1}(t_i)] \\ + \frac{\lambda \Delta t}{8(\Delta x)^2} [h_{n+1}(t_i) - h_{n-1}(t_i)]^2 + \sqrt{\Delta t} \xi_{ni}$$

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

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



# Application to 1d KPZ equation: Results



- 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

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# Literature:

## Recommendations for further reading

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