

DE LA RECHERCHE À L'INDUSTRIE



# EIGENVALUE PROBLEMS IN THREE-DIMENSIONAL RANDOM MEDIA

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**CEA/SACLAY**

Workshop MaNu |

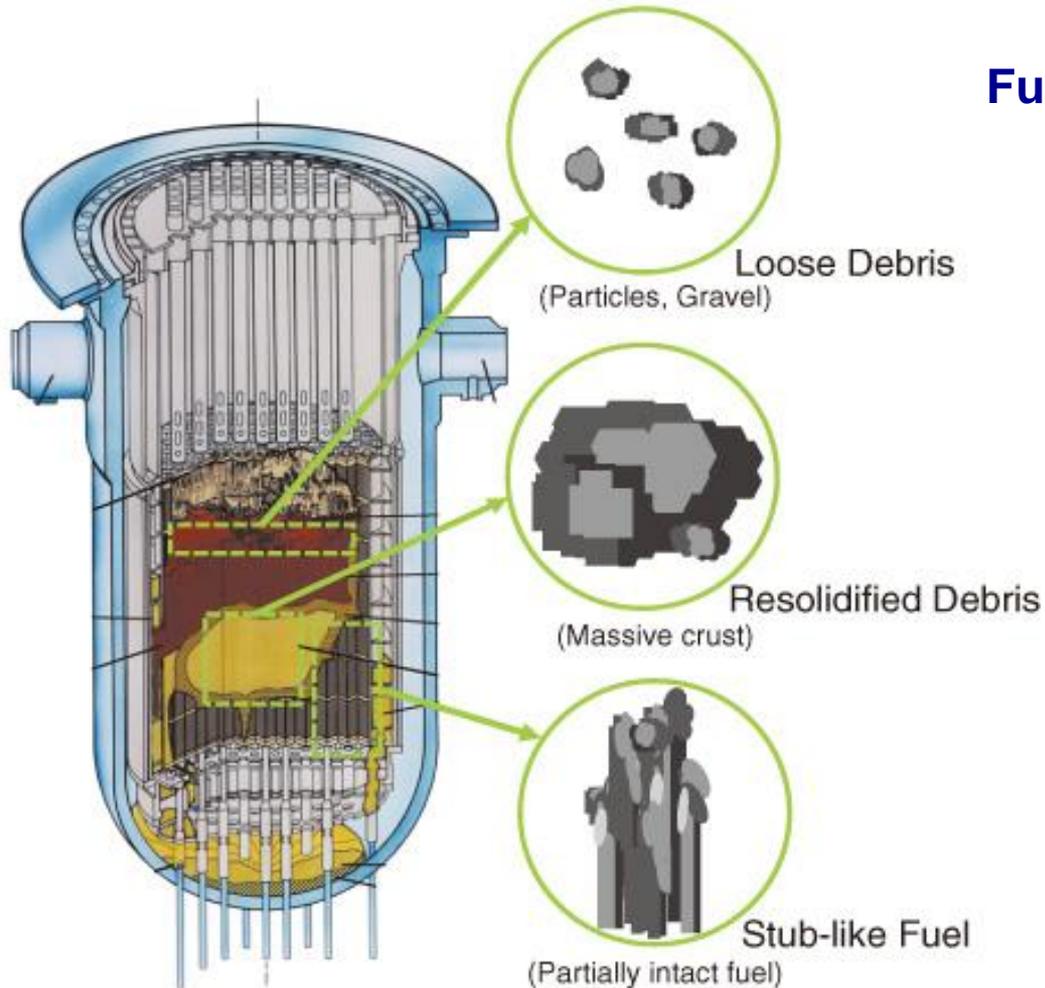
Coline LARMIER | DEN/DANS/DM2S/SERMA/LTSD

November 30th 2017

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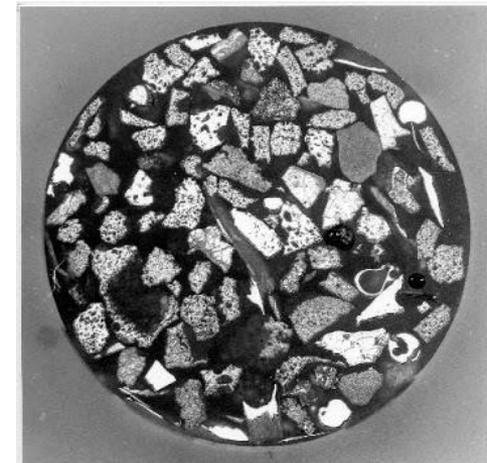
- ❑ Eigenvalue problems in random media
- ❑ Stochastic tessellations
- ❑ Analysis of fuel assemblies
- ❑ Perspectives

