— RV Seminars—

Critical probability of percolation over bounded region in $N-$dimensional Euclidean space

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05/04/2019

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Journal of Statistical Mechanics: Theory and Experiment
An IOP and SISSA journal

PAPER: Disordered systems, classical and quantum

Critical probability of percolation over bounded region in N-dimensional Euclidean space

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Received 28 October 2015
Accepted for publication 7 February 2016
Published 22 March 2016

Online at stacks.iop.org/JSTAT/2016/033306
doi:10.1088/1742-5468/2016/03/033306

Outline

Morphological model based on correlated Random Fields

Outline

Macro vs Meso

Problematic: Take into account the **internal variability** of the material

Macroscopic point of view

Mesoscopic point of view

Macro vs Meso

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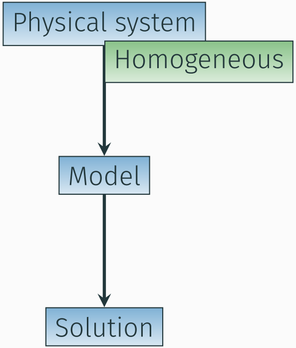

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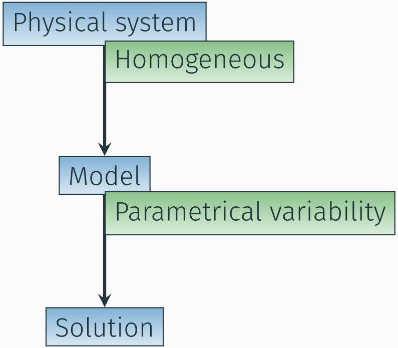

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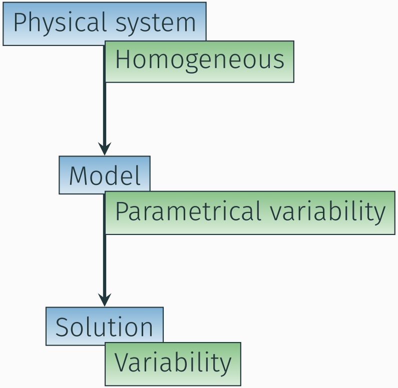

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Macroscopic point of view

Physical system
Homogeneous
↓
Model
Parametrical variability
↓
Solution
Variability

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Heterogeneities

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New sets of variabilities

Morphological variability

Local parametrical variability

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- Morphological variability
- Local parametrical variability

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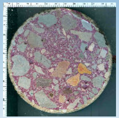

New sets of variabilities

Morphological variability

Local parametrical variability

Necessity of a **morphological model**

Morphological models

Goals:

- **Random** aspect of heterogeneities shape and positions
- **Discrete** aspect
- Size distribution of the heterogeneities…

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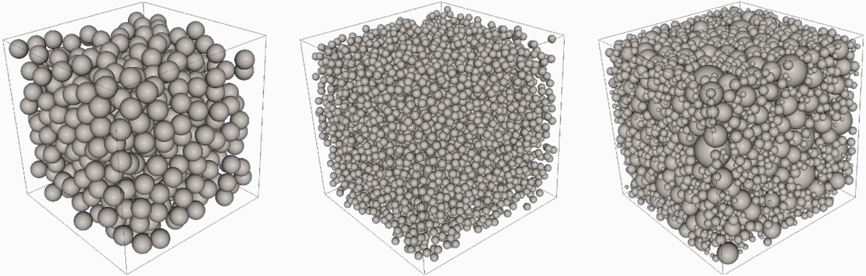

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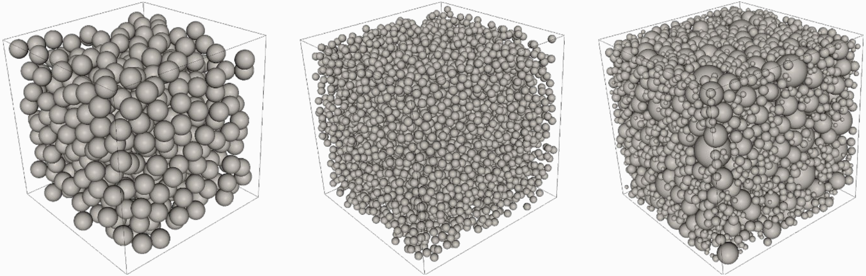

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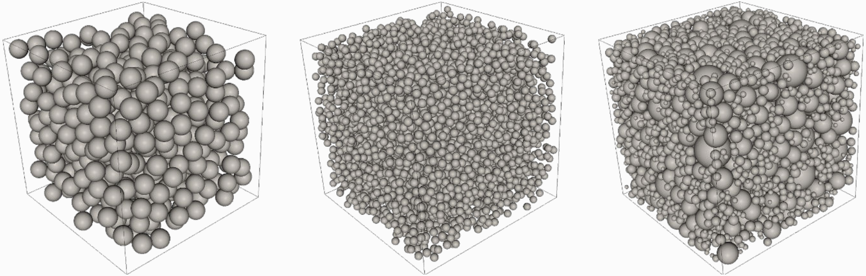

Simple, natural and efficient , one “kind” of morphology, ideal shapes, heavy

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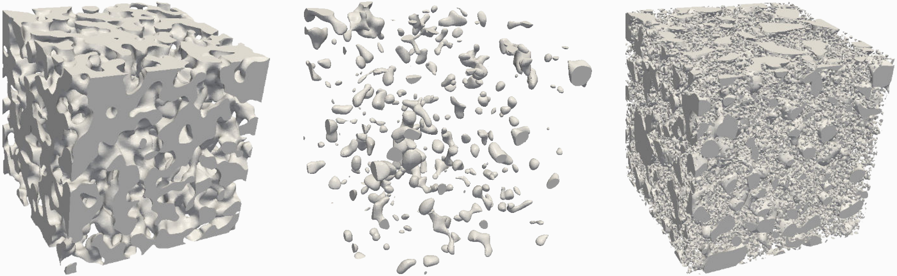
Morphological models

Excursion set of correlated Random Fields:



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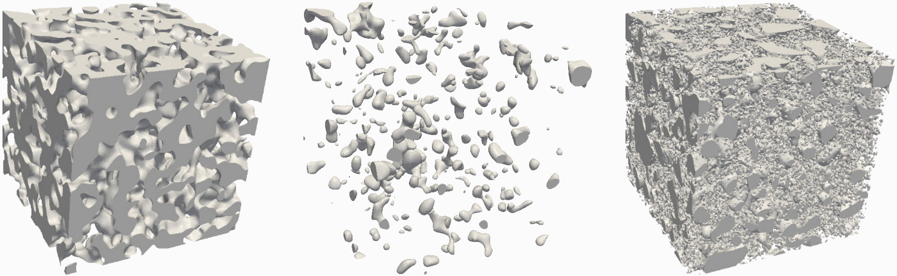

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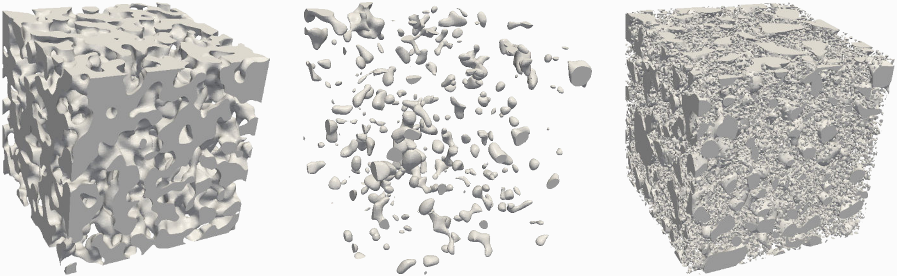

- Different "kinds" of morphologies, light, random shapes, evolutive
- Hard to control, distribution less natural, smooth surfaces (for now)

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Outline

Probabilistic framework

Random Variables

It represents a phenomenon possessing an **unpredictible output** which, **with repetition** can possess a **regular nature**.
The **theory of probability** is mathematical framework to model those processes.

A. Kolmogorov, *Foundations of the Theory of Probability*, 1933.

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To put in simply, in our case we can define a Random Variable as a function: $X : \Omega \mapsto E$ where Ω the set of all the possible results of the experiment.

If A is a subset of E we often note the event $X^{-1}(\omega) = \{\omega \in \Omega, X(\omega) \in A\}$: $\{X \in A\}$

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Ω is set with a probability function P measuring the chance of such an event to occur:

$$P(X \in A) = \int_A f_X(x)dx \quad \forall A \subset E$$

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Probability function of a Random Variable

Here, RV take value in $\mathbb{R}$. The density probability function $f_X : \mathbb{R} \mapsto \mathbb{R}^+$:
The probability function is:

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From this distribution the first two moments are known as:

The **expected value:** $\mathbb{E}(X) = \int_{\mathbb{R}} x f_X(x)dx$ and the **variance:** $\mathbb{V}(X) = \int_{\mathbb{R}} x^2 f_X(x)dx$

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Lack of spatial structure

Correlated Random Fields

Based on the same definition, a **correlated Random Field** (RF) is defined by adding to the function X a space parameter. If g is such a field, it is defined over both

- Ω, the probability space
- $M \subset \mathbb{R}^N$, an Euclidean space

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

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Covariance functions

In order to statistically control the spatial structure of the field a **covariance function** is defined (for a zero mean distribution):

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- If $g(\boldsymbol{x})$ and $g(\boldsymbol{y})$ are independent: $C(\boldsymbol{x}, \boldsymbol{y}) = \mathbb{E}(g(\boldsymbol{x}))\mathbb{E}(g(\boldsymbol{y})) = 0$
- $C(\boldsymbol{x}, \boldsymbol{x}) = \mathbb{E}(g(\boldsymbol{x})^2) = \mathbb{V}(g(\boldsymbol{x}))$

Correlated Random Fields

Technically to define a **stricly stationary correlated Random Field** we have to define:

- A constant probability distribution over the spatial parameter $\boldsymbol{x}$. $g(\boldsymbol{x})$ can be seen as a RV X. A classical distribution is the **Gaussian distribution** $\mathcal{N}(\mu, \sigma)$ where μ is the mean value and σ the standard deviation:

$$f_X(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-(x-\mu)^2/2\sigma^2}$$

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- A covariance function wich depends on the distance between two points in space $d = \|\boldsymbol{x} - \boldsymbol{y}\|$. A classical choice is the **Gaussian covariance function**:

$$C(d) = \sigma^2 e^{-d^2/L_c^2}$$

Correlation length L_c

The Gaussian correlation function

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has a single structural parameter L_c called the **correlation length**.

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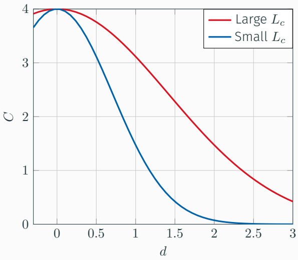
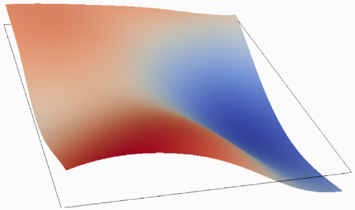
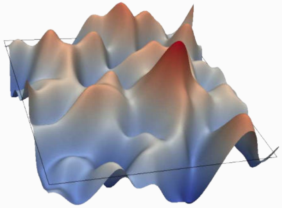




Large L_c



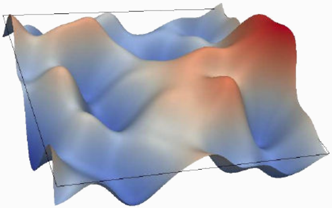
Small L_c

Correlated Random Fields

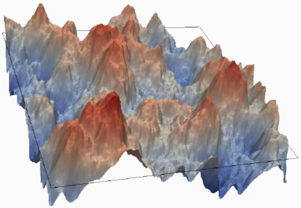
Out of topic... but other classes of covariance functions bring more flexibilty.

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

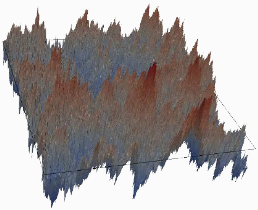
$$C(d) = \frac{\sigma^2}{\Gamma(\nu)2^{1-\nu}} \left(\frac{\sqrt{2\nu}d}{L_c} \right)^{\nu} K_{\nu} \left(\frac{\sqrt{2\nu}d}{L_c} \right)$$



$\nu \to \infty$
Gaussian



$\nu = 3/2$



$\nu = 1/2$
Exponential

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

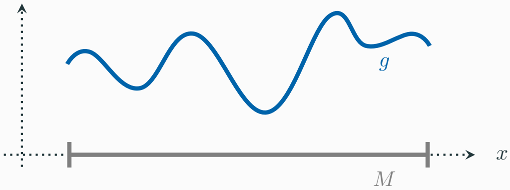
Outline

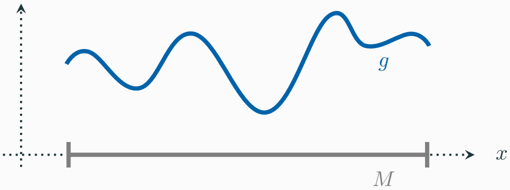
Definition of an excursion set

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**.





