Stochastic Geometry days — 2023

Morphological modeling of the microstructure of geo-materials

Current limitations of the excursion set theory. . . as I understand it.

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2023/06/15

Laboratoire 3SR
Université Grenoble Alpes (France)

Who am I?

I'm a **classical physisist** in **geo-mechanics**.

I study the mechanical behavior of geo-materials (rocks, clays, earth, concrete, ...) and related physical phenomena (thermo-hydro-meca...)

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Scale: $>$ m

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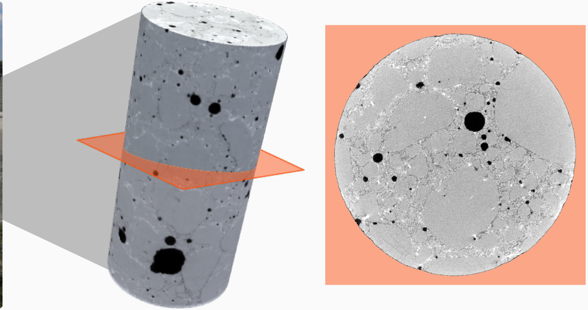
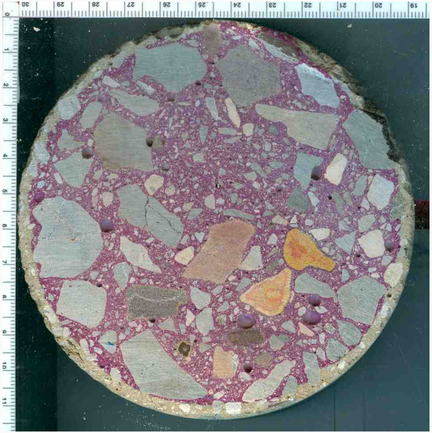


Material
Scales: mm, µm, nm

Why am I here?



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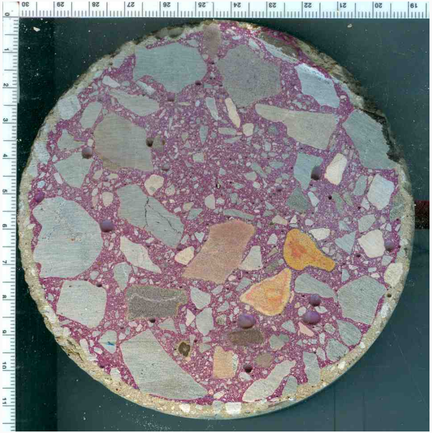
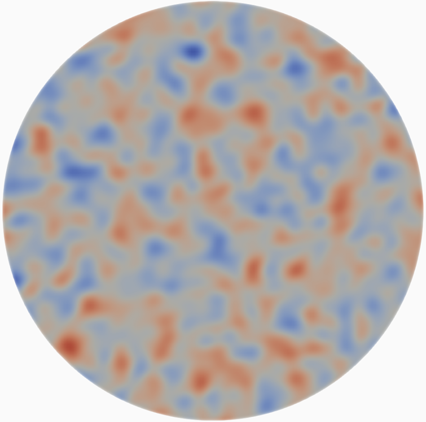


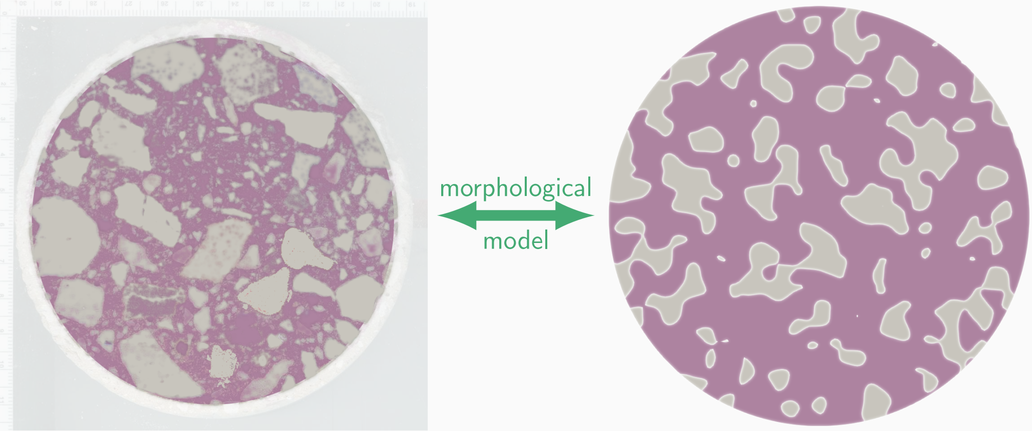
morphological

model



Correlated Random Field

Why am I here?

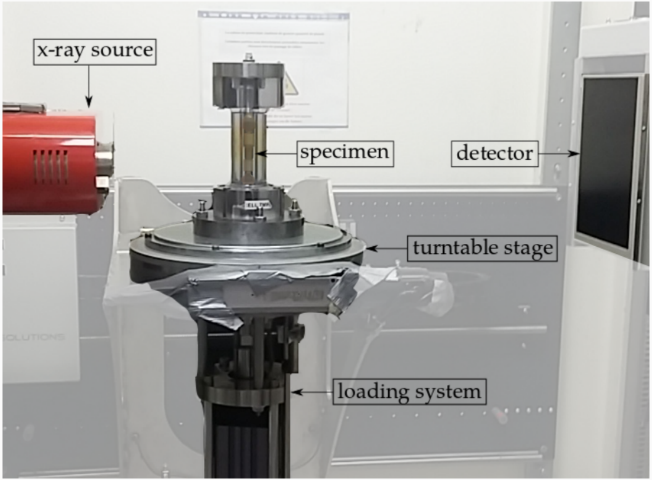


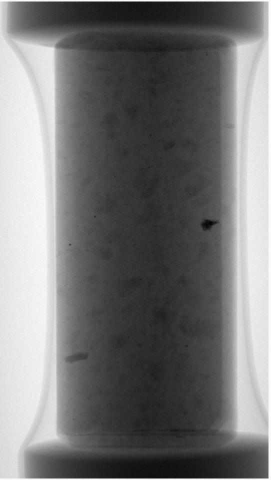
Excursion of Correlated Random Field

Outline

1. Motivations
   - Tomography
   - From images to simulations
2. Excursions as a morphological model
   - Morphological models
   - Excursions of correlated Random Fields
3. The Excursion Set Theory
   - Global descriptors
   - Expectations of the measures
4. Limitations of the model
   - Percolation and topology
   - Solutions?

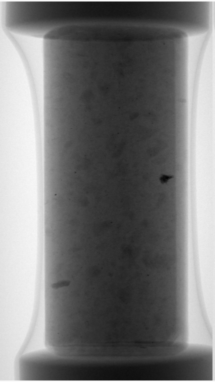
Tomographic images



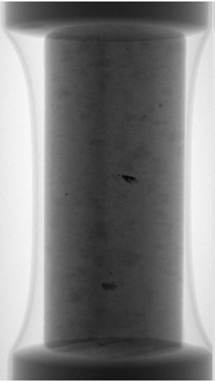


Apparatus for *in situ* tension test

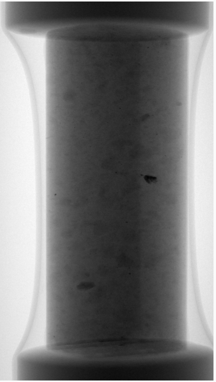
Tomographic images



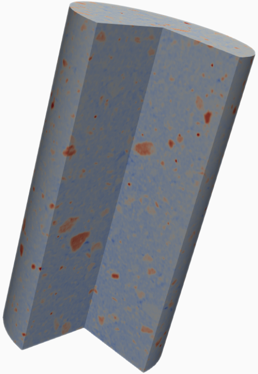
Projection θ_1



Projection θ_i

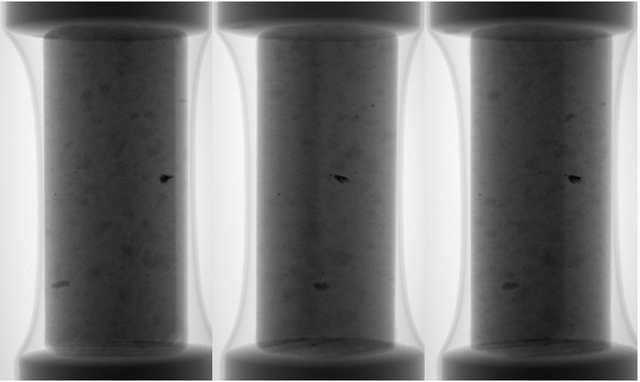


Projection θ_n

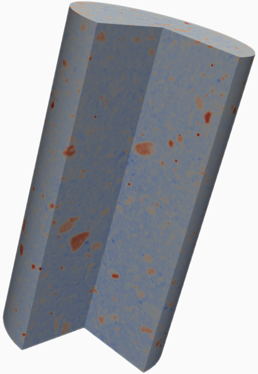


Reconstruction

Tomographic images



Projection θ_1 Projection θ_i Projection θ_n



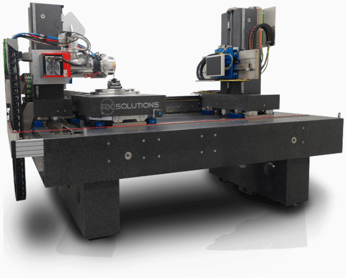
Reconstruction

Attenuation field $\neq$ correlated Random Field

Noise + heterogeneous phases $\Rightarrow$ bi/trinarisation needed

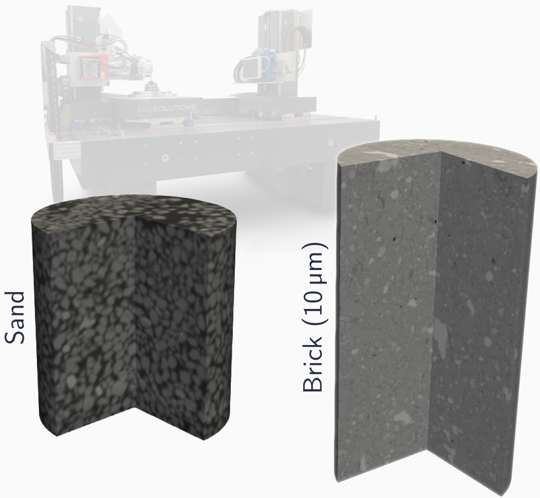
Tomographic images

Laboratory tomographs



International facilities

Laboratory tomographs



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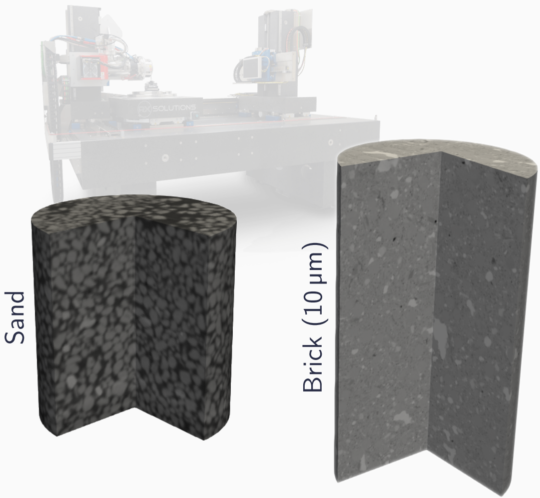

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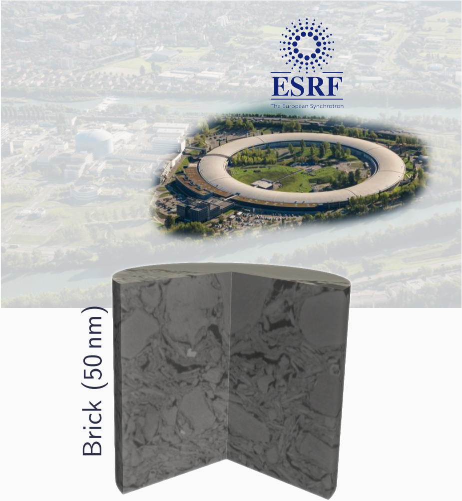