## Analysis of **re-criticality** probability following **severe core accidents**



### Fuel degradation:

- **melting** and **solidification**
- **random** configurations

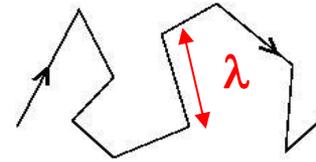


TMI corium sample

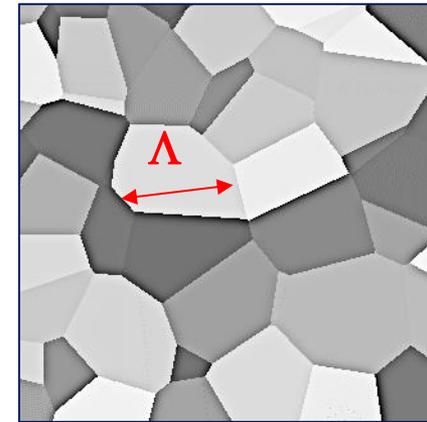
The **randomness** of a medium is measured w.r.t. **neutron transport**

Define :

□  $\lambda = 1 / \Sigma =$  neutron mean free path



□  $\Lambda =$  typical disorder size (*correlation length*) :  
average size of homogeneous regions



Three possible **regimes** :

$\Lambda \ll \lambda$

$\Lambda \approx \lambda$

$\Lambda \gg \lambda$

$\Lambda$

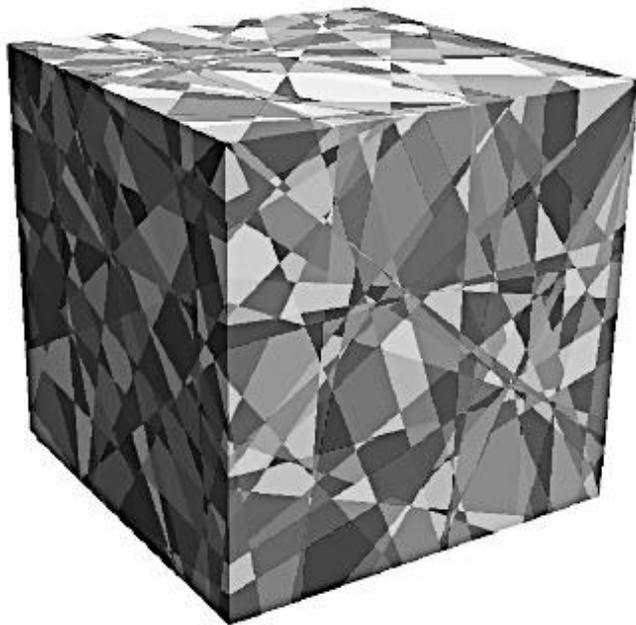
▪ **Microscopically homogeneous** medium  
(« *atomic mix* »)

▪ **Microscopically heterogeneous** medium  
▪ Disorder can be described by **probabilistic models**

▪ **Macroscopically heterogeneous** medium  
(homogeneous « by blocks »)

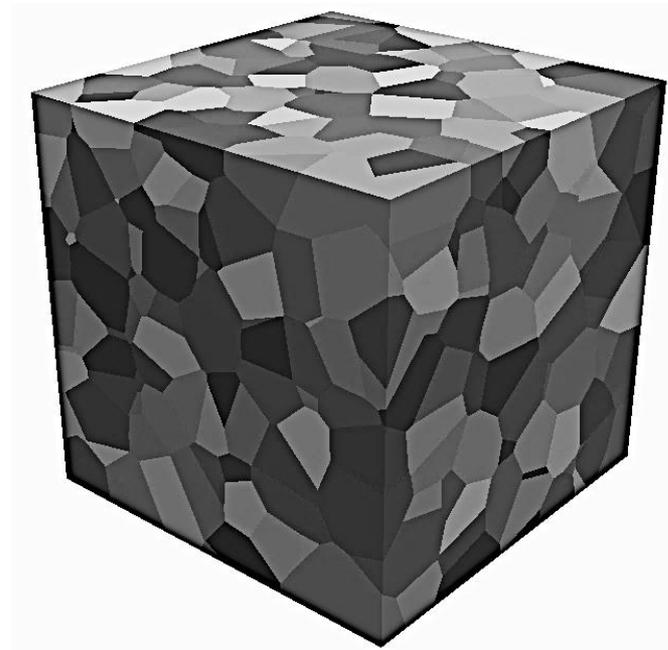
**Stochastic tessellations** [Miles, Santalo] are a convenient model for disorder