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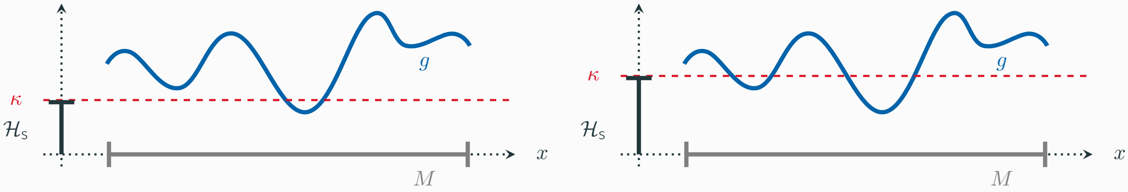

Excursion with “low” threshold

Excursion with “high” threshold

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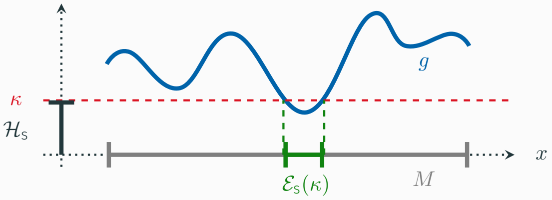
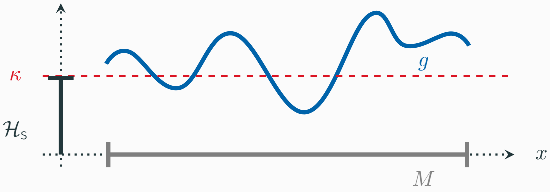


Excursion with "low" threshold



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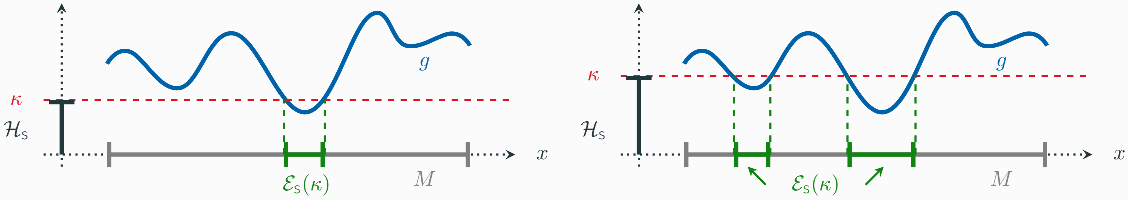

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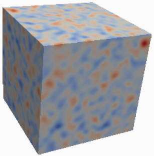
Excursion with "high" threshold

Excursion sets and scale factor

Medium L_c



Correlated Random Fields

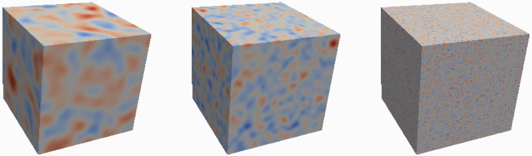
$g : \Omega \times \mathbb{R}^3 \mapsto \mathbb{R}$

Continuous aspect

parametric variability

Excursion sets and scale factor

Large L_c Medium L_c Small L_c



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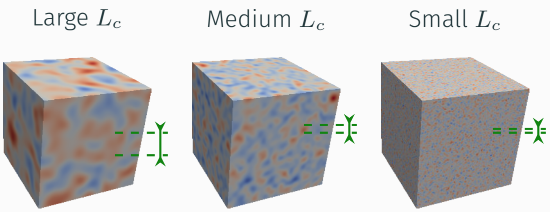

Heterogeneity sizes

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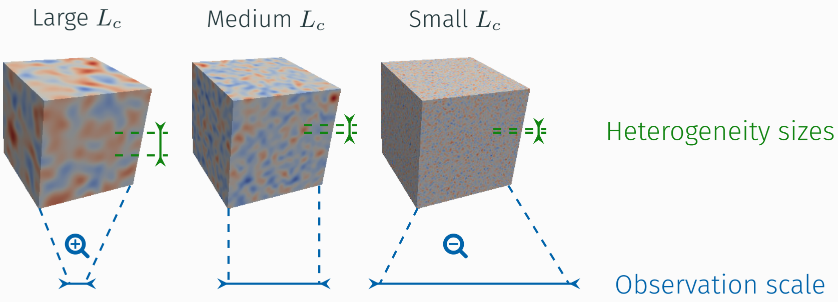

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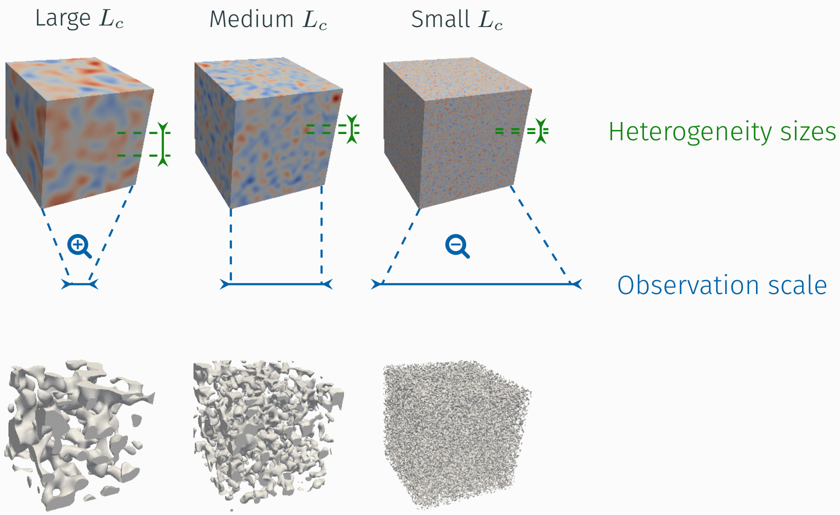
Discrete aspect

explicit morphology



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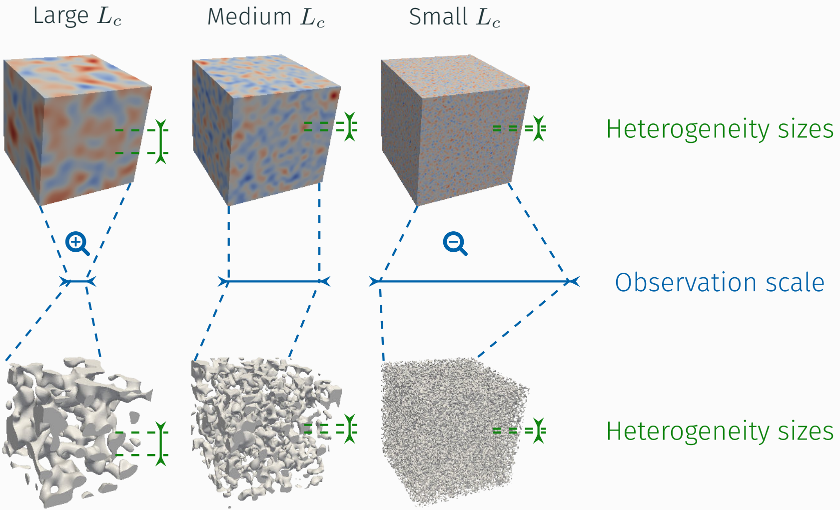

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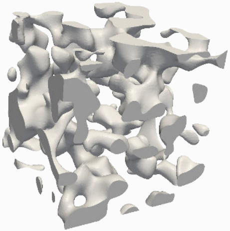
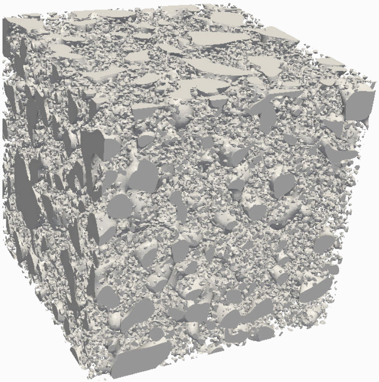
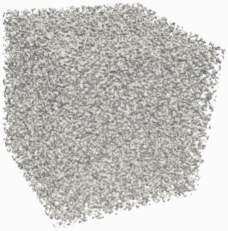
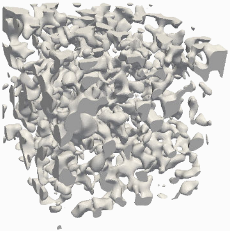
Discrete aspect
explicit morphology

A large set of morphologies









Standard mathematical measures of manifolds

Outline

Family of measures

It exists several **family of measures** (Minkowski functionals, Lipschitz-Killing curvatures...). In an $N-$dimensional space, the size of the family 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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Here we simplify by using known **linear combinasions** of those which gives:

In 2D

$n = 2$: Surface area

$n = 1$: Total curvature

$n = 0$: Euler Characteristic

Family of measures

It exists several **family of measures** (Minkowski functionals, Lipschitz-Killing curvatures...). In an $N-$dimensional space, the size of the family 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** $(n = 0)$

Here we simplify by using known **linear combinasions** of those which gives:

In 2D

$n = 2$: Surface area

$n = 1$: Total curvature

$n = 0$: Euler Characteristic

In 3D

$n = 3$: Volume

$n = 2$: Surface area

$n = 1$: Total curvature

$n = 0$: Euler Characteristic

The Euler Characteristic

The Euler Characteristic: a topological measure

The Euler Characteristic is a mathematical measure that gives information on the topology of the morphology.
It enumerates $n-$dimensional features.

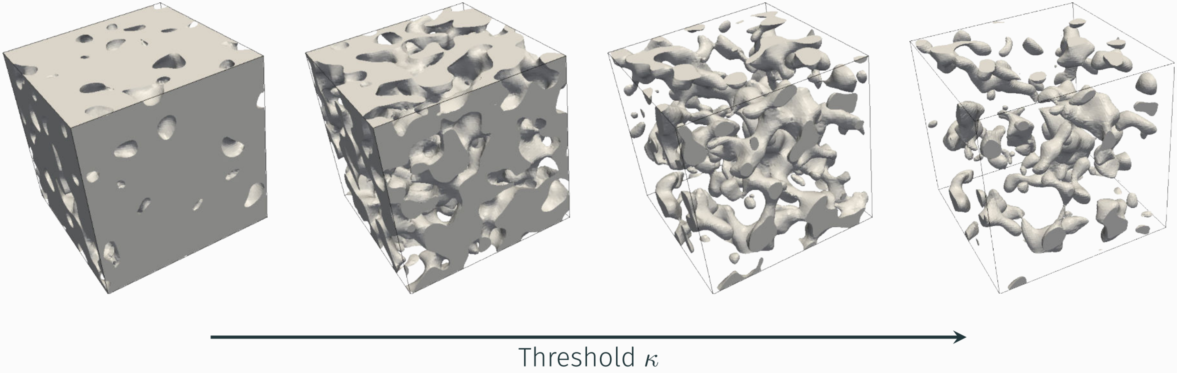
- In 2D

$$\chi = \#\{\text{connected components}\} - \#\{\text{holes}\}$$

- In 3D

$$\chi = \#\{\text{connected components}\} - \#\{\text{handles}\} + \#\{\text{holes}\}$$

Mean value of the measures over the threshold



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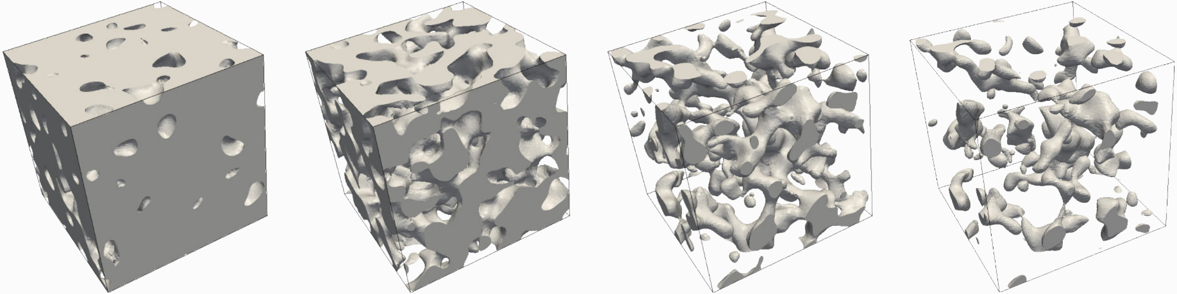
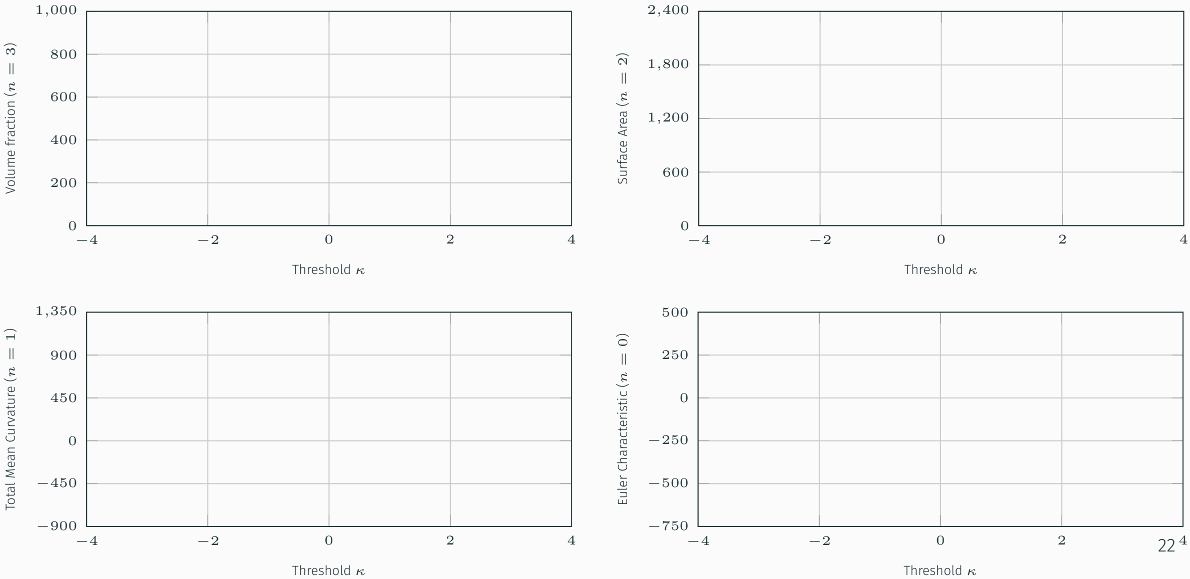


Threshold κ

Evolution of the 4 measures?