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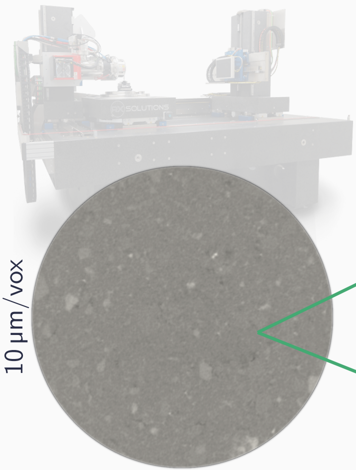

10 µm/vox

International facilities

50 nm/vox

Tomographic images

Laboratory tomographs

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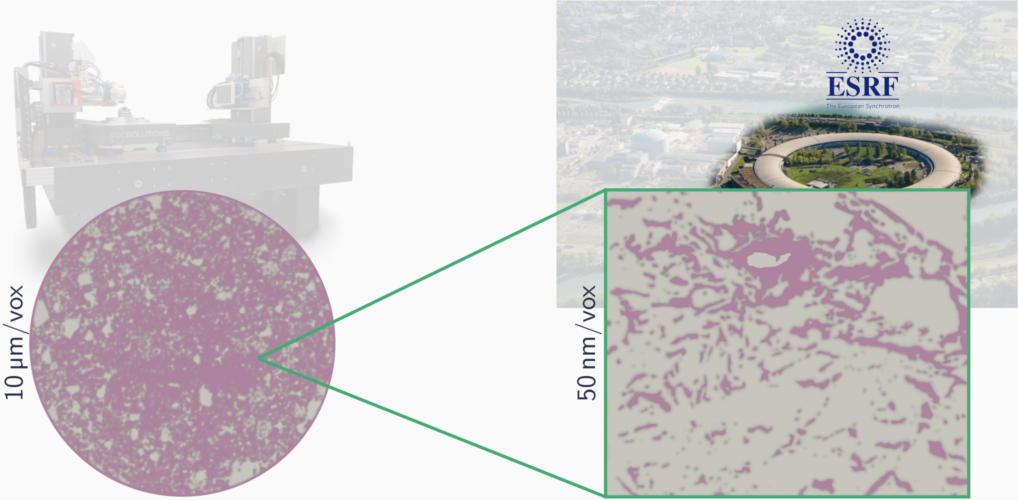

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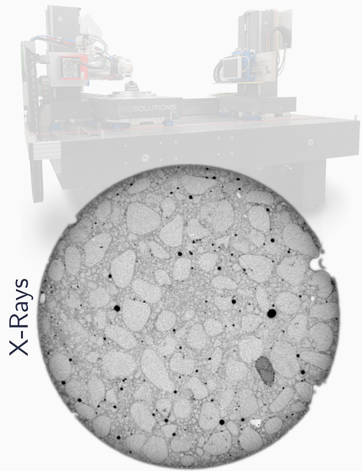
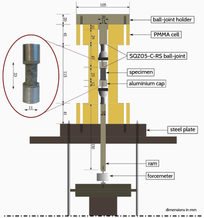


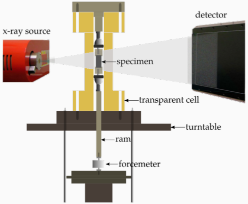
International facilities

From images to simulations



Specimen

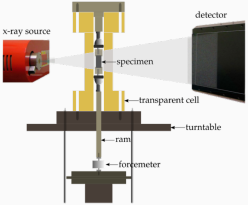
From images to simulations

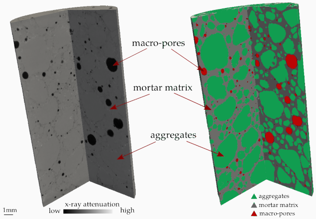


Specimen

X-Ray Tomography

From images to simulations



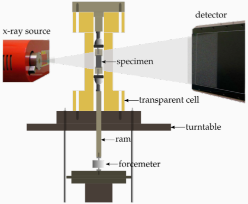


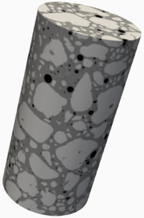
Specimen

X-Ray Tomography

Morphology Identification

From images to simulations





Specimen

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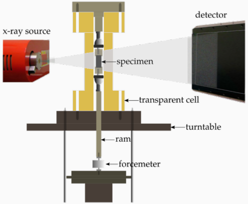
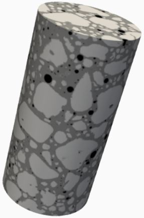
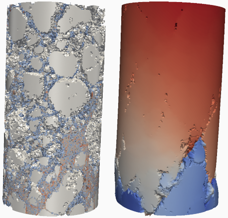






Specimen

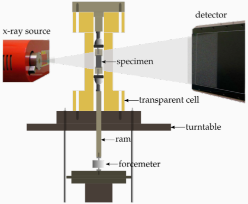
X-Ray Tomography

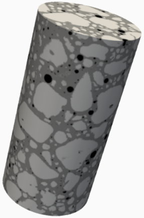
Morphology Identification

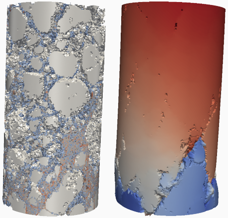
Simulations (model)
Cracks / displacements

From images to simulations

Morphological model







Specimen

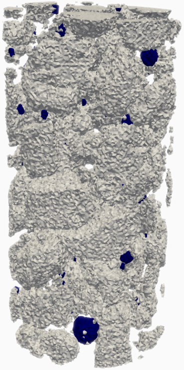
X-Ray Tomography

Morphology Identification

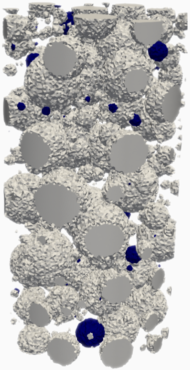
Simulations (model)
Cracks / displacements

Tomography takes a lot of time $\Rightarrow$ We need **morphological models**

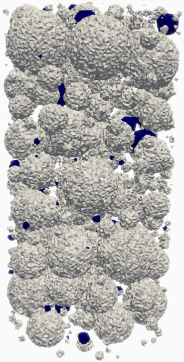
From images to simulations



Real morphology

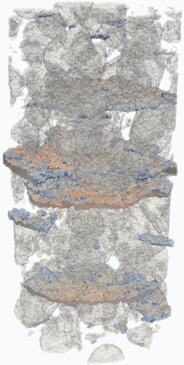


Equivalent spheres

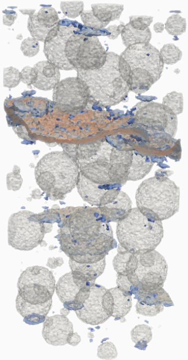


Other positions

From images to simulations



Real morphology



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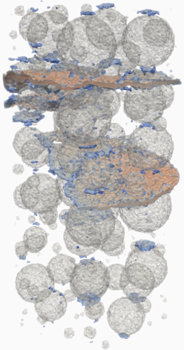


Other positions

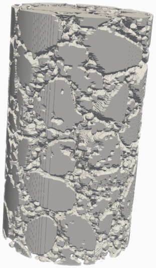
Getting an accurate representation of the morphology is of crucial importance!

Outline

Morphological models

Goals

- **Random** aspect in terms of shapes and positions
- **Discrete** aspect
- **Control** geometrical and topological quantities



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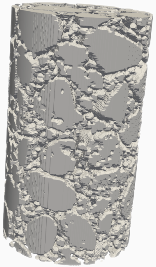
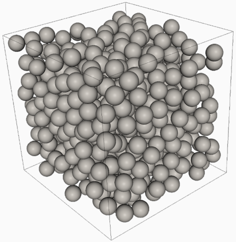
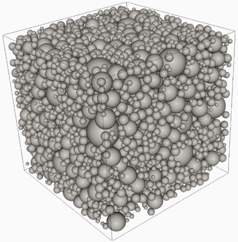
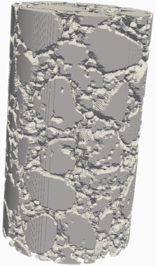


Hard sphere packing





Morphological models



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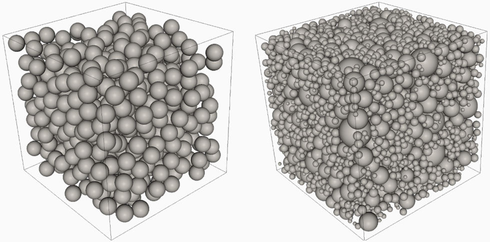
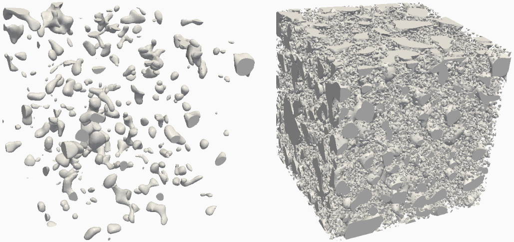


Excursion sets



Correlated Random Fields

Stricly stationnary correlated Random Field with:

- Gaussian distribution
- Gaussian covariance function

Correlated Random Fields

Stricly stationnary correlated Random Field with:

- Gaussian distribution, or Gaussian related
- Gaussian covariance function

Correlated Random Fields

Stricly stationnary correlated Random Field with:

- Gaussian distribution, or Gaussian related
- Gaussian covariance function or anything that makes MS differentiable RF

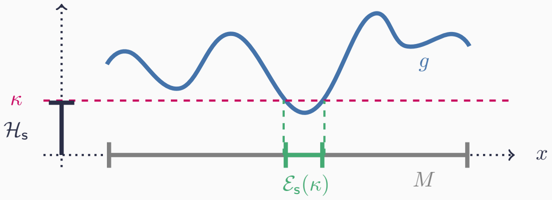
Excursion sets

An **excursion set** $\mathcal{E}_s$ is the result of the **"threshold"** of a realisation of a RF:

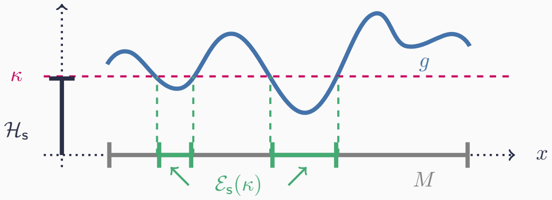
$$\mathcal{E}_s = \{\boldsymbol{x} \in M \mid g(\boldsymbol{x}) \in \mathcal{H}_s\}$$

where M is the domain of definition of the RF and $\mathcal{H}_s$ the so called **Hitting Set**.