- Idea: **partition** a d-dimensional region according to a given **probability law**  $P(q)$



**Poisson tessellations**

- Random hyper-planes
- Markov property



**Voronoi tessellations**

- Poisson point process
- Voronoi diagrams

Eigenvalue Boltzmann equation for the neutron flux  $\varphi$  :

$$\underbrace{\omega \cdot \nabla \varphi_k^{(q)}}_{\text{Leakage}} + \underbrace{\Sigma_t^{(q)} \varphi_k^{(q)}}_{\text{Collisions}} - \int \overbrace{\Sigma_s^{(q)}(\mathbf{r}, \mathbf{v}' \rightarrow \mathbf{v}) \varphi_k^{(q)}(\mathbf{r}, \mathbf{v}') d\mathbf{v}'}^{\text{Scattering}} = \frac{\chi^{(q)}(\mathbf{r}, v)}{k^{(q)}} \int \underbrace{\nu^{(q)}(v') \Sigma_f^{(q)}(\mathbf{r}, v') \varphi_k^{(q)}(\mathbf{r}, \mathbf{v}') d\mathbf{v}'}_{\text{Fission}}$$

For a single geometry realization  $q$

In compact form:

$$\mathcal{L}^{(q)} \varphi_k^{(q)}(\mathbf{r}, \mathbf{v}) = \frac{1}{k^{(q)}} \mathcal{F}^{(q)} \varphi_k^{(q)}(\mathbf{r}, \mathbf{v})$$

For random geometries: we search the ensemble-averaged eigenpairs

$$\begin{cases} \langle \varphi_k \rangle = \int \mathcal{P}(q) \varphi_k^{(q)}(\mathbf{r}, \mathbf{v}) dq \\ \langle k \rangle = \int \mathcal{P}(q) k^{(q)} dq \end{cases}$$

**Quenched disorder:**  
reference solutions

# HOMOGENEISATION: « ANNEALED DISORDER »

Instead of solving the exact equation and taking ensemble averages

Introduce **effective transport kernels**  $\mathcal{L}'$  and  $\mathcal{F}'$

$$\text{such that } \mathcal{L}' \varphi'_k = \frac{1}{k'} \mathcal{F}' \varphi'_k \quad \text{Annealed disorder}$$

with the constraints

$$\begin{cases} k' \simeq \langle k \rangle \\ \varphi'_k \simeq \langle \varphi_k \rangle \end{cases}$$

➤ **Advantages :**

- solve the eigenvalue problem just once
- no need to generate random tessellations

➤ **Drawbacks :**

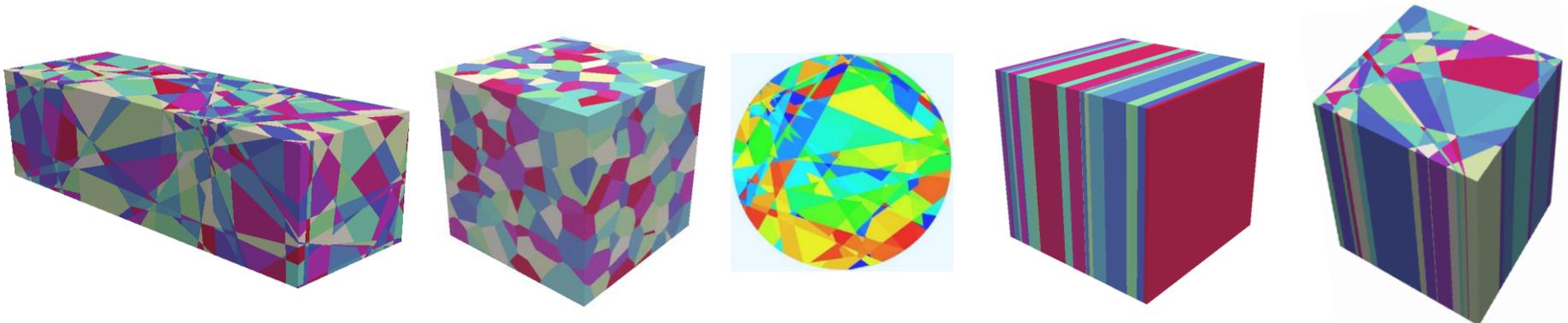
- suppressing correlations: no memory of the media already traversed
- approximate method: need reference solutions for validation