Mean value of the measures over the threshold



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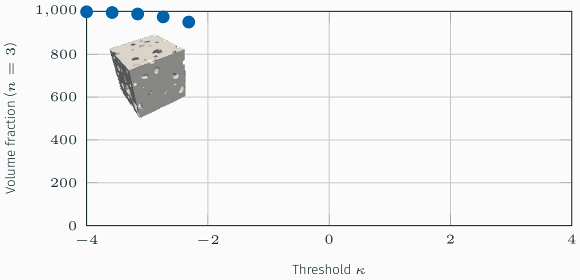

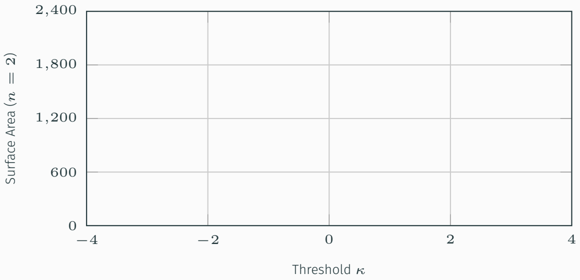

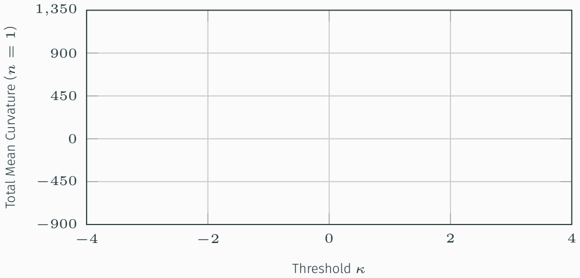

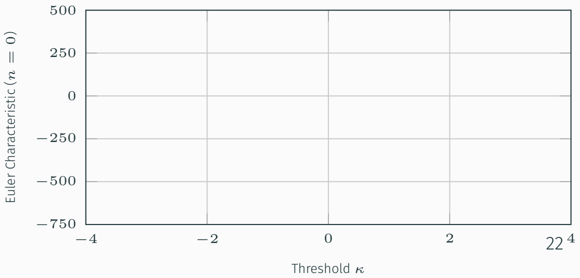

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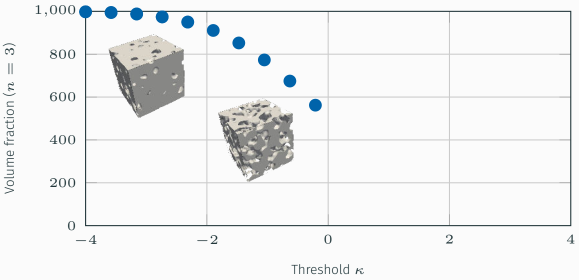

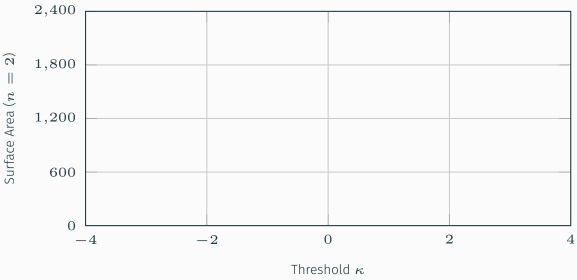

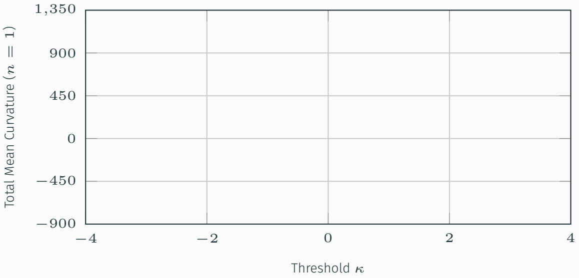

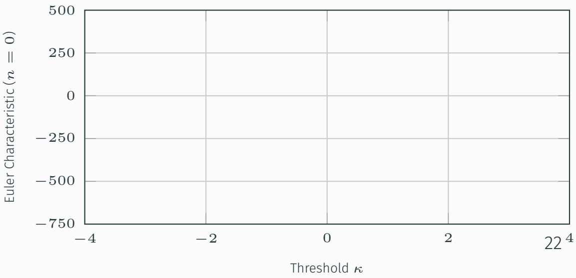

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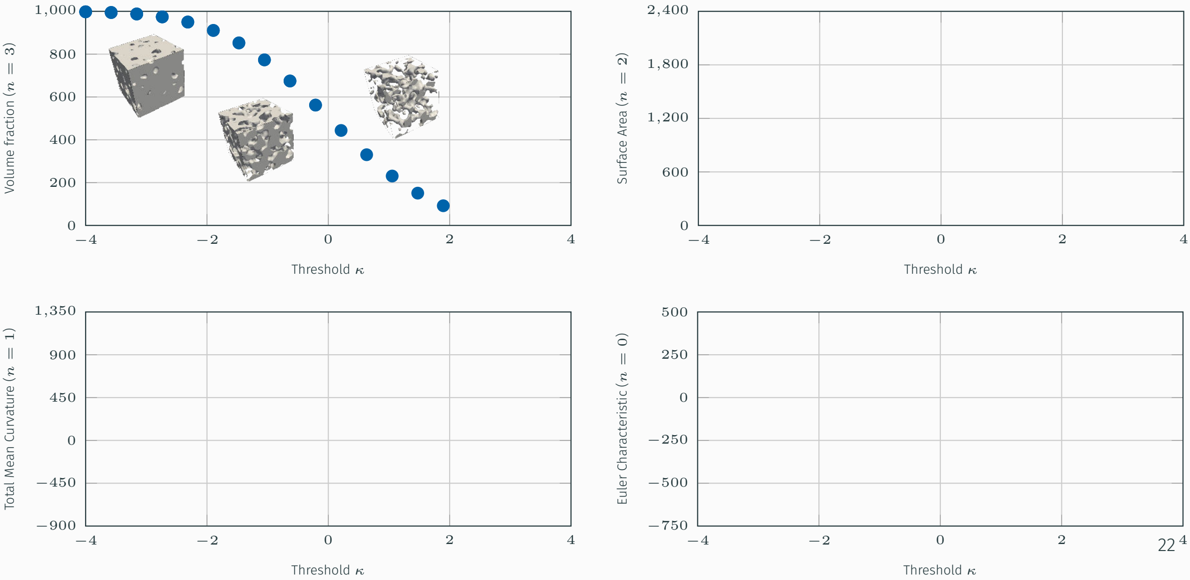

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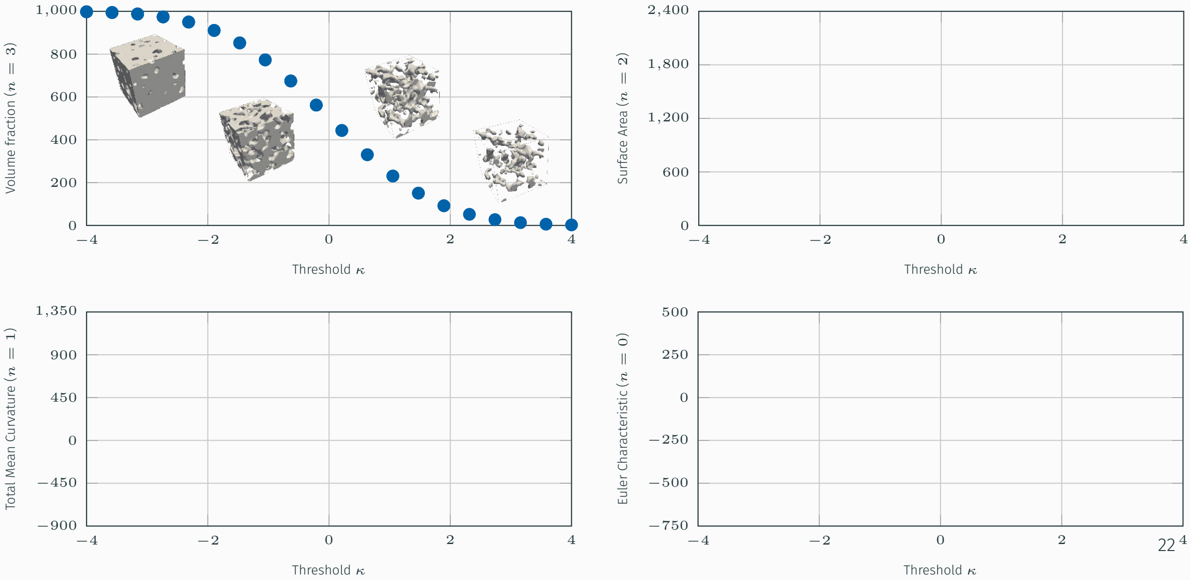

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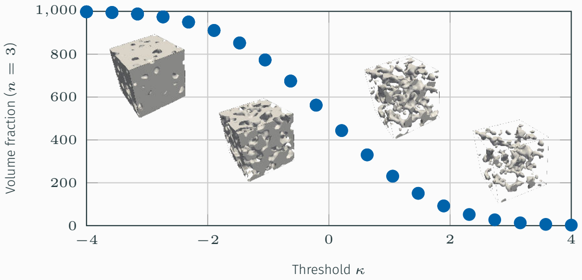

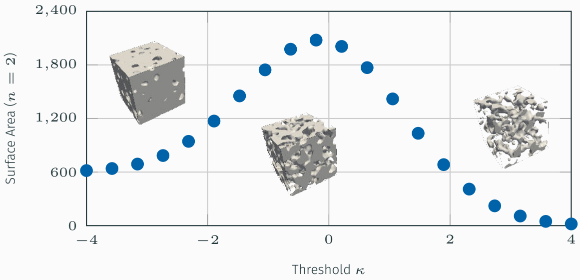

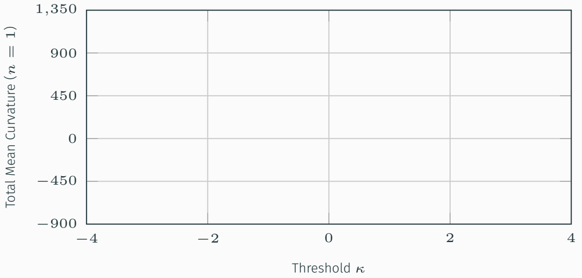

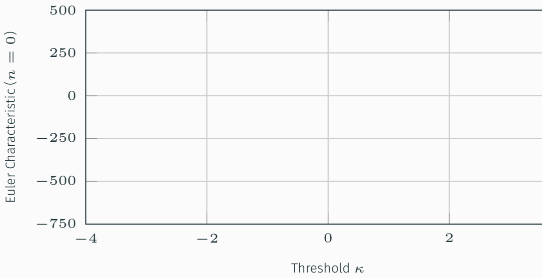

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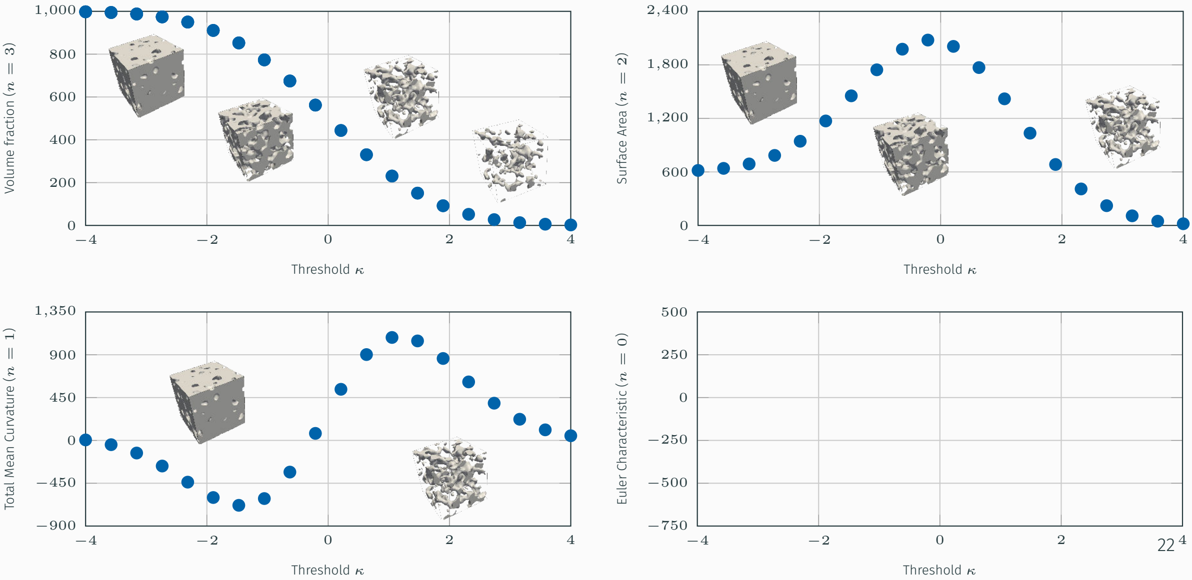