For example if we set $\mathcal{H}_s =]-\infty; \kappa]$ we have $\mathcal{E}_s(\kappa) = \{\boldsymbol{x} \in M \mid g(\boldsymbol{x}) \leq \kappa\}$



Excursion with "low" threshold



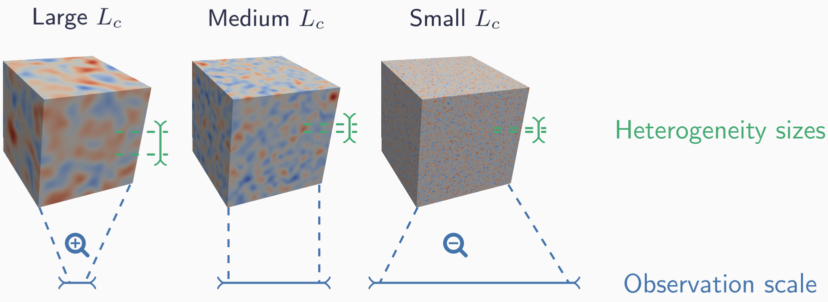
Excursion with "high" threshold

Correlated Random Fields

$g : \Omega \times \mathbb{R}^3 \mapsto \mathbb{R}$

Continuous aspect

parametric variability



Excursion sets

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$g : \Omega \times \mathbb{R}^3 \mapsto \mathbb{R}$

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Excursion sets

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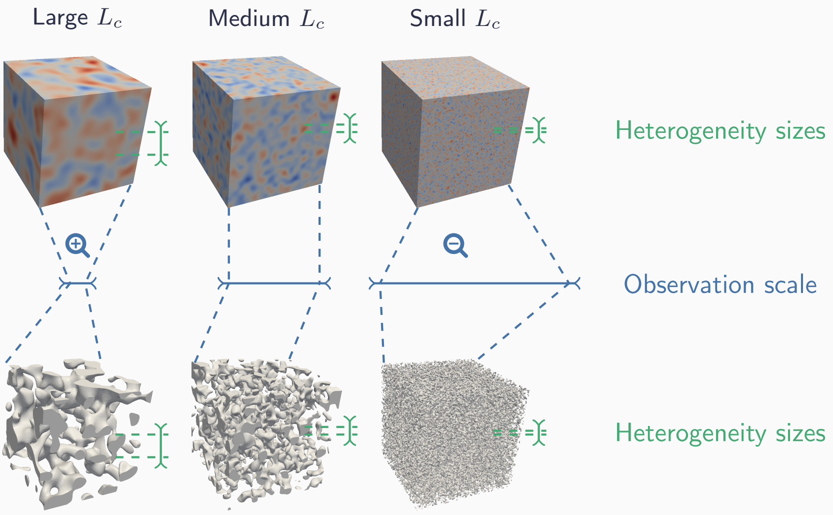
Discrete aspect

explicit morphology



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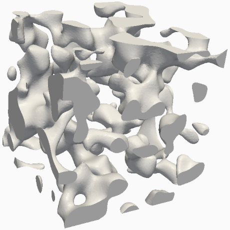

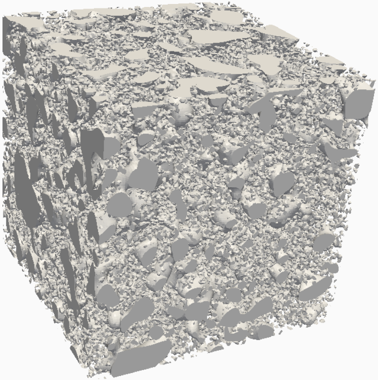

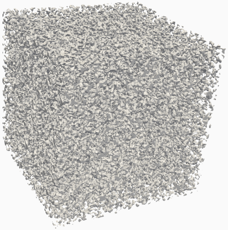

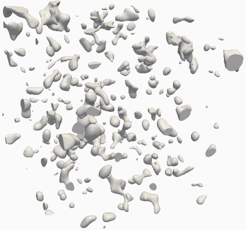

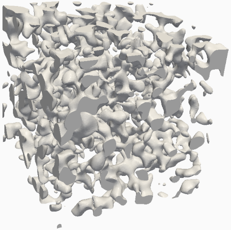

Outline

Families of measures

It exists several **families of measures** (Minkowski functionals, Lipschitz-Killing curvatures...). In an $N-$dimensional space, the size of the base is $N+1$ where each element can be seen as a $n-$dimensional measure.

Each measure can be classified into two types:

- **geometrical measures** $(1 \leq n \leq N)$
- **topological measure** $(n = 0)$

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In 3D it's equivalent of considering:

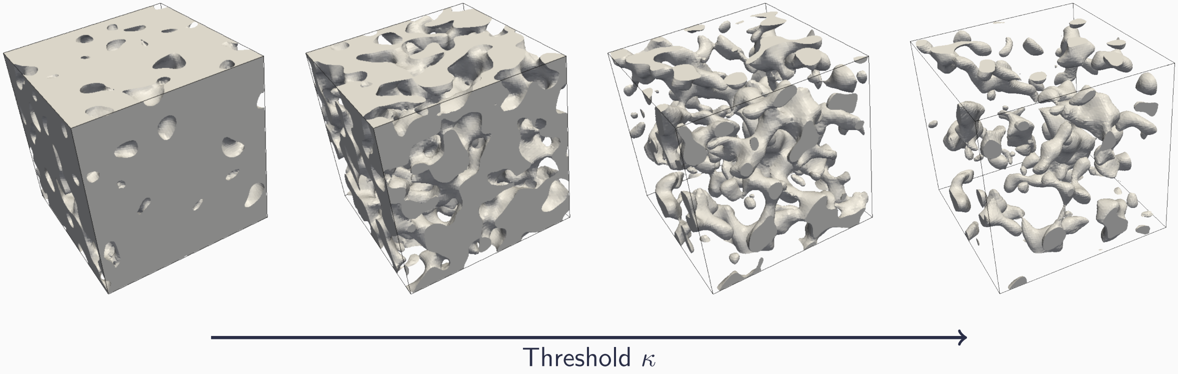
$n = 3$: Volume

$n = 2$: Surface area

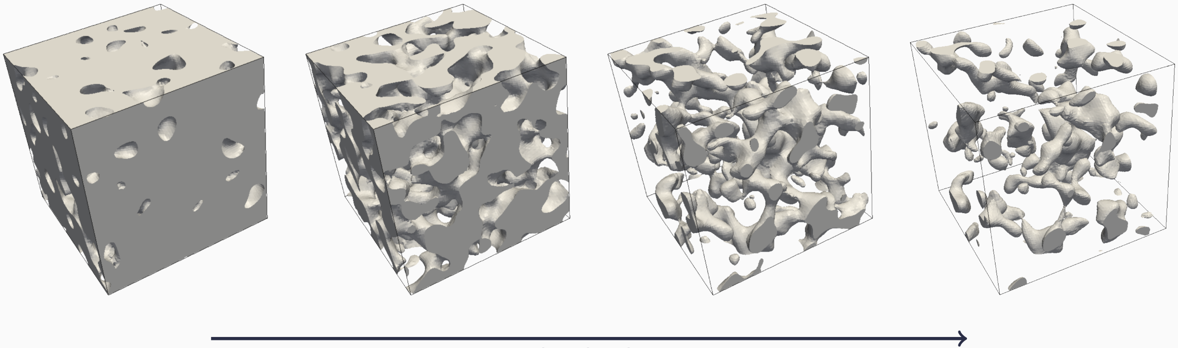
$n = 1$: Total curvature

$n = 0$: Euler Characteristic

Average of the measures over the threshold

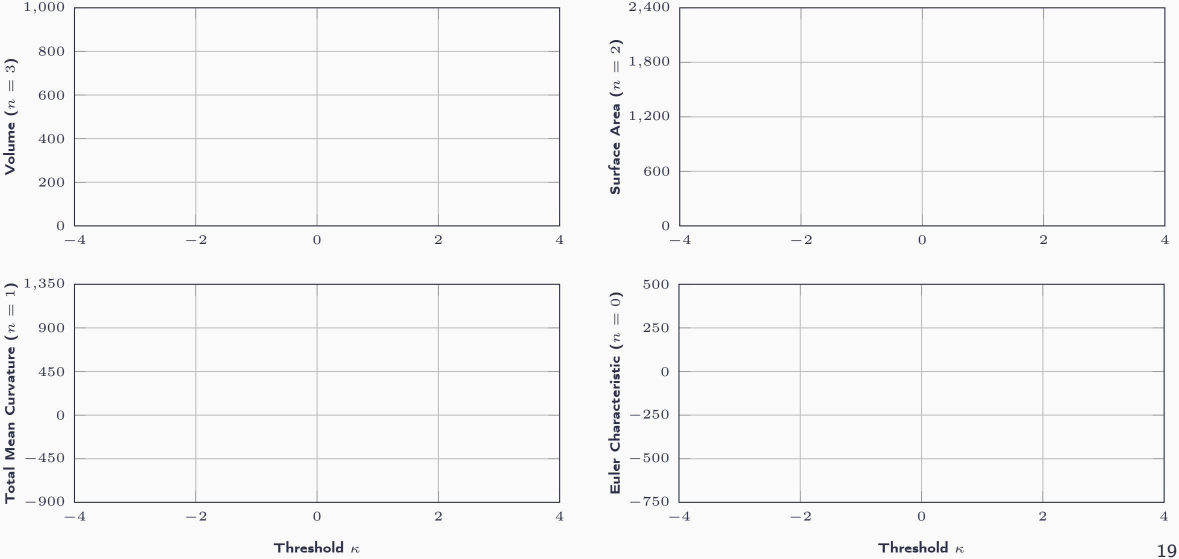


Average of the measures over the threshold

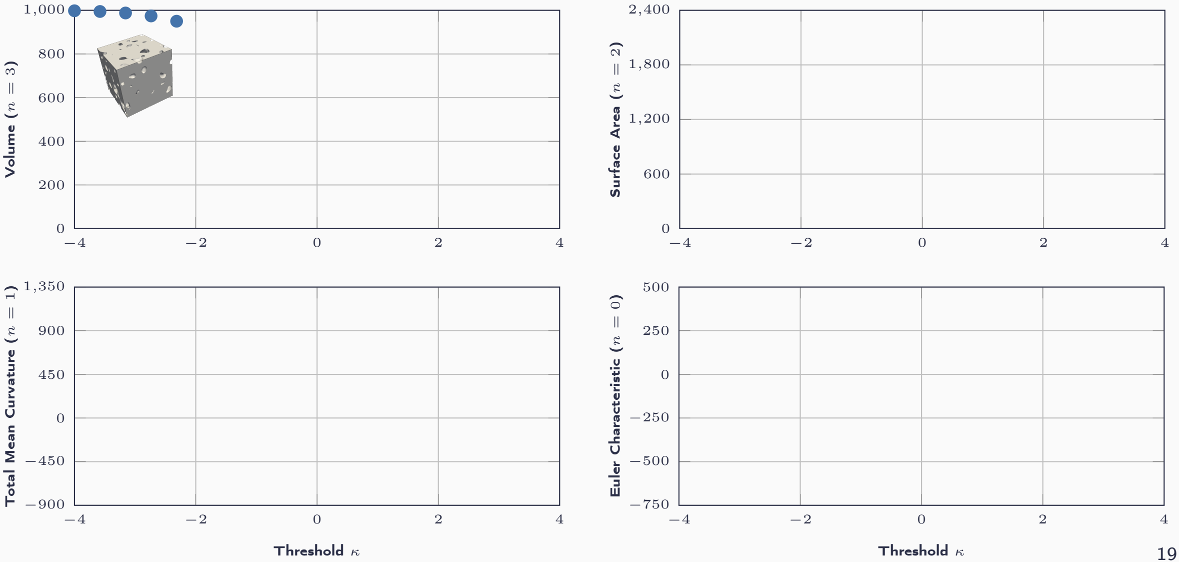


Threshold κ

Evolution of the 4 measures?