## Eigenvalue problems in stochastic (Poisson) tessellations :

- ❑ Analytical results via perturbation theory [Pomraning; Williams]
- ❑ Numerical simulations for 1d configurations (slab or rod)

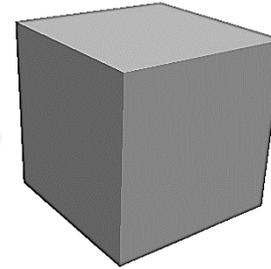
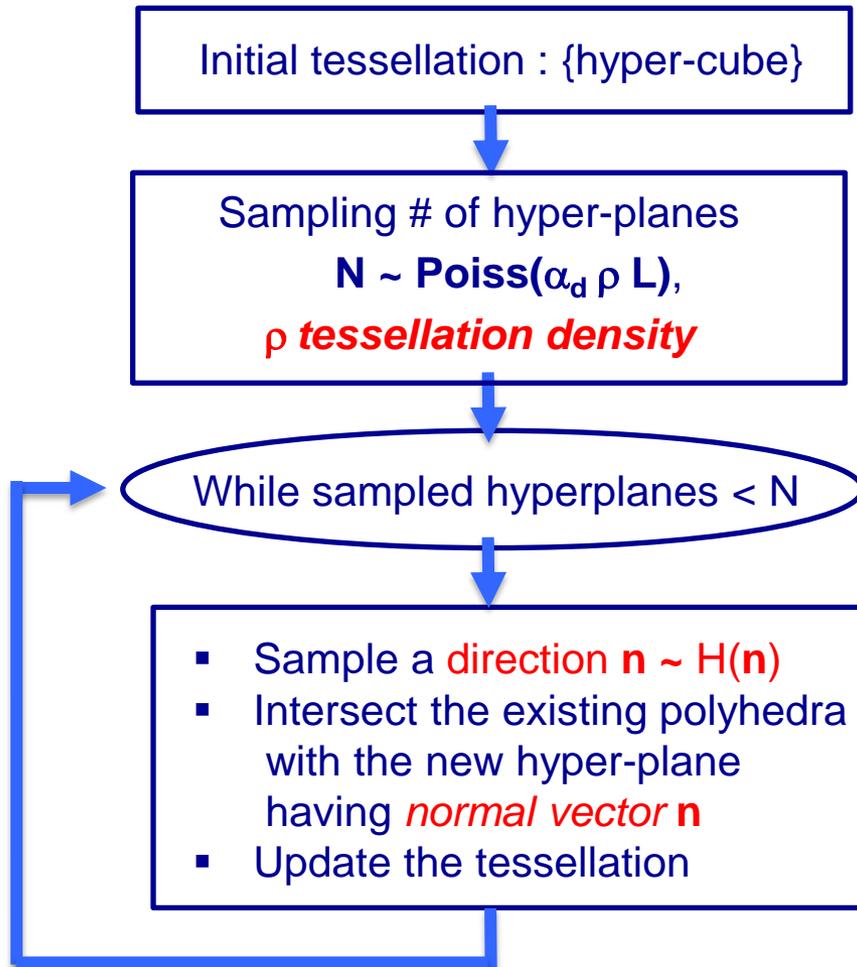
## We have developed a **c++ code** to generate random tessellations

- Several **geometrical forms**: d-parallelepipeds, spheres, cylinders, ...
- Dimensions: **1d** (rod or slab); **2d** (flat or extruded); **3d**
- Several **mixing statistics**: Poisson (Markov), Voronoi, Box
- **Interface** for the Monte Carlo transport code **TRIPOLI-4**