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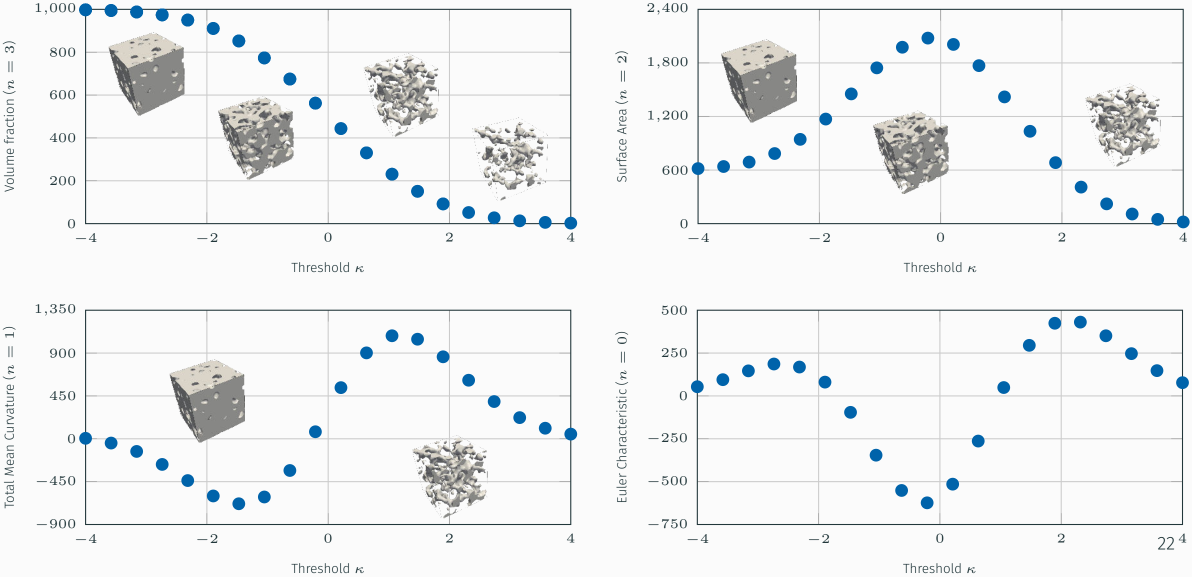

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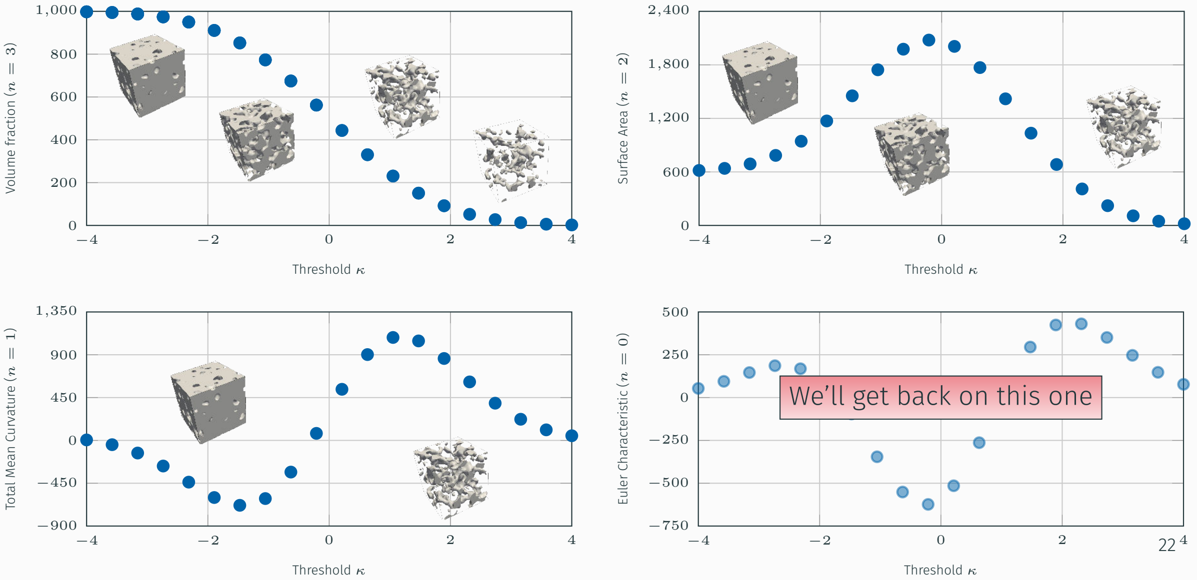

Outline

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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$$\mathbb{E}(\mathcal{L}_j(\mathcal{E}_\mathrm{s})) = f(j, L_c, \mu, \sigma, M, \kappa)$$

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

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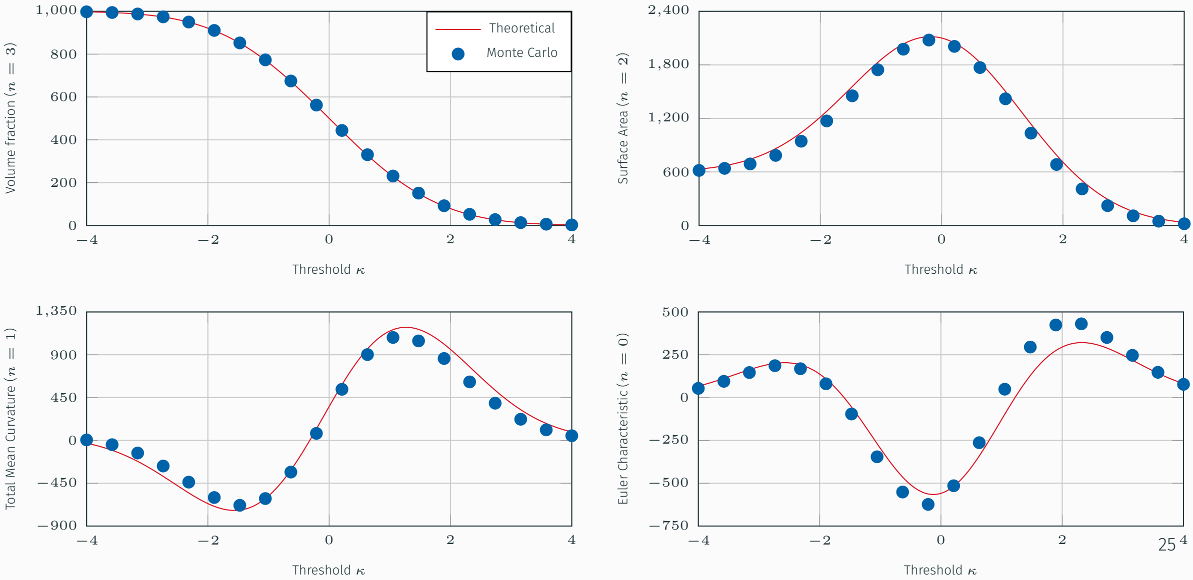

The Excursion Set Theory and percolation

Outline

- Morphological model based on correlated Random Fields
  - Motivations
  - Correlated Random Fields
  - Excursions of correlated Random Fields
- Standard mathematical measures of manifolds
  - $N+1$ measures for $N-$dimensional spaces
  - Expectation of the measures for excursion: **The Excursion Set Theory**
- The Excursion Set Theory and percolation
  - Our positioning
  - The Euler Characteristic: percolation criterion
  - Results

The pioners

Summary

A diagrammatic scheme has been presented for representing the structure of a three-dimensional polymer in a way which facilitates statistical analysis. It has been shown that the general condition for the formation of infinitely large molecules is expressed by $\alpha > 1/(f-1)$, where f is the functionality of the branch units and α is the probability of chain branching as opposed to chain termination. Methods have been presented for

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PERCOLATION PROCESSES

I. CRYSTALS AND MAZES

BY S. R. BROADBENT AND J. M. HAMMERSLEY

Received 15 August 1956

ABSTRACT. The paper studies, in a general way, how the random properties of a 'medium' influence the percolation of a 'fluid' through it. The treatment differs from conventional diffusion theory, in which it is the random properties of the fluid that matter. Fluid and medium bear general interpretations: for example, solute diffusing through solvent, electrons migrating over an atomic lattice, molecules penetrating a porous solid, disease infecting a community, etc.

S. R. Broadbent and J. M. Hammersley, *Percolation process I and II*, 1957.

The Critical Percolation Probabilities p_c

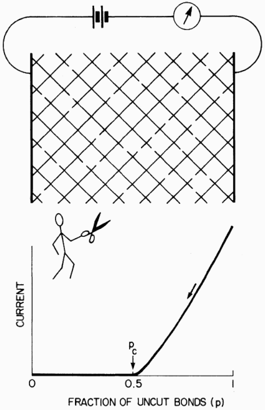

Figure 4.1 The randomly cut network as an example of percolation.

R. Zallen, *The Physics of Amorphous Solids: Chapter 4 The Percolation Model*, 1983.

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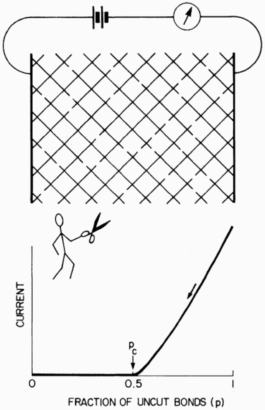

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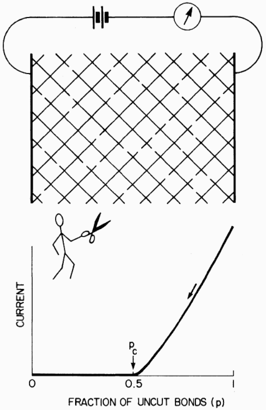
From (7.1), if K is singular at p_c then it is also singular at $1 - p_c$, and if there is only one singularity these must be identical points, or

$$p_c = \tfrac{1}{2}. \qquad (7.2)$$

This establishes two important percolation probabilities as $\frac{1}{2}$—that for the site problem on the triangular lattice and that for the bond problem on the simple quadratic lattice. The result (7.2) holds for any fully triangulated lattice.

M. F. Sykes and J. W. Essam, *Exact Critical Percolation Probabilities for Site and Bond Problems in Two Dimensions*, 1964.



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M. F. Sykes and J. W. Essam, *Exact Critical Percolation Probabilities for Site and Bond Problems in Two Dimensions*, 1964.