Volume ($n = 3$)
1,000
800
600
400
200
0
Surface Area ($n = 2$)
2,400
1,800
1,200
600
0
Total Mean Curvature ($n = 1$)
1,350
900
450
0
−450
−900
Euler Characteristic ($n = 0$)
500
250
0
−250
−500
−750
−4
−2
0
2
4
Threshold κ

Mean value of the measures over the threshold



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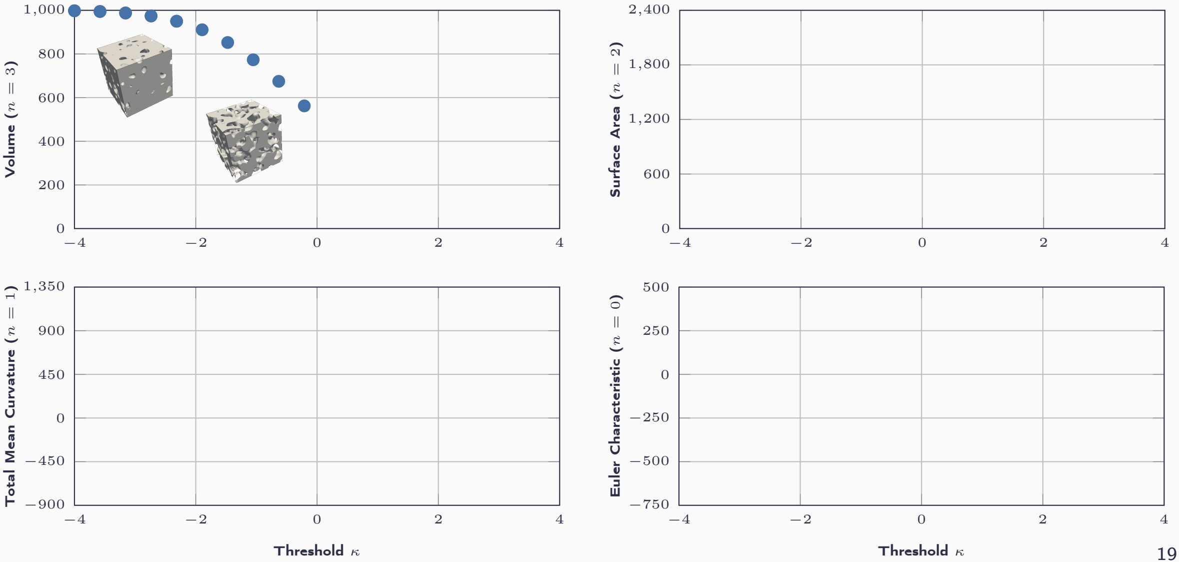

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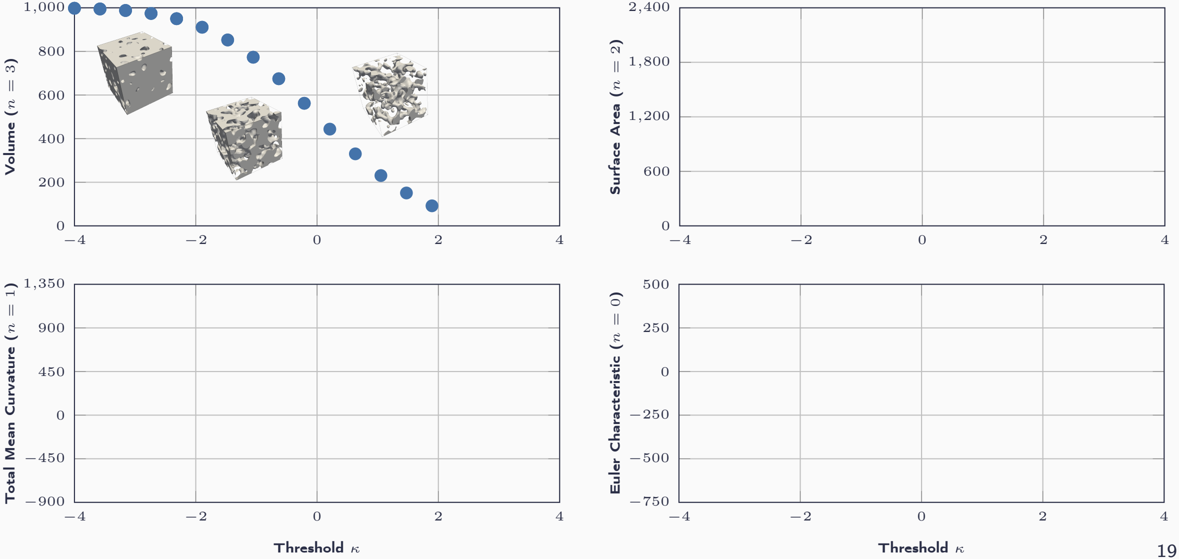
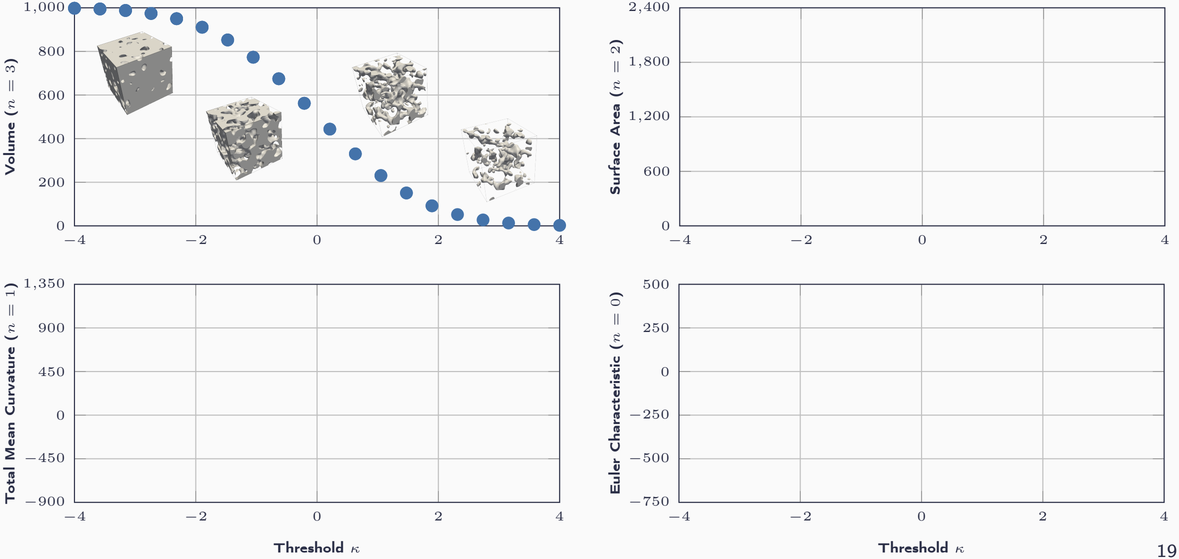


Mean value of the measures over the threshold



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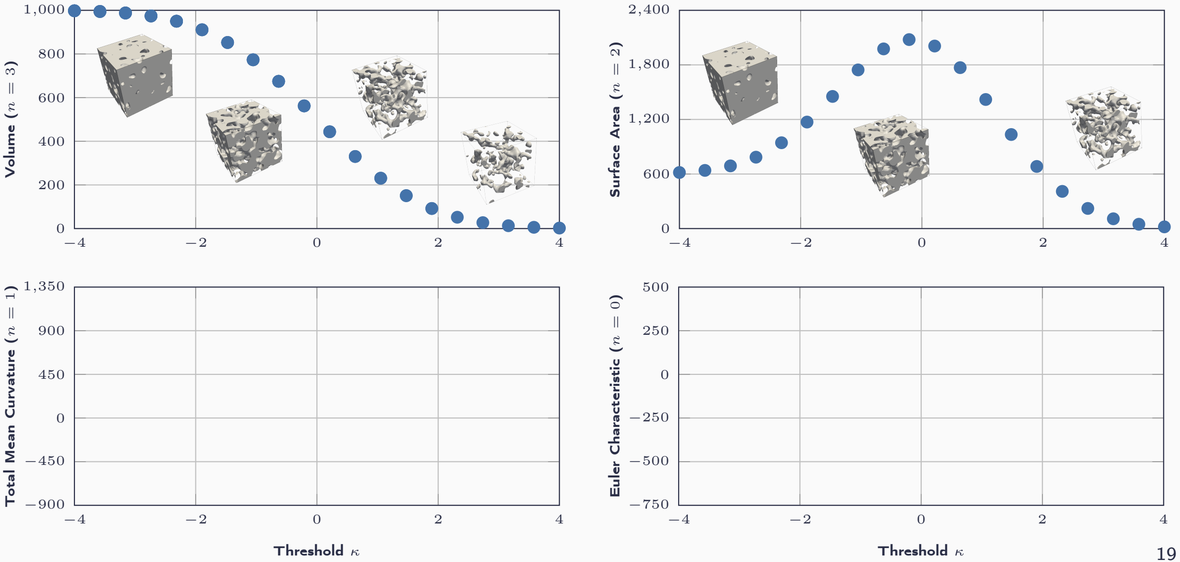

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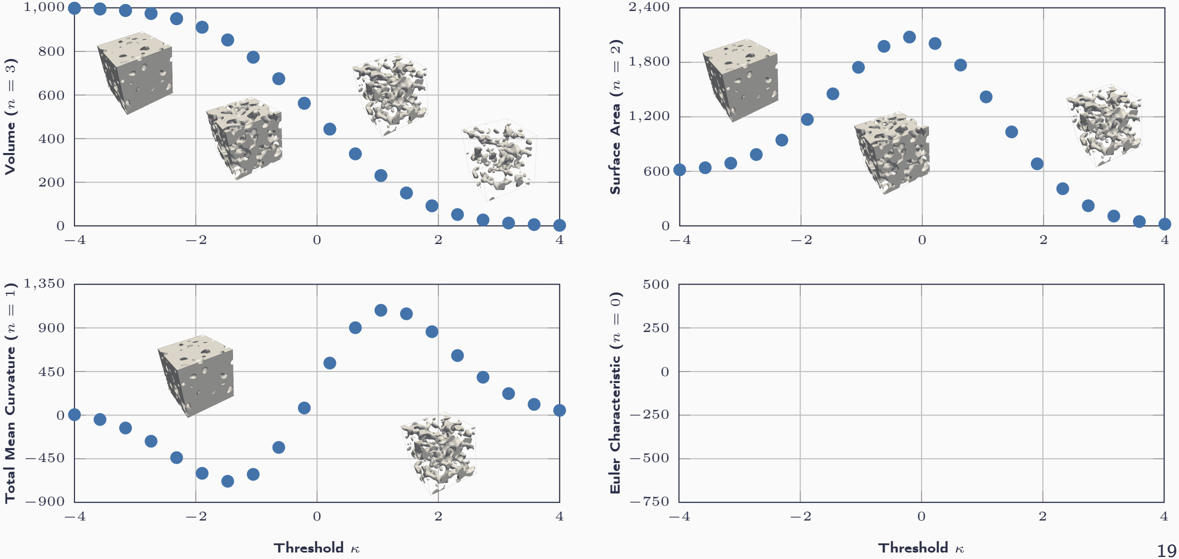

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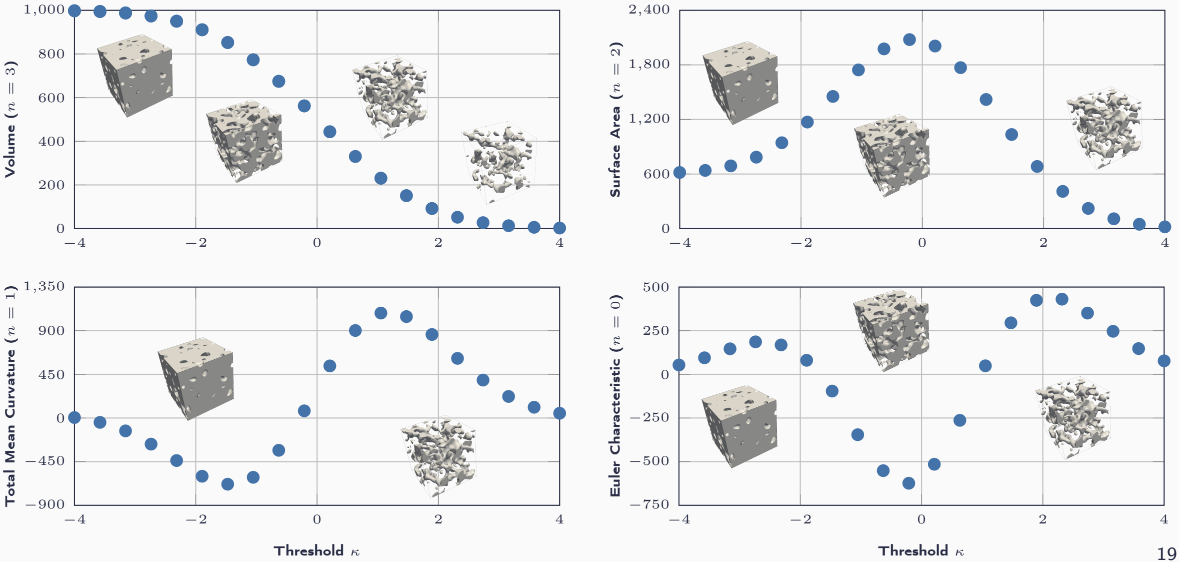