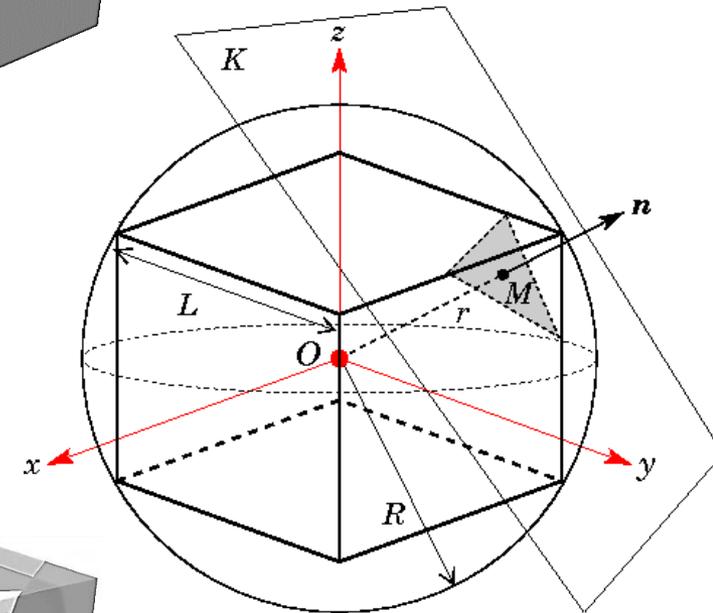


# Analysis of Poisson tessellations

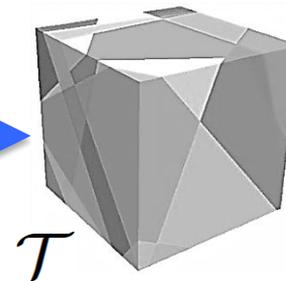
## □ Tessellation of a box of side L



$$\alpha_d = 2\sqrt{\pi} \frac{\Gamma\left(\frac{d+1}{2}\right)}{\Gamma\left(\frac{d}{2}\right)}$$