- Only on lattices (graphs)
- Depends much on the lattice type
- No analytical results in 3D
- Volumetric approach to regularise

R. Zallen, *Critical density in percolation processes*, 1970.

Links between percolation theory and topology

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

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- Often with analytical solutions
- Often limited to boolean problems in infinite spaces

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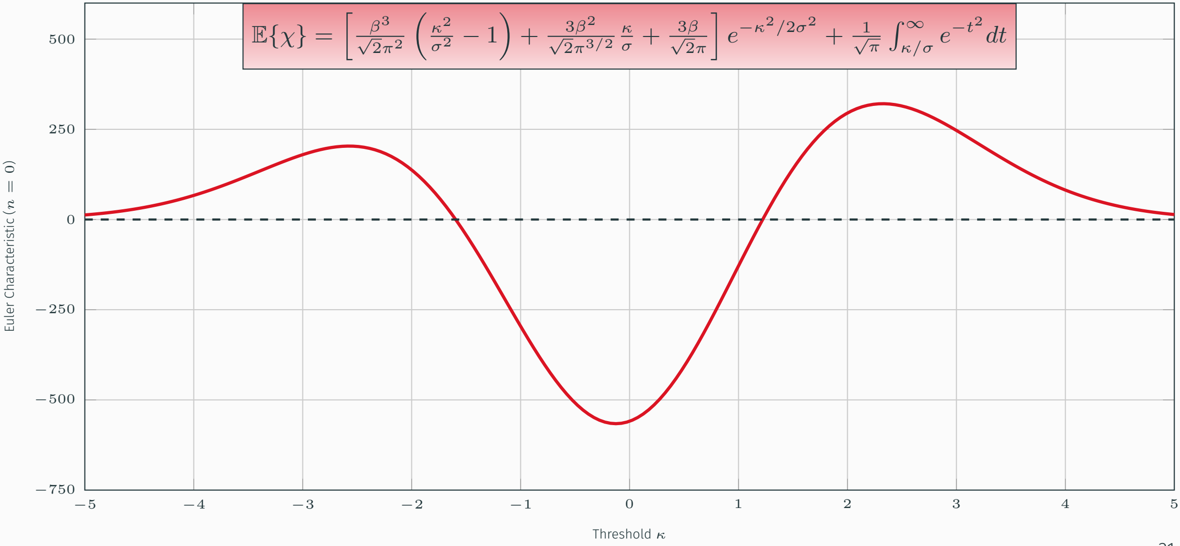
Outline

The Euler Characteristic



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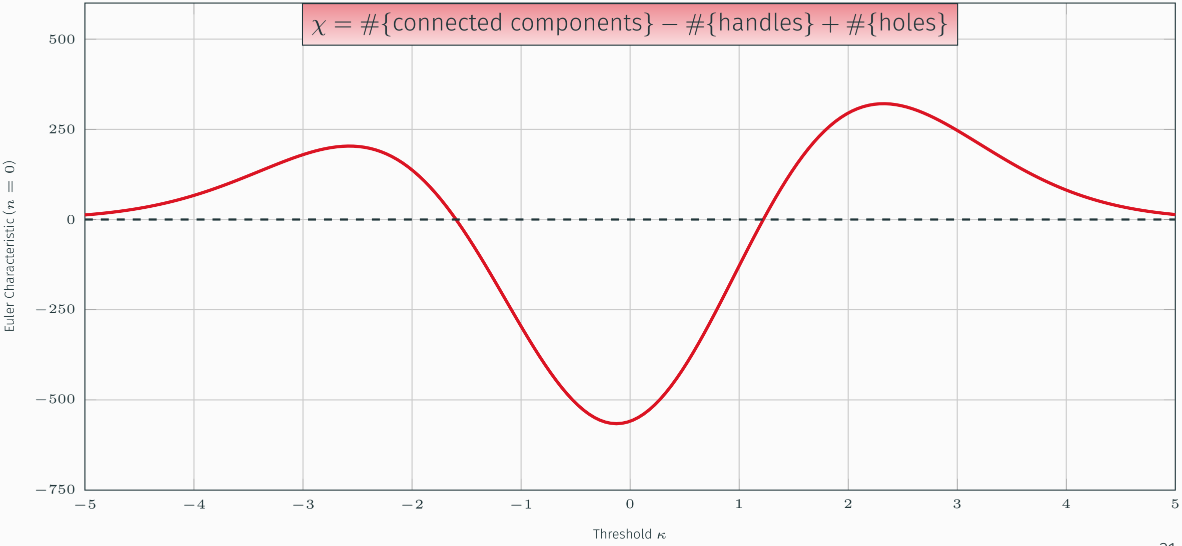

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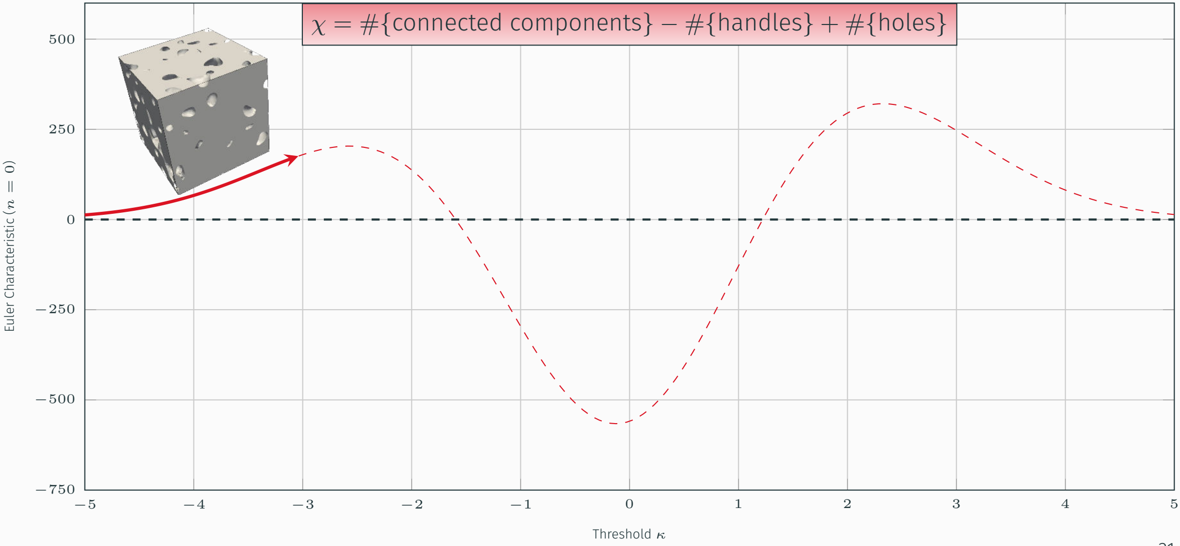

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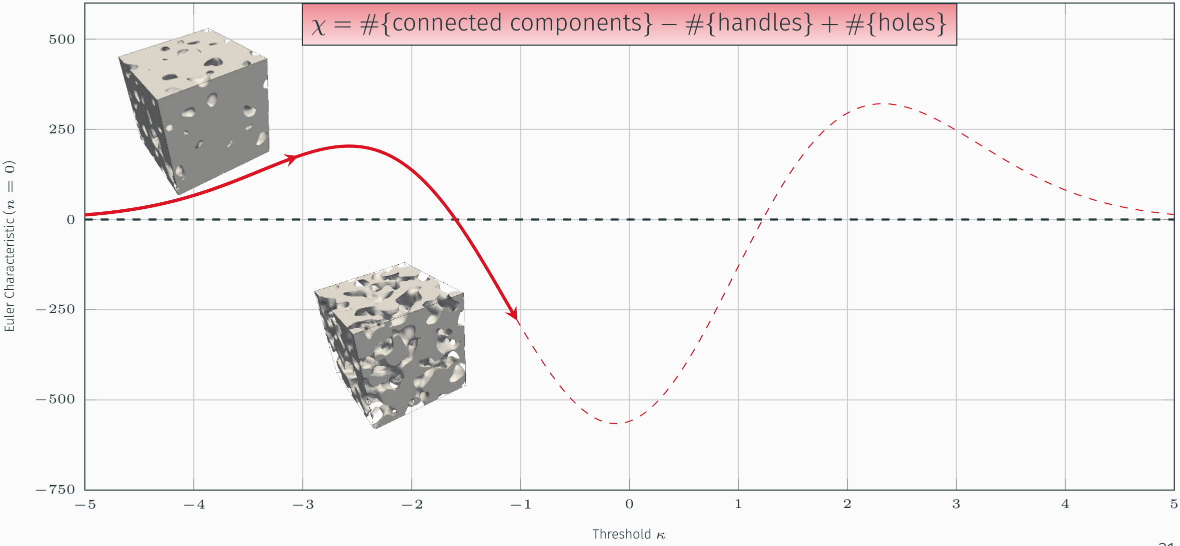

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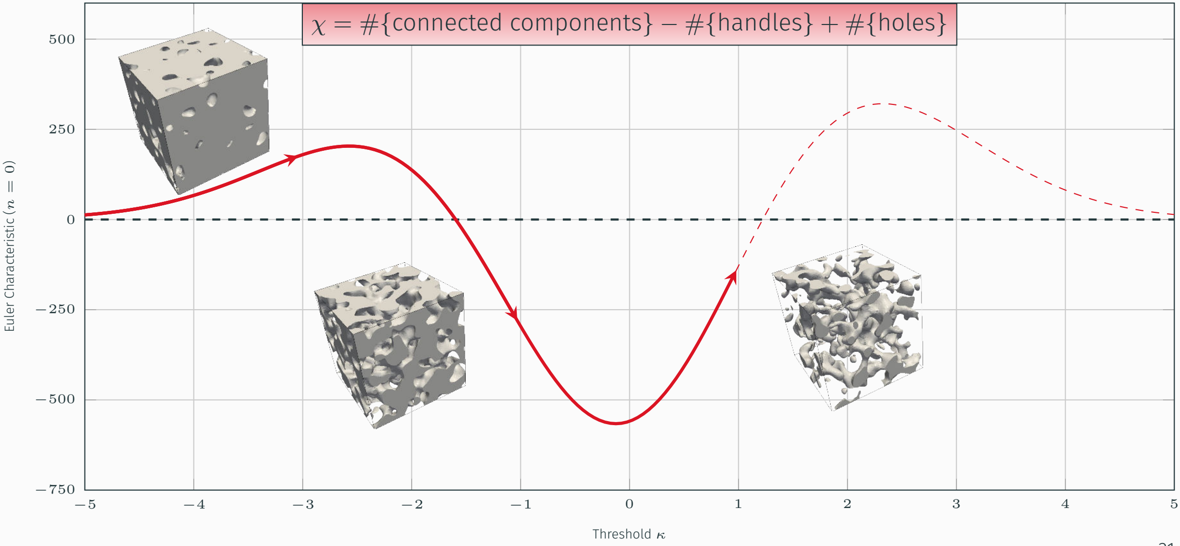

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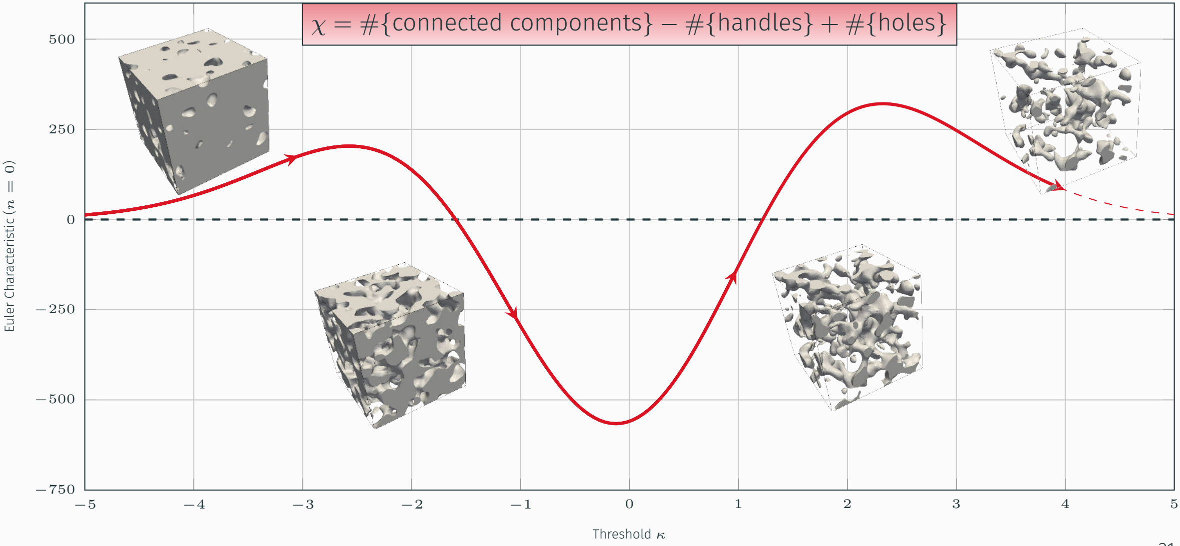