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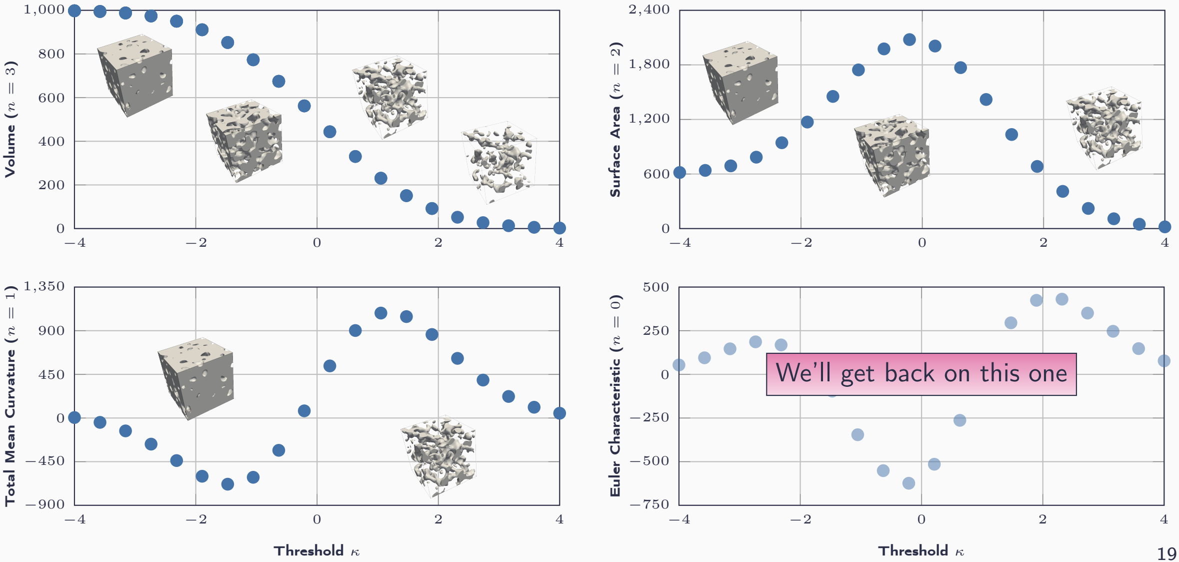

The expectation formula

In the context of **excursion sets of correlated Random Fields** each measure $\mathcal{L}_j$ is a **Random Variable**.

They have a distribution that depends on:

- the parameters of the correlated Random Field $(C(\boldsymbol{x}, \boldsymbol{y}), f_X(x), M)$
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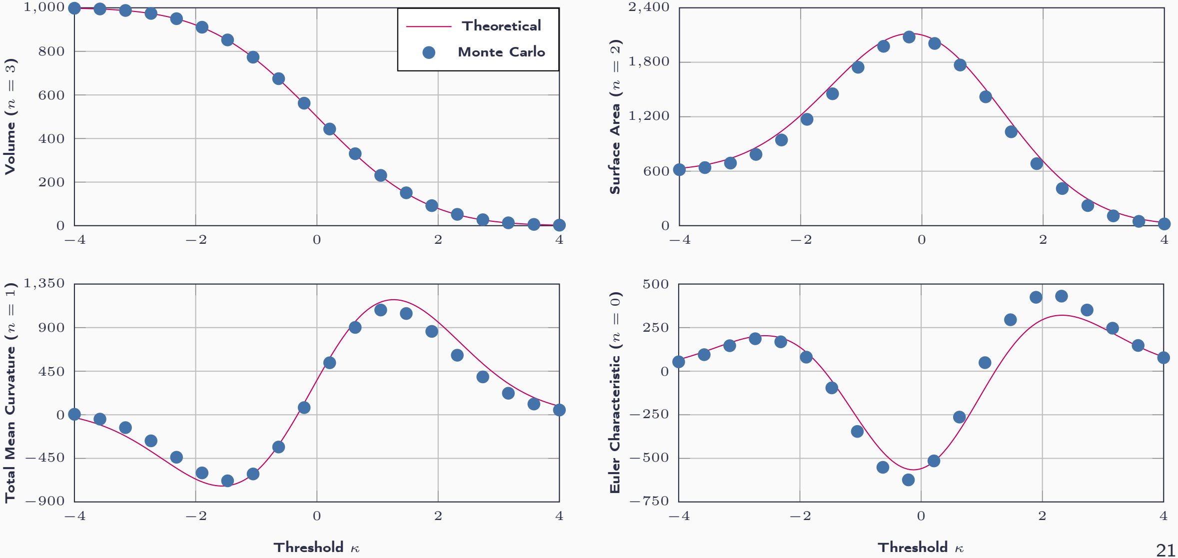
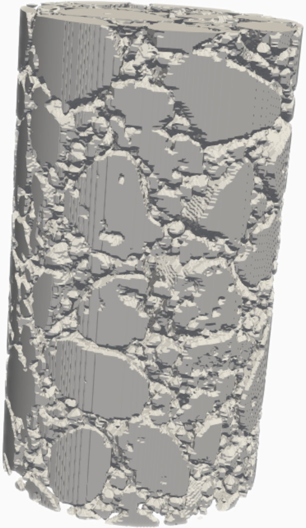


Outline

Let's simplify our goals



- 3D manifold
- with high volume fractions ($\mathcal{L}_3 > 50\,\%$)
- made of disconnected components ("$\mathcal{L}_0 > 0$")

Links between percolation theory and topology

DISCLAIMER

To be taken with a grain of salt as it's not an exact result (for $N > 2$)...
But it's good enough to proove my point ☺

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Percolation and topological quantification

They are **two different concepts**.

Percolation: find the existence of clusters of the size of the system

Topology: measure the connectivity

It has been observed that **critical behaviour** takes place close to when **Euler Characteristic changes sign**.

B. L. Okun, *Euler Charachteristic in Percolation Theory*, 1989 K. R. Mecke and H. Wagner, *Euler characteristic and related measures for random geometric sets*, 1991 H. Tomita and C. Murakami, *Percolation pattern in continuous media and its topology*, 1994

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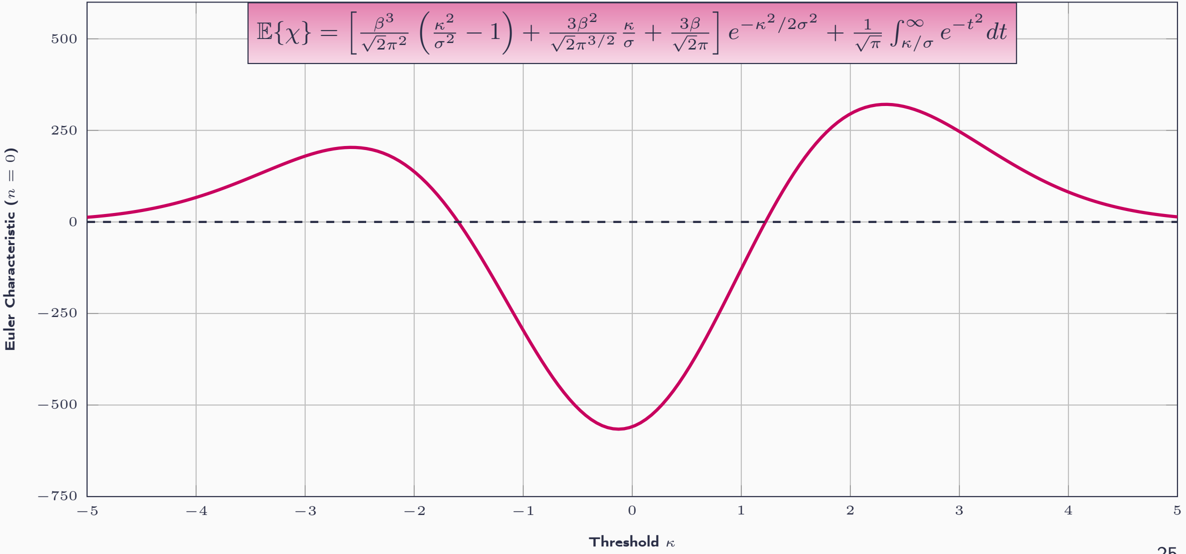

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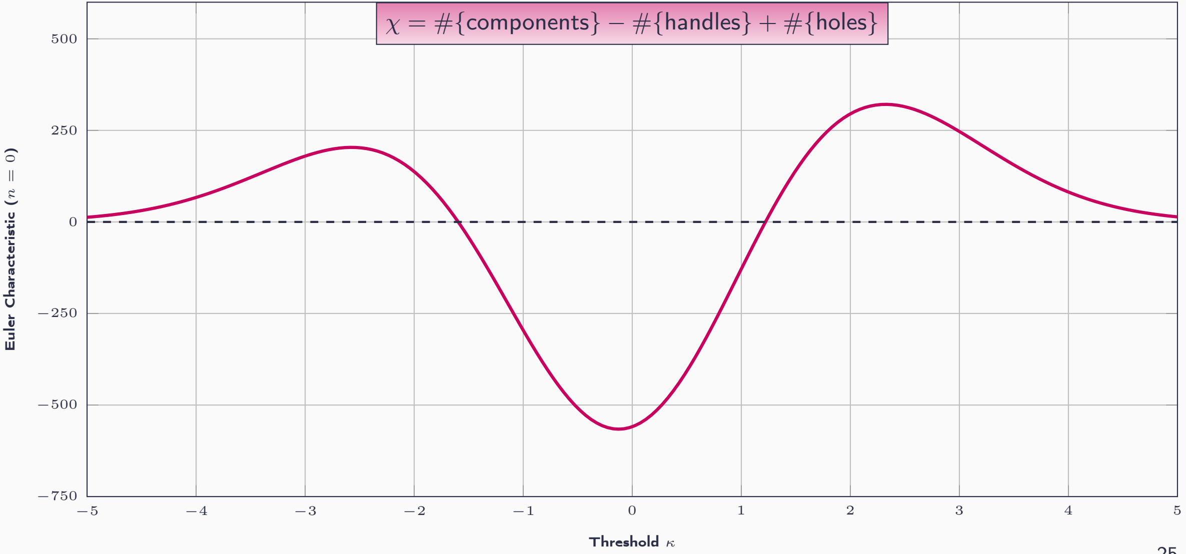