$H(\mathbf{n})$  : degree of anisotropy

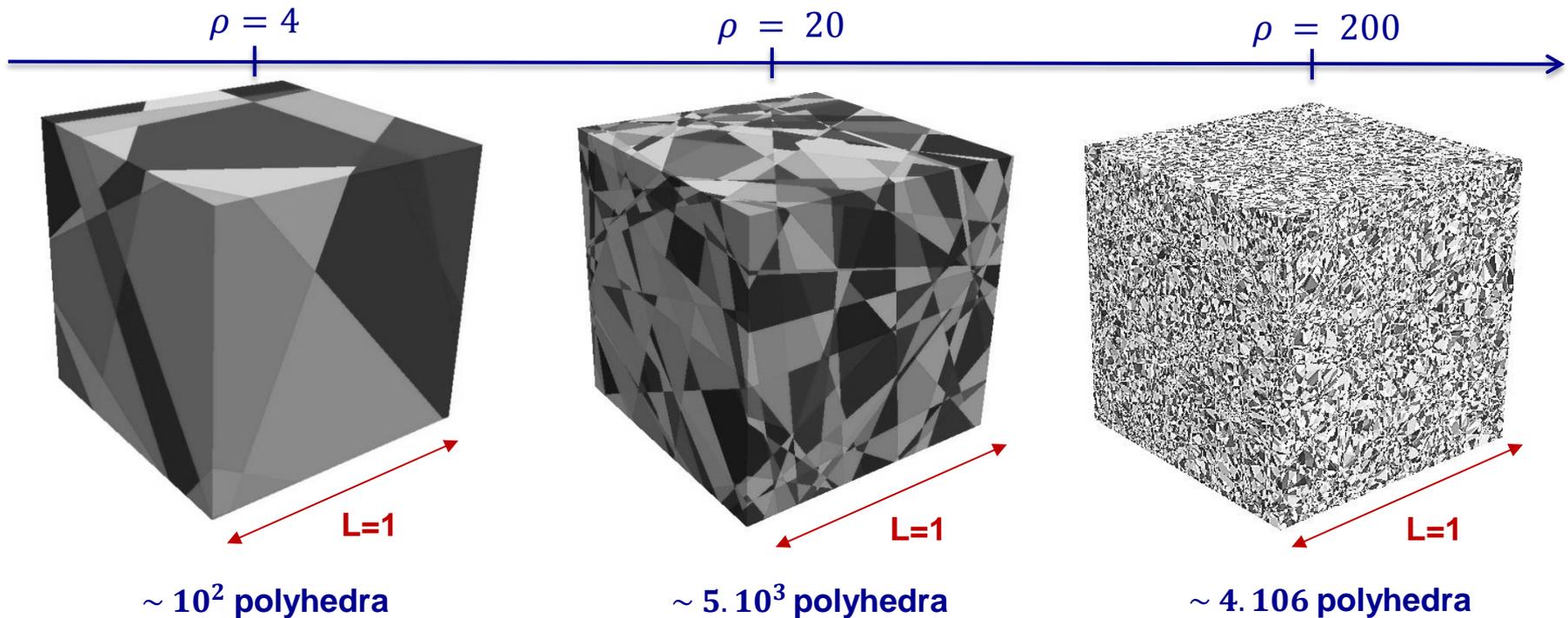


# Effects of the tessellation density $\rho$

## Analysis of the tessellation density $\rho$

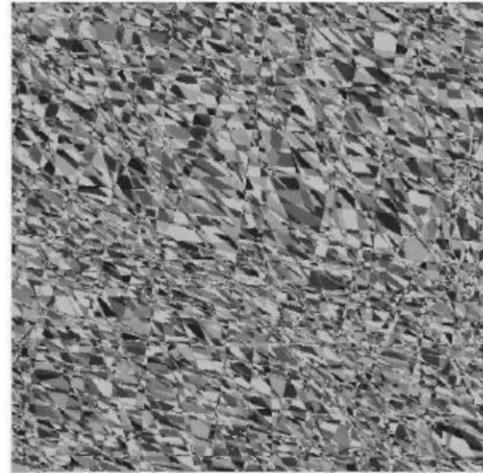
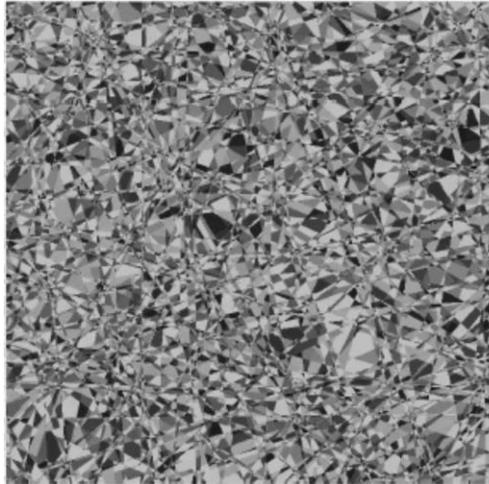
- $1 / \rho = \Lambda =$  correlation length = typical disorder size (for infinite tessellations)
- The number  $N_p$  of **d-polyhedra** increases with increasing  $\rho$  :  $N_p \sim (\rho L)^d$

## 3d tessellations : examples of realizations

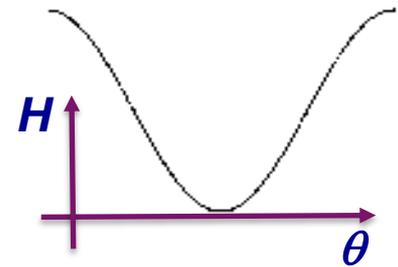


# Effects of anisotropy: $H(n)$

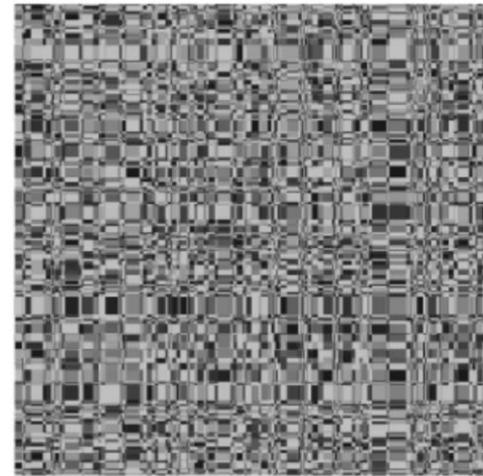