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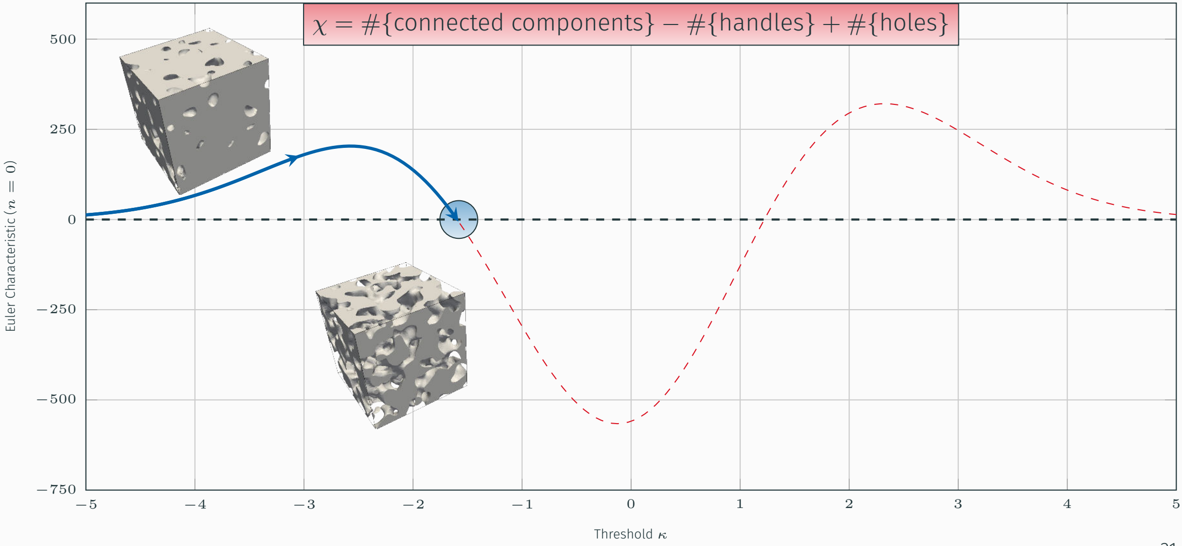

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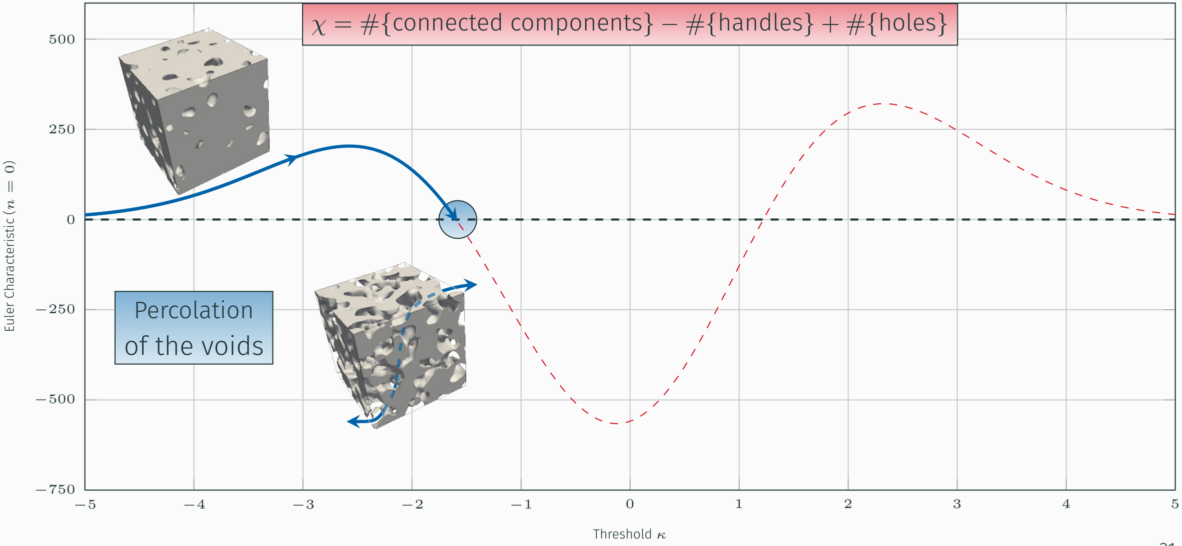

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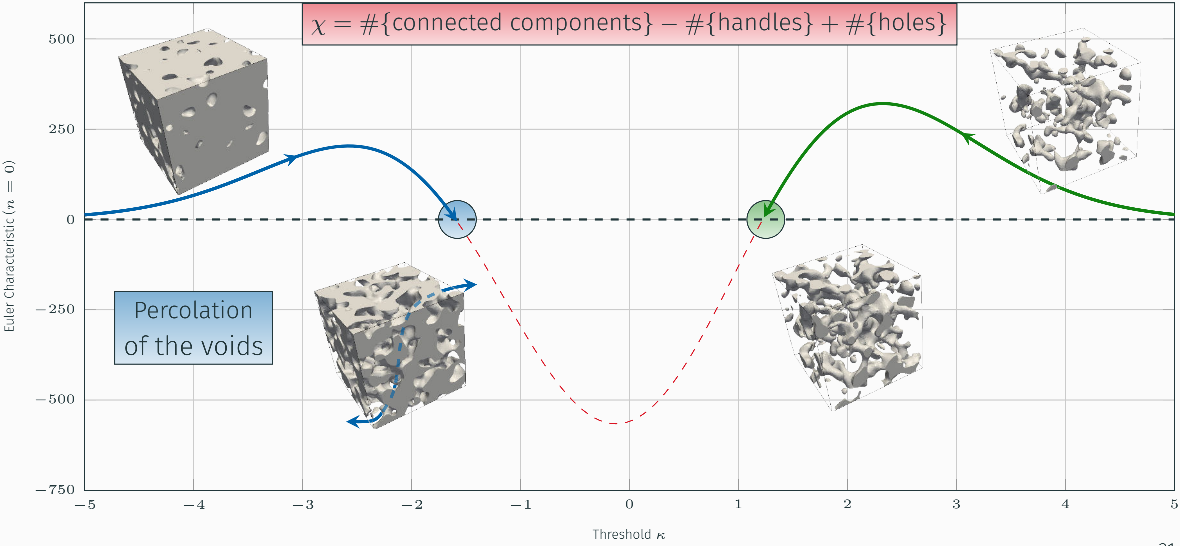

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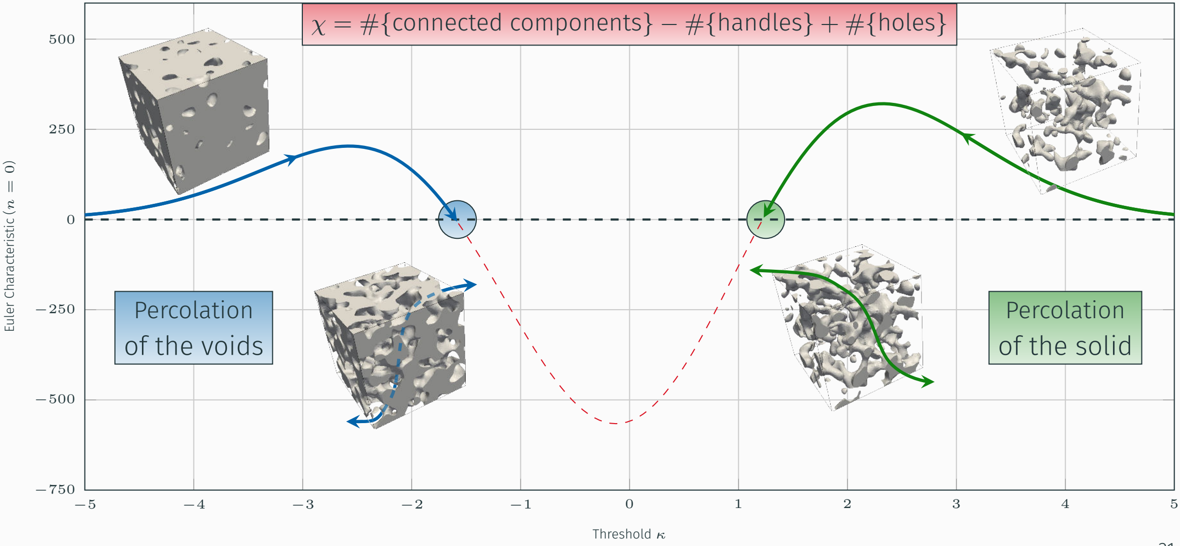

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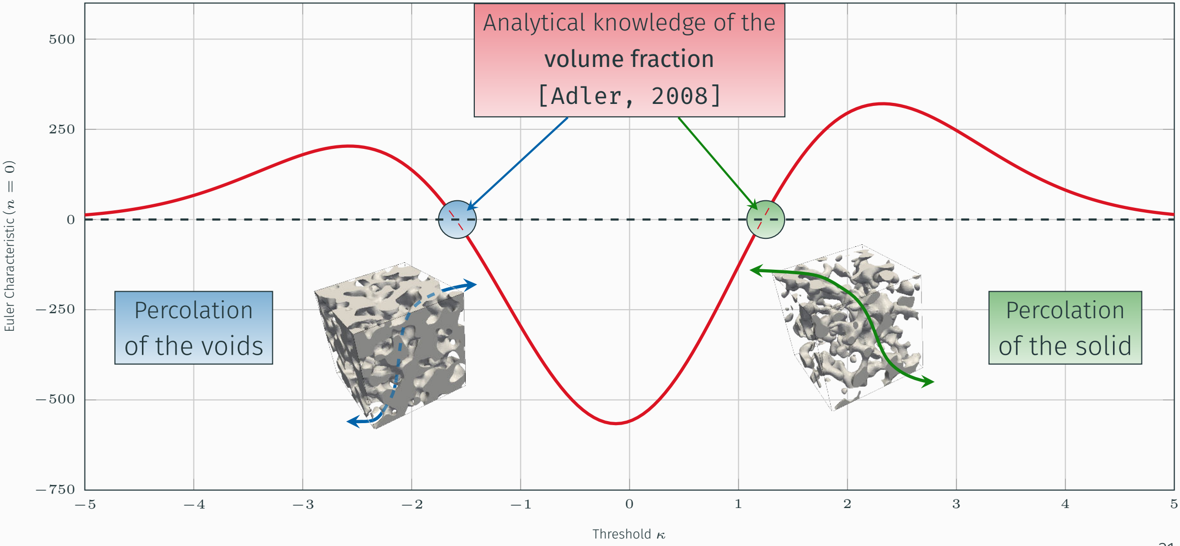
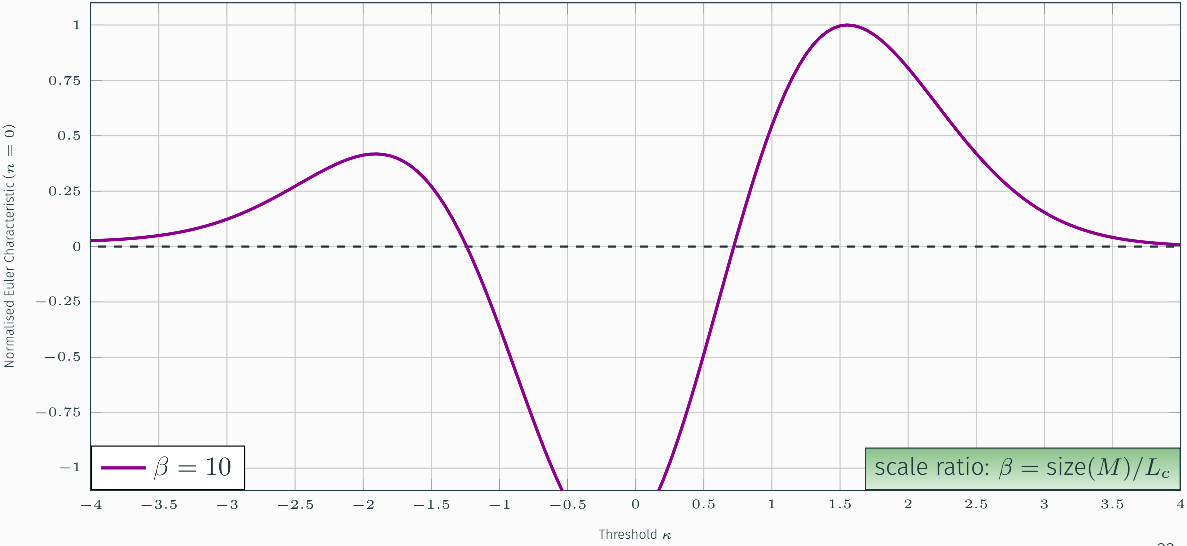