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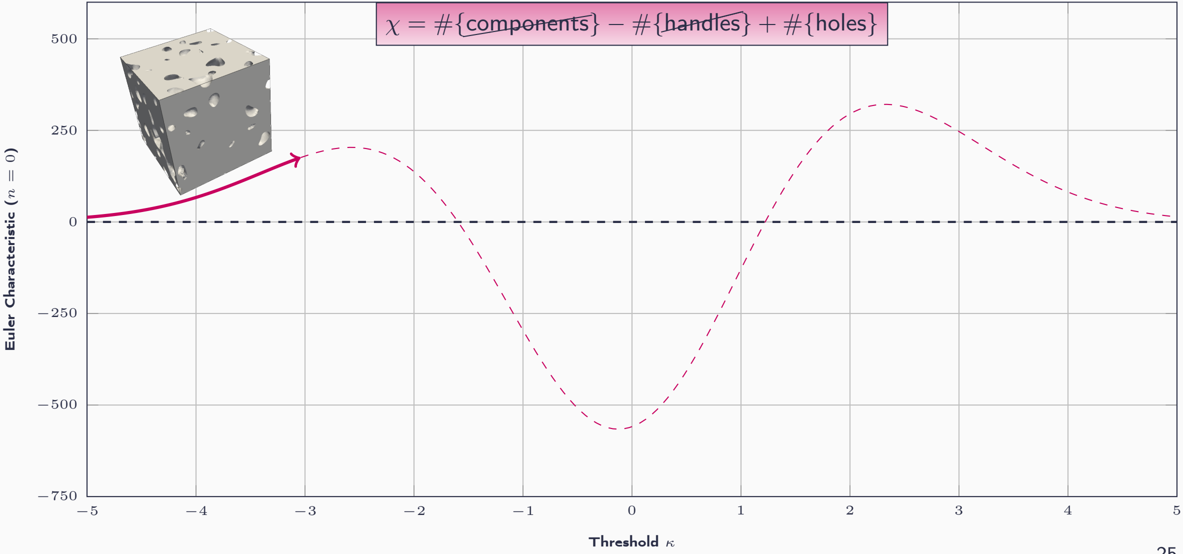

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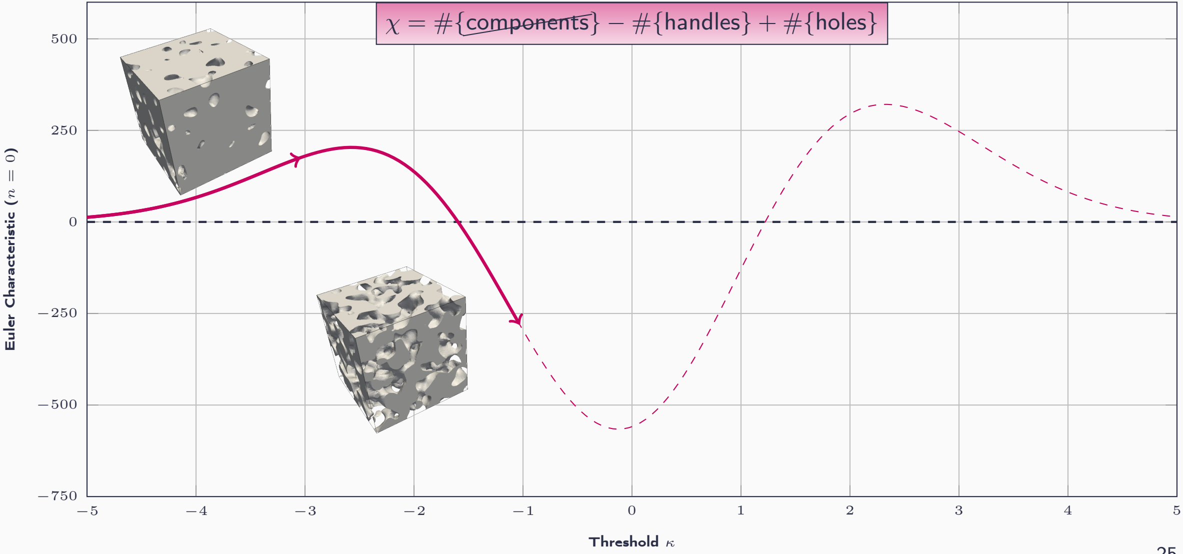

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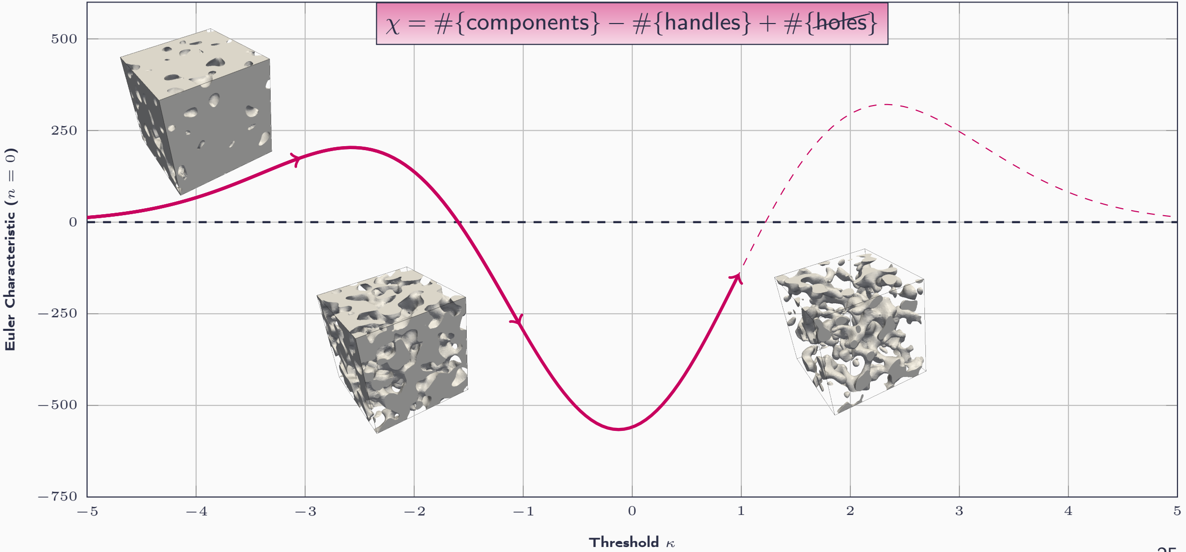

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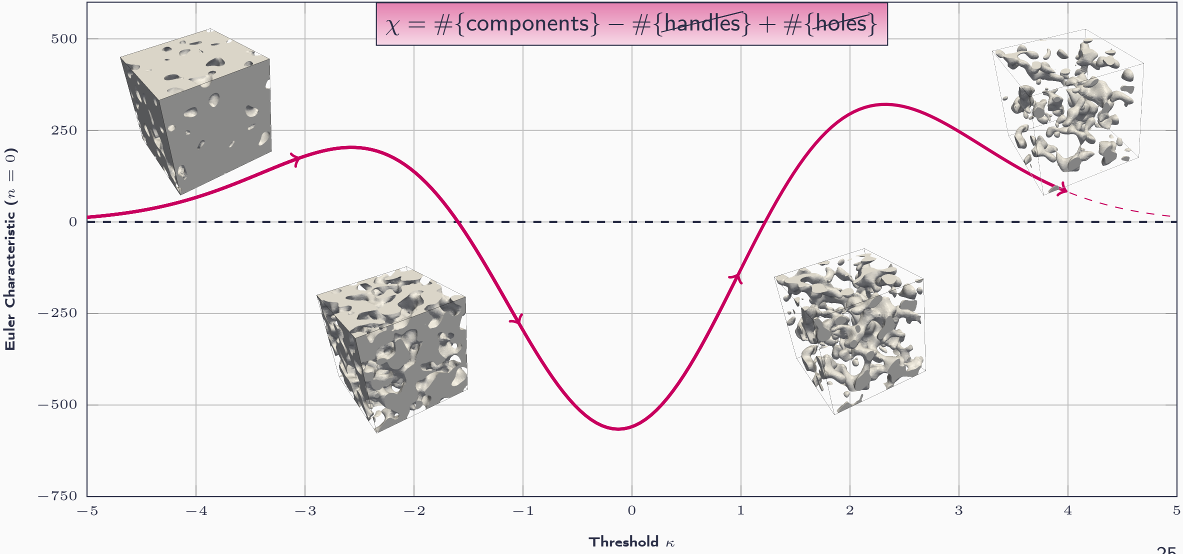

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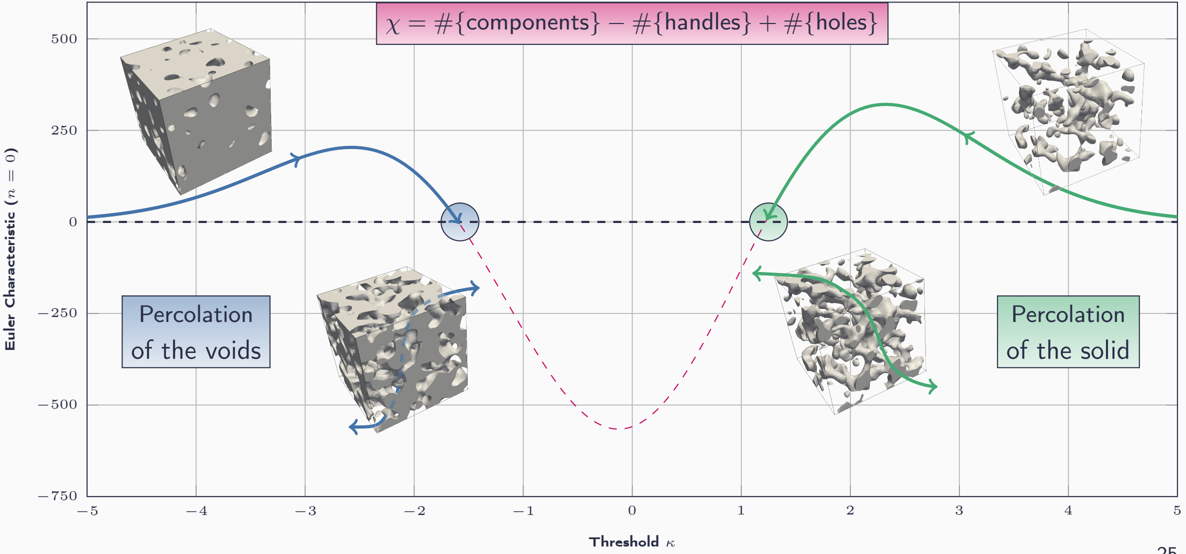

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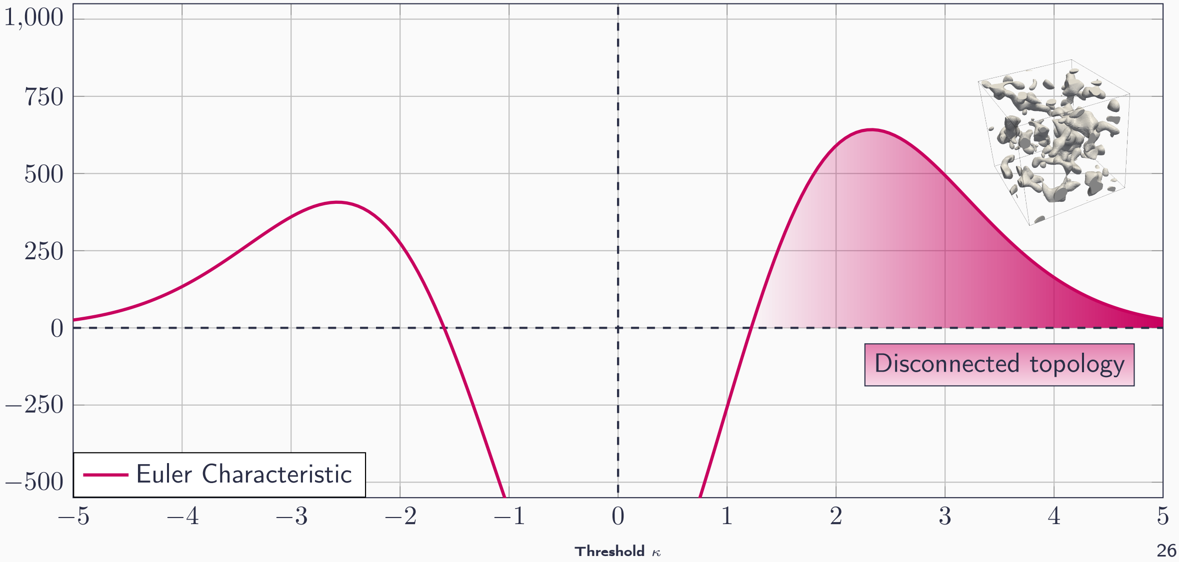