The Euler Characteristic: scale ratio



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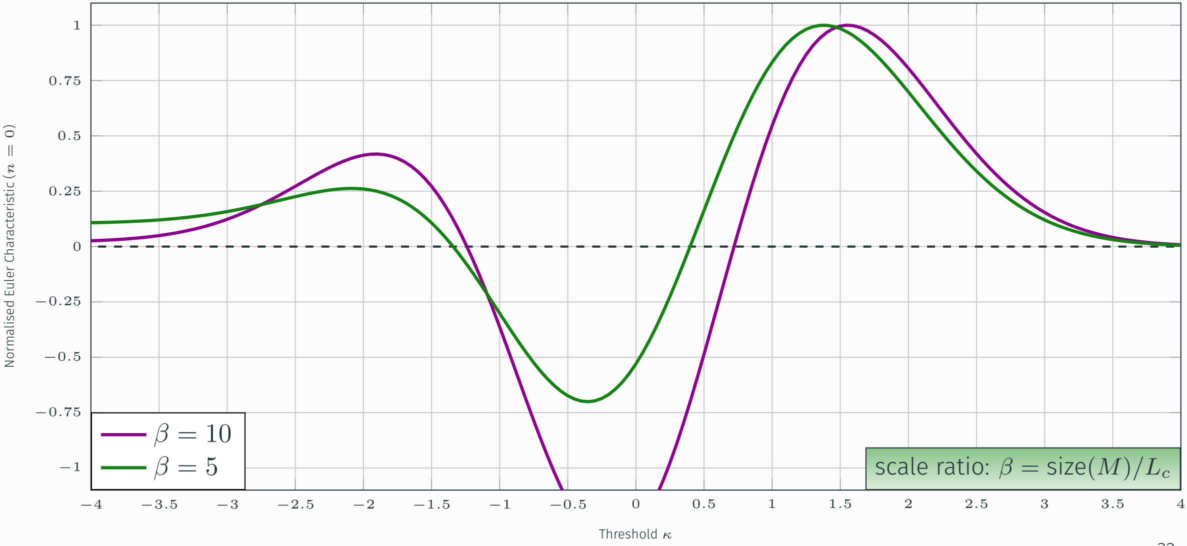

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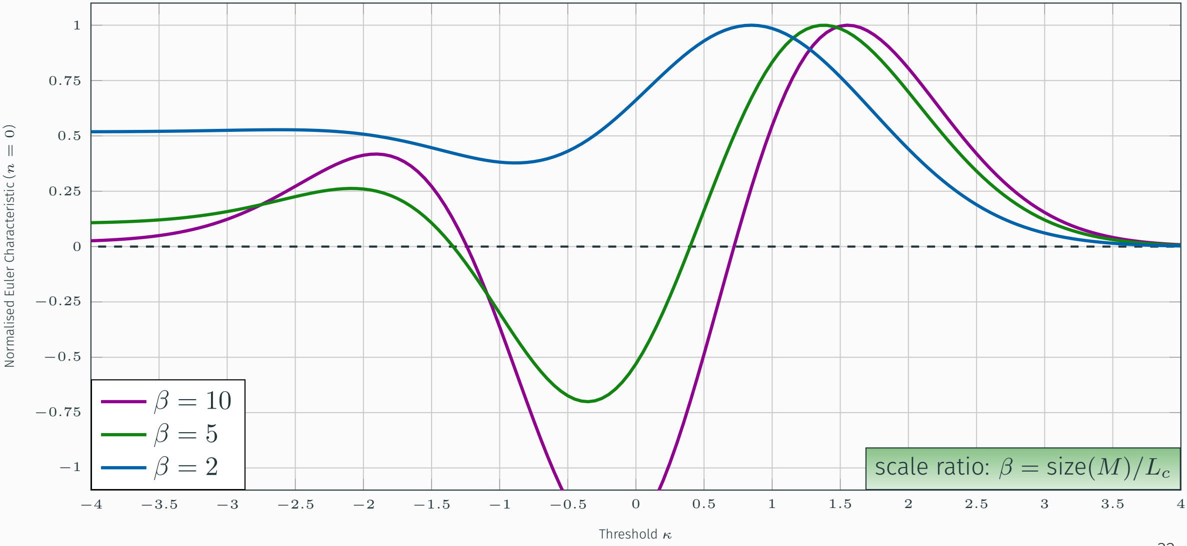

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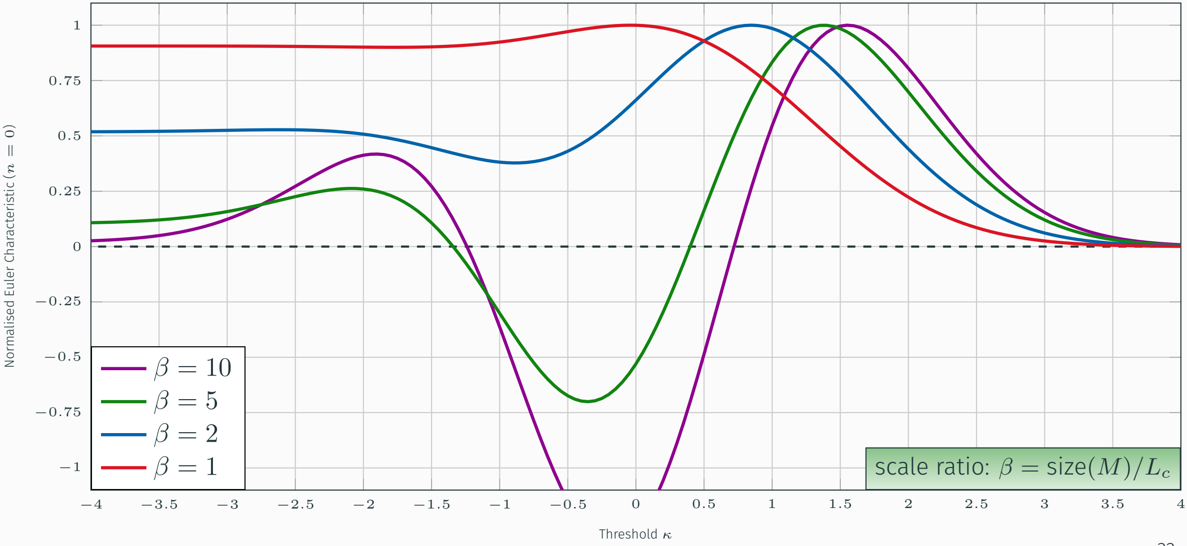
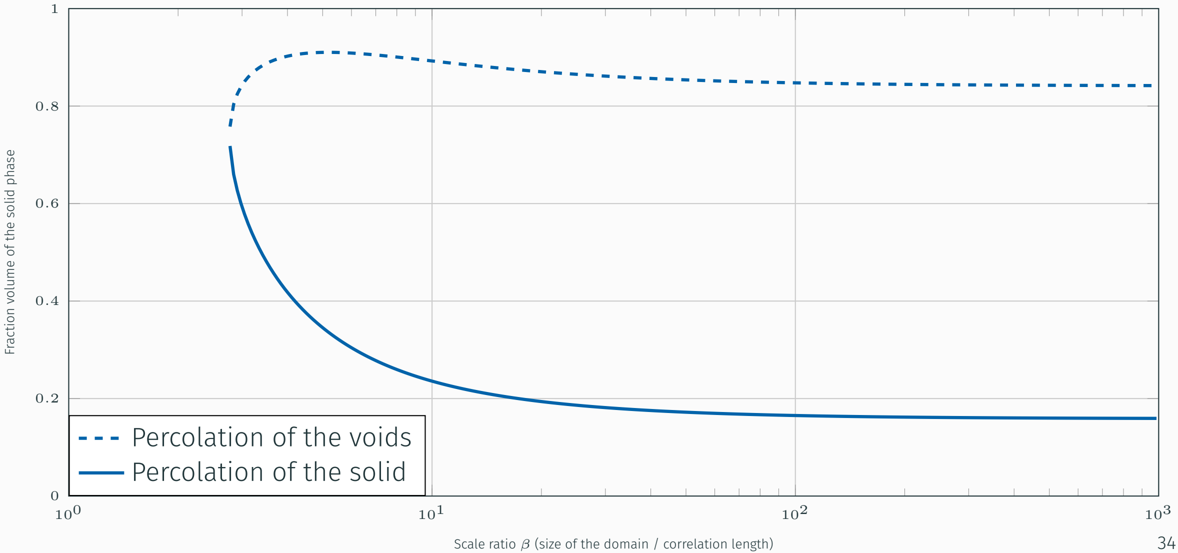


Outline

Phase diagram



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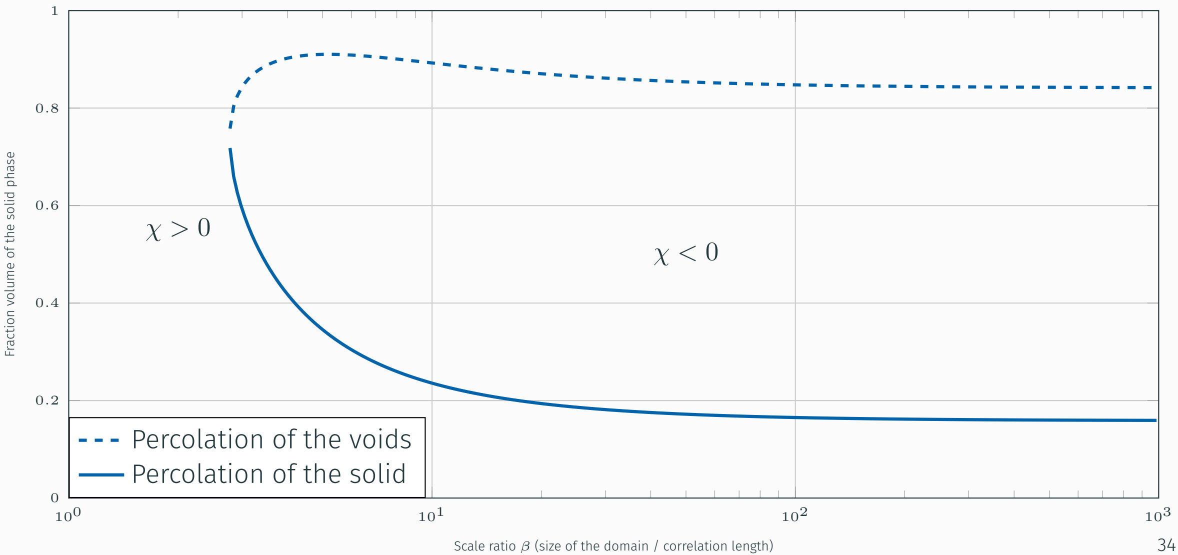

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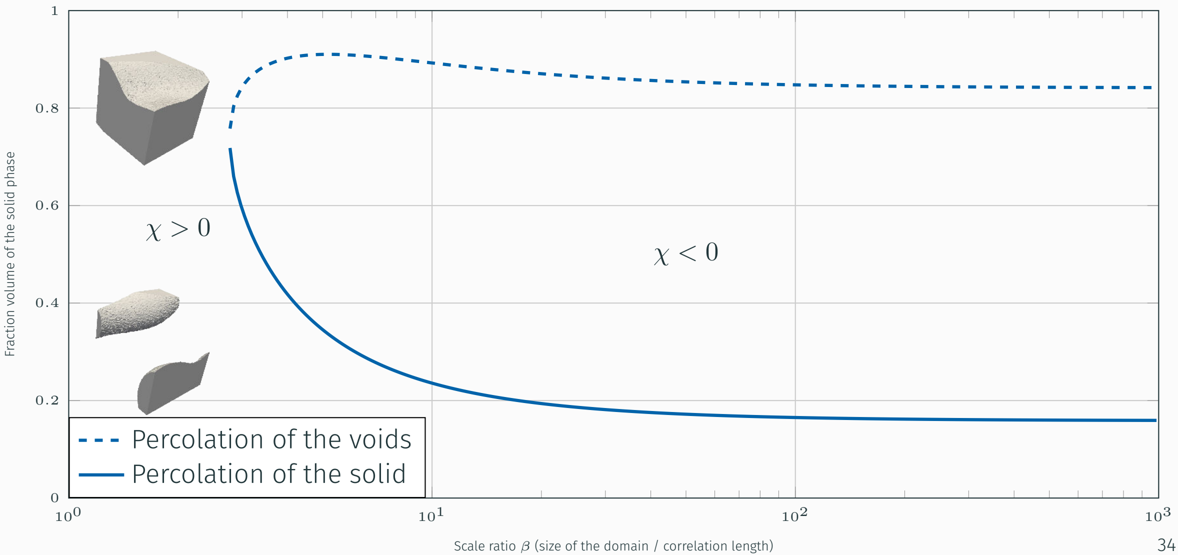

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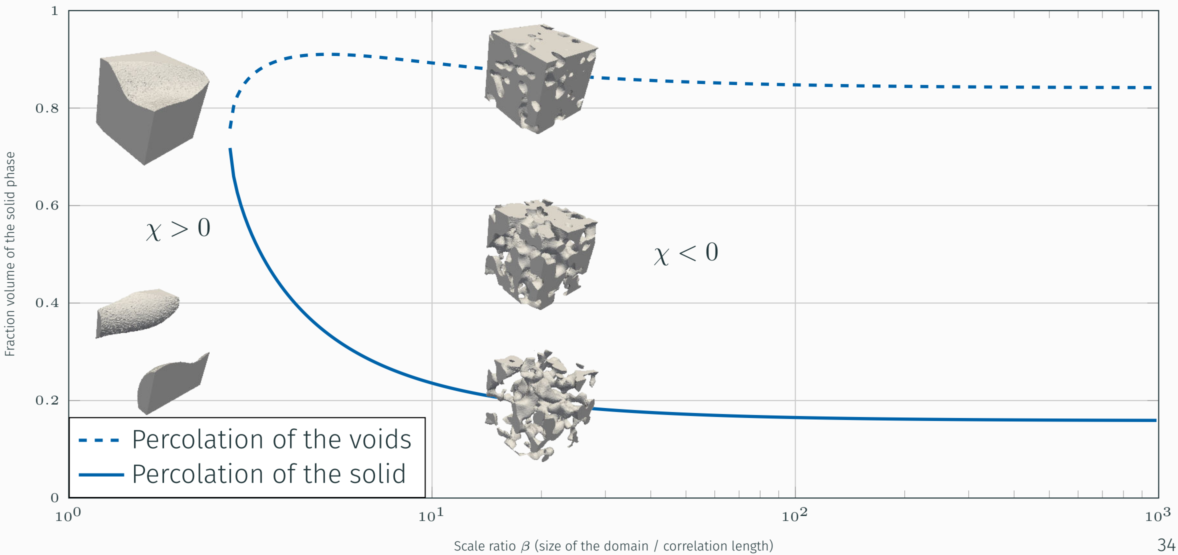

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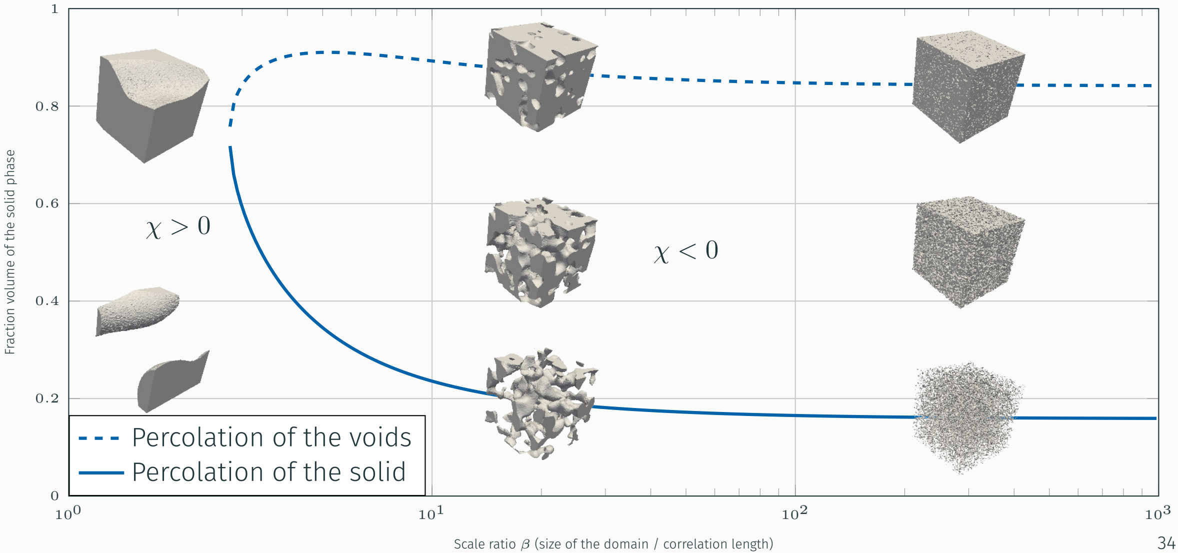

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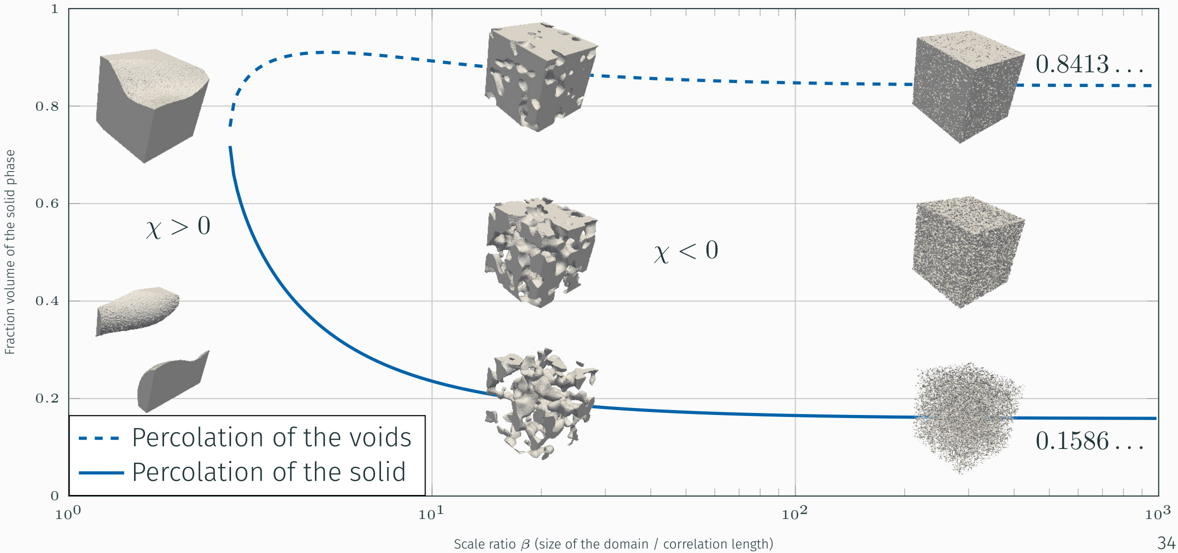

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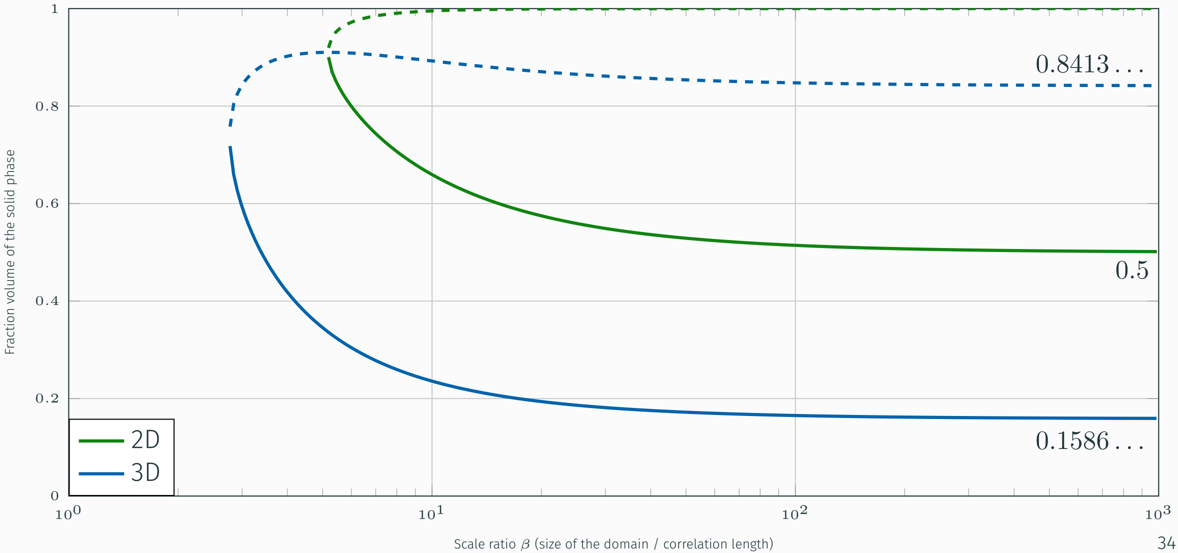

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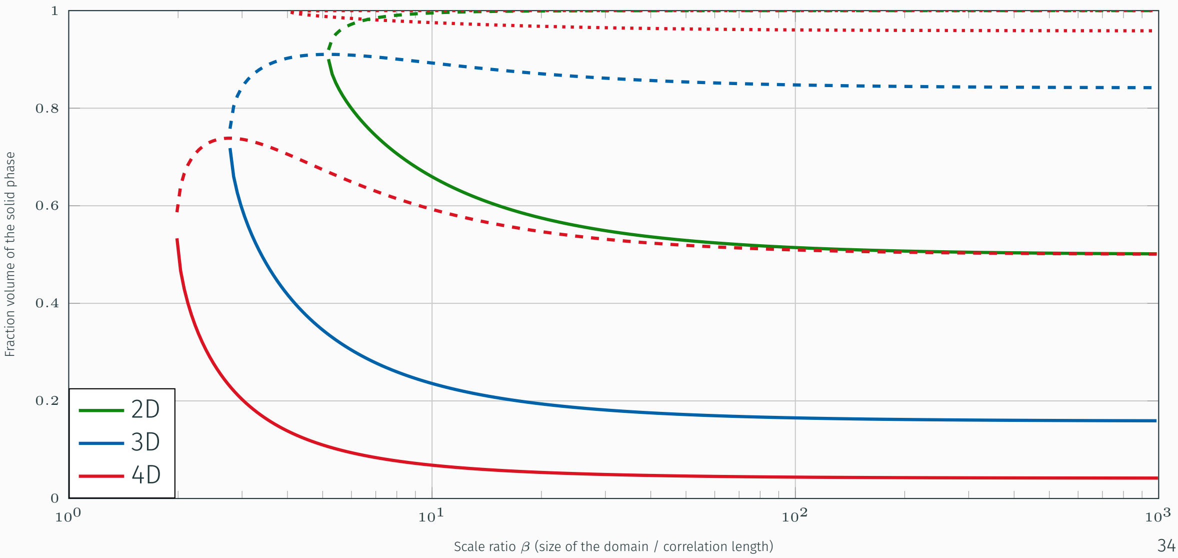
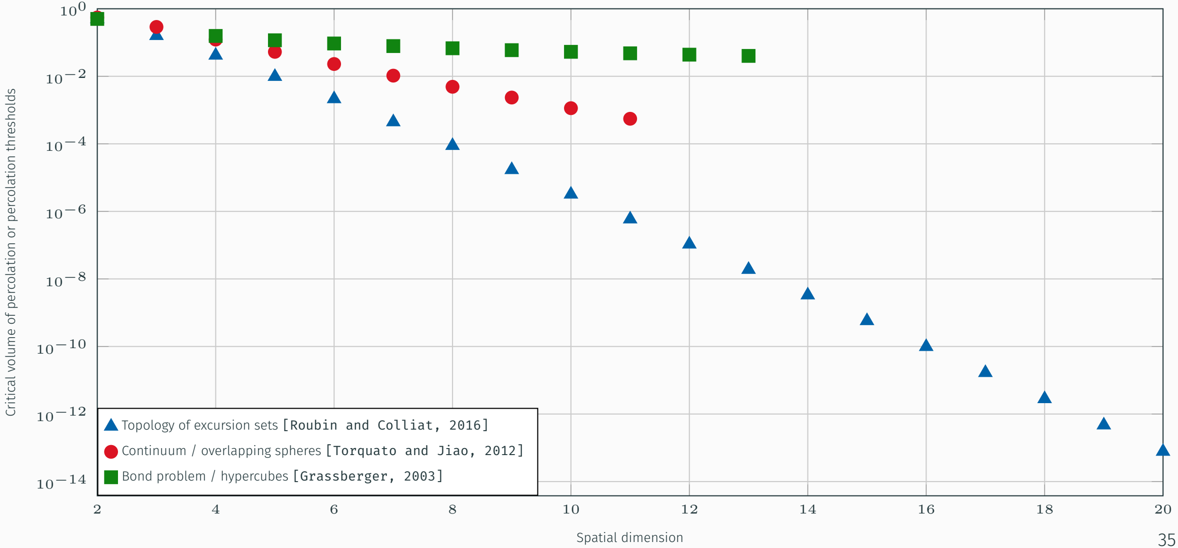


Percolation of the solid phase in N dimensions



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Statistical procedure to define RVE

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We can define analyticaly the error as: $\epsilon(\beta) = \dfrac{\Phi_c(\beta) - \Phi_c^\infty}{\Phi_c^\infty}$

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RVE with the Excursion set theory

We have access to the **infinite domain volume of percolation Φ_c^∞** that we take as **the reference** (not possible to compute in the previous case).

We can define analyticaly the error as: $$\epsilon(\beta) = \frac{\Phi_c(\beta) - \Phi_c^\infty}{\Phi_c^\infty}$$

By inverting the error we have $\beta(\epsilon)$ and thus, the RVE for a given error.

RVE for percolation

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Comparison to RVE for water diffusivity in cement paste

It is linked with percolation. In [Zhang, Ye and Breugel, 2011] they found for a 1% error a scale ratio of 100.

- Not the same property of interest (mechanical vs topological)
- Polydisperse spheres

M. Zhang, Ye G. and K. van Breugel, *Microstructure-based modeling of water diffusivity in cement paste*, 2011.

Perspectives and possible applications

Further investigations

- Role of the distribution on the model (non isotropic fields)
- Investigation on the $\chi = 0 \Leftrightarrow$ percolation with numerical simulations

Applications

- Prediction of percolation in evolutive heterogeneous media
- Estimation of local parameters in phenomenological laws (diffusion, ...)
- Analytical model for size effect for heterogeneous brittle materials (lack of mechanics)