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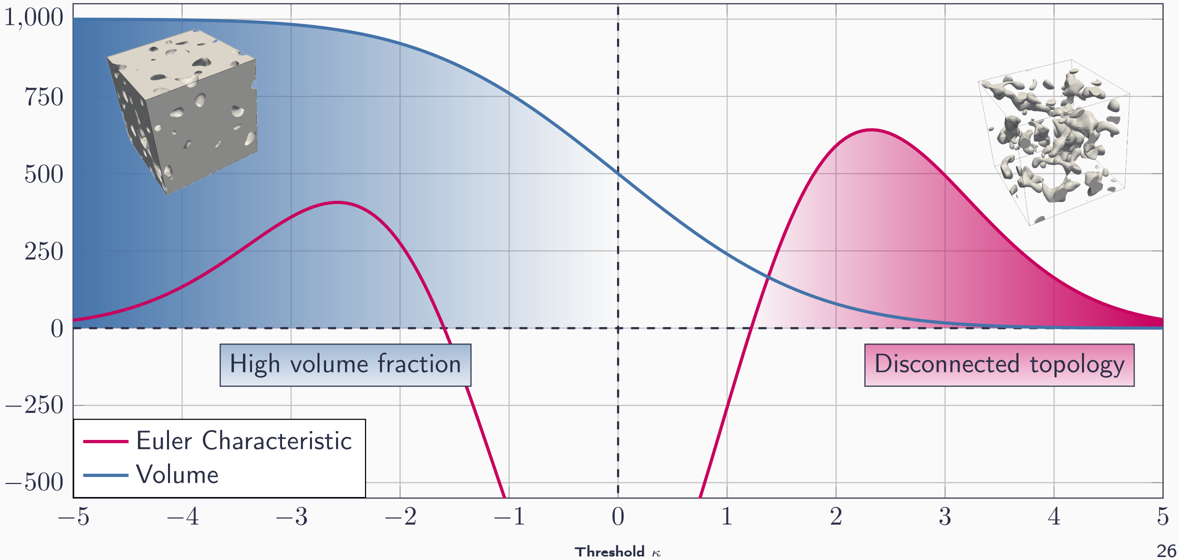

“Parameters” we can play with

So far we have restricted ourself.

$$\mathbb{E}(\mathcal{L}_j(\mathcal{E}_\mathsf{s})) = \sum_{i=0}^{N-j} \binom{i+j}{i} \frac{\omega_{i+j}}{\omega_i \omega_j} \left(\frac{\lambda_2}{2\pi}\right)^{i/2} \mathcal{L}_{i+j}(M)\, \mathcal{M}_i(\mathcal{H}_\mathsf{s})$$

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We can use any covariance function that yield a mean square differentiable RF
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Hitting set 1D (scalar RF) and $\mathcal{H}_s = [\kappa; \infty[$

- other subsets of $\mathbb{R}$ like $\mathcal{H}_s =]-\infty; \kappa] \cup [\kappa; \infty[$
- and vector valued RF leading to N-**dimensional hitting sets**.

Covariance function

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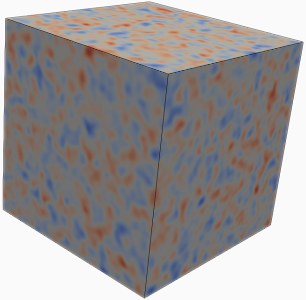
Regarding the covariance, only the **second spectral moment**

$$\lambda_2 = \left.\frac{\partial^2 \boldsymbol{C}(d)}{\partial d^2}\right|_{d_0}$$

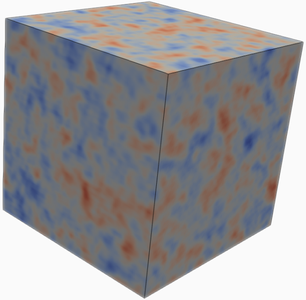
has an impact on the measure. . . which means that only the **second derivative of the covariance at 0** plays a part 😐

With the **Matérn class** we can play with the roughness (additional parameter ν):

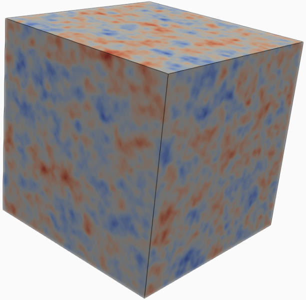
$$\boldsymbol{C}_\nu(d) = \frac{\sigma^2}{\Gamma(\nu)2^{1-\nu}} \left(\frac{\sqrt{2\nu}d}{L_c} \right)^\nu K_\nu \left(\frac{\sqrt{2\nu}d}{L_c} \right)$$



$\nu \to \infty$ (Gaussian)



$\nu = 3/2$



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Rasmussen and Williams, *Gaussian Processes for Machine Learning*, 2006

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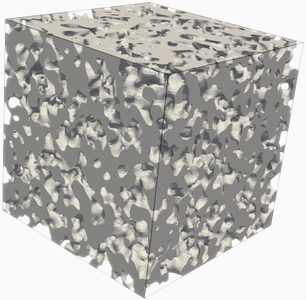

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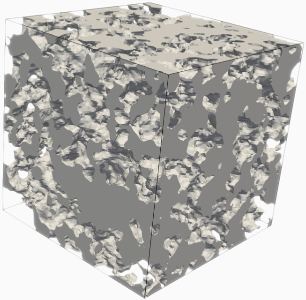

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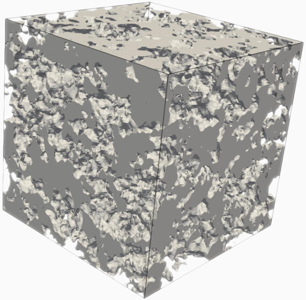

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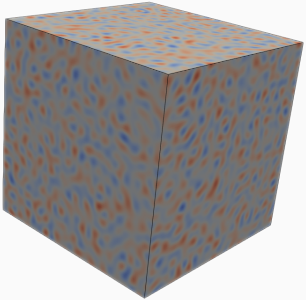

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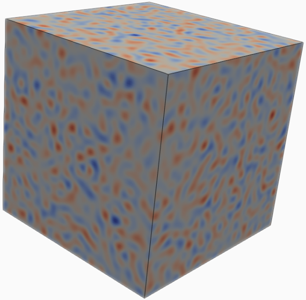

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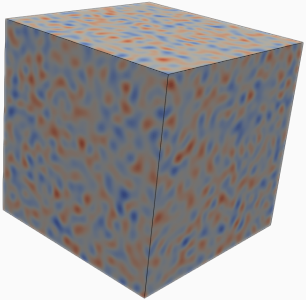

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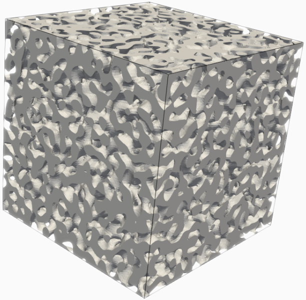

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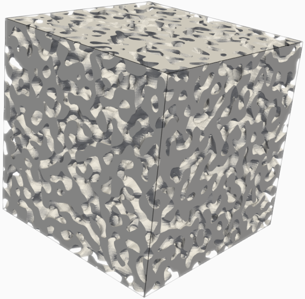

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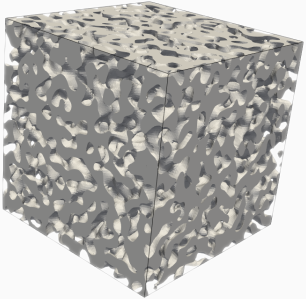

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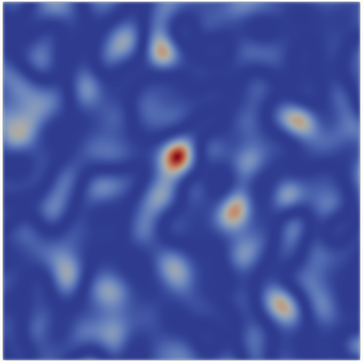
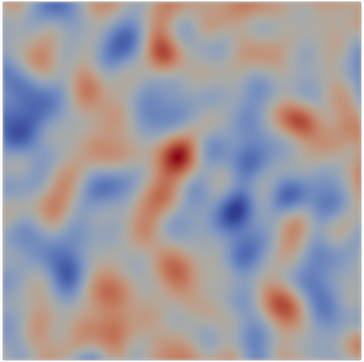
But we are still going to see a simple example with the χ_k^2 to smoothly enter the real matter of **hitting sets** and vectored valued RF.

χ_1^2

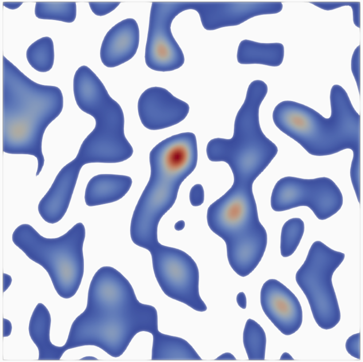


Gaussian



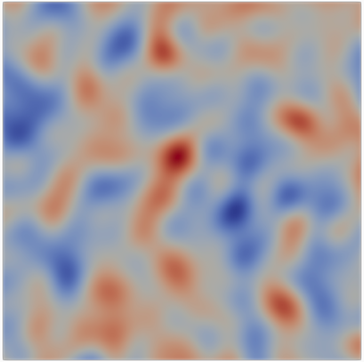
Gaussian related distributions: χ^2_k

χ^2_1



$\mathcal{H}_\mathsf{s} = [\kappa; \infty[$

Gaussian



Gaussian related distributions: χ_k^2

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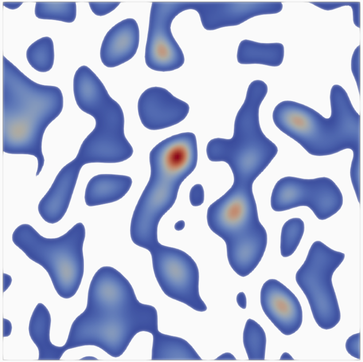

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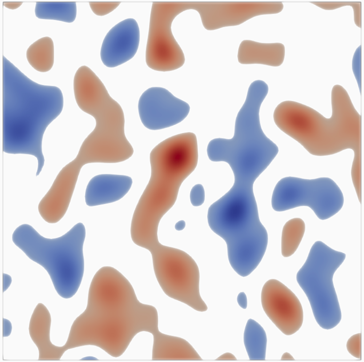

$\mathcal{H}_s = \,]-\infty; -\sqrt{\kappa}] \cup [\sqrt{\kappa}; \infty[$

χ^2_1

$\mathcal{H}_s = [\kappa; \infty[$

=

Gaussian

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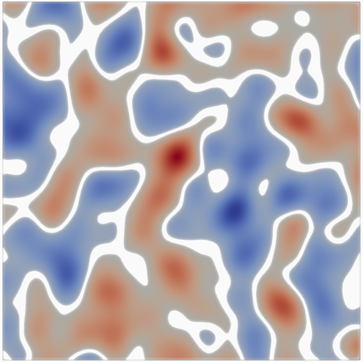
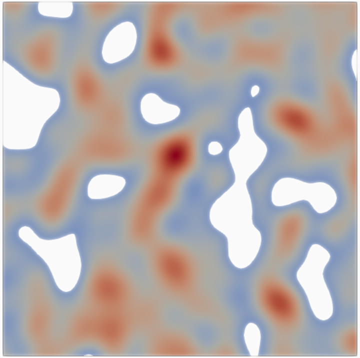
Topology of the hitting set

$\mathcal{H}_s =]-\infty; -\kappa_1] \cup [\kappa_1; \infty[$



$\mathcal{H}_s = [\kappa_2; \infty[$



κ_1, κ_2 such that we have the same surface area

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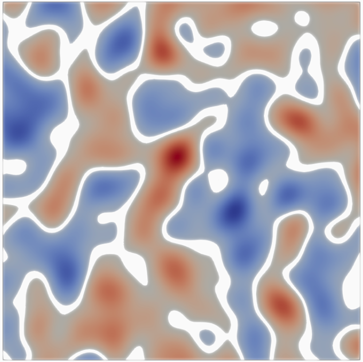

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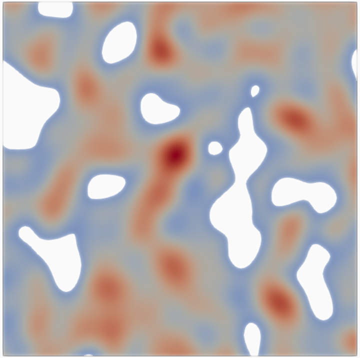

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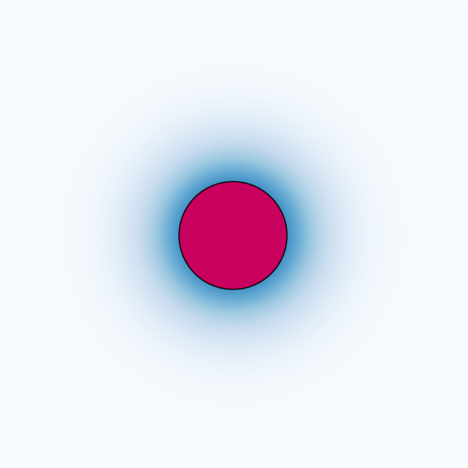
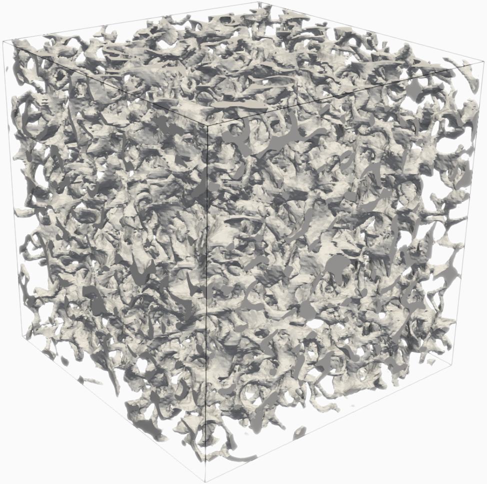
Somehow the **topology of the hitting set** is reflected onto the **topology of the excursion**.

Hitting sets in higher dimensions

Bivariate density function

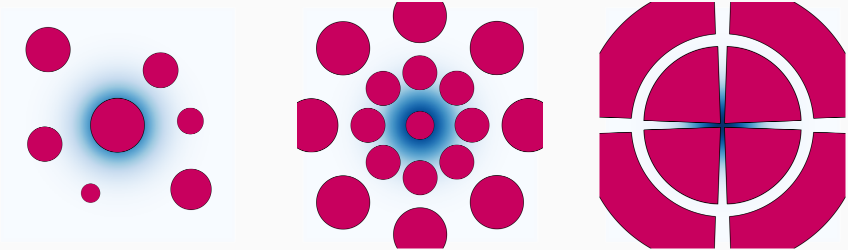
Bivariate density function





2D hitting set **3D excursion**

Hitting sets in higher dimensions



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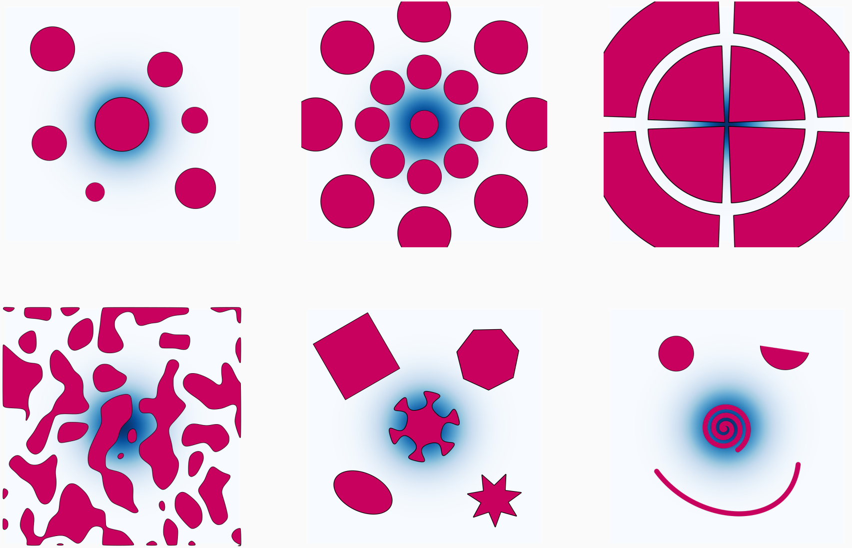

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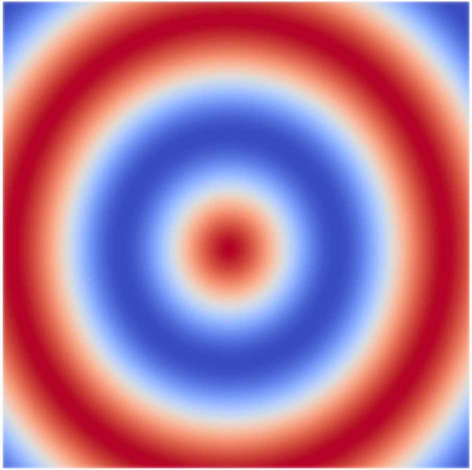
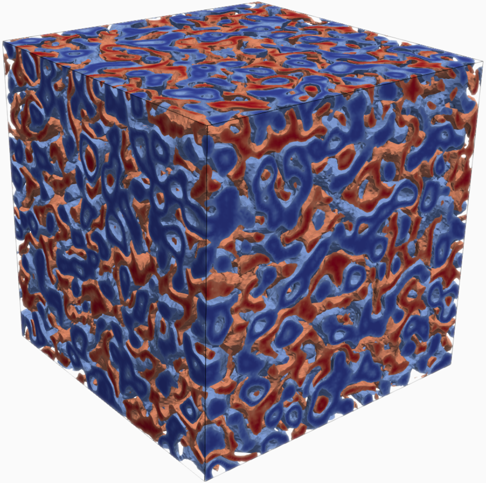
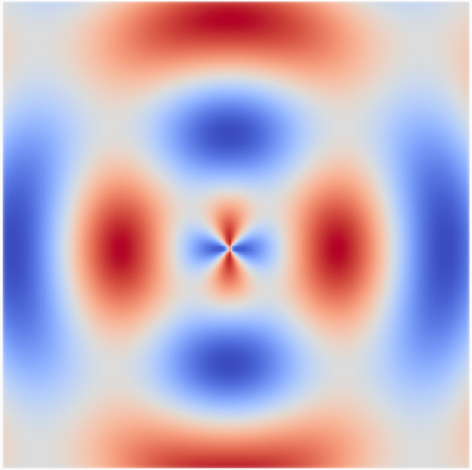
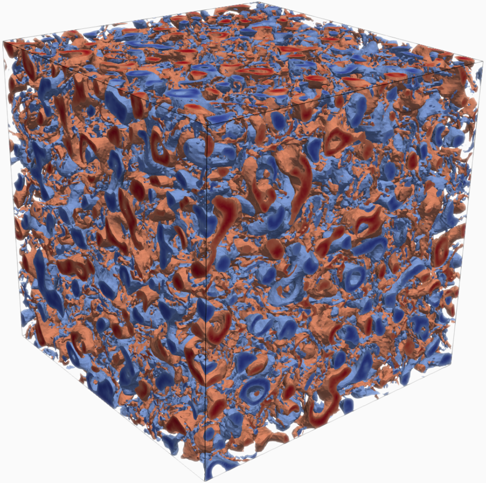




Hitting sets in higher dimensions





Questions

$$\mathbb{E}(\mathcal{L}_j(\mathcal{E}_\mathsf{s})) = \sum_{i=0}^{N-j} \binom{i+j}{i} \frac{\omega_{i+j}}{\omega_i \omega_j} \left(\frac{\lambda_2}{2\pi}\right)^{i/2} \mathcal{L}_{i+j}(M)\, \mathcal{M}_i^{\gamma}(\mathcal{H}_\mathsf{s})$$

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- Is there a solution?
- How can we have a more pragmatic approach to explore the possibilites?
- Am I missing some “parameters” we can play with?

The expectation formula

Gaussian Minkowski functionals: $\mathcal{M}_i^{\gamma_k}(\mathcal{H}_\mathsf{s})$

- They measure the probability of the Random Field to be in the hitting set $\mathcal{H}_\mathsf{s} \subset \mathbb{R}^k$.
- They are Minkowski functionals associated with the measure of a Gaussian distribution γ_k.

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Kinematic formula

If $\boldsymbol{X} = X_i$ is a standard Gaussian vector of size k in which $X_i \sim \mathcal{N}(0, \sigma^2)$ are independant and $\mathcal{H}_\mathsf{s} \subset \mathbb{R}^k$:

$$\gamma_k(\mathcal{H}_\mathsf{s}) = P(\boldsymbol{X} \in \mathcal{H}_\mathsf{s}) = \frac{1}{\sigma^k (2\pi)^{k/2}} \int_{\mathcal{H}_\mathsf{s}} e^{-\|\boldsymbol{x}\|^2/2\sigma^2} d\boldsymbol{x}$$

J. Taylor, *A Gaussian kinematic formula*, 2006

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If $\mathcal{K}(A, \rho)$ is the tube of A or ray ρ we have the following Taylor expansion:

$$\gamma_k(\mathcal{K}(\mathcal{H}_\mathsf{s}, \rho)) = \sum_{j=0}^{\infty} \frac{\rho^j}{j!} \mathcal{M}_i^{\gamma_k}(\mathcal{H}_\mathsf{s})$$

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Application to scalar valued Gaussian Random Fields: $\mathcal{M}_i^\gamma(\mathcal{H}_\mathsf{s})$

Hitting set, Tube and expansions

$\mathcal{H}_\mathsf{s}$ and Tube $\mathcal{H}_\mathsf{s} = [\kappa, \infty[$ and $\mathcal{K}(\mathcal{H}_\mathsf{s}) = [\kappa - \rho, \infty[$

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Identification of the Gaussian Minkowski Functionals

$$\mathcal{M}_i^\gamma(\mathcal{H}_s) = (-1)^j \bar{F}^{(i)}(\kappa)$$

The expectation formula

Volume Fraction

$$\mathbb{E}\{\Phi\} = \frac{1}{\sqrt{\pi}} \int_{\kappa/\sigma}^{\infty} e^{-t^2} dt$$

Euler Characteristic

With the scale ratio $\beta = \text{size}(M)/L_c$

$$\mathbb{E}\{\chi\} = \left[\frac{\beta^3}{\sqrt{2}\pi^2} \left(\frac{\kappa^2}{\sigma^2} - 1 \right) + \frac{3\beta^2}{\sqrt{2}\pi^{3/2}} \frac{\kappa}{\sigma} + \frac{3\beta}{\sqrt{2}\pi} \right] e^{-\kappa^2/2\sigma^2} + \frac{1}{\sqrt{\pi}} \int_{\kappa/\sigma}^{\infty} e^{-t^2} dt$$

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R.J. Adler, *Random Fields and Geometry*, 1976

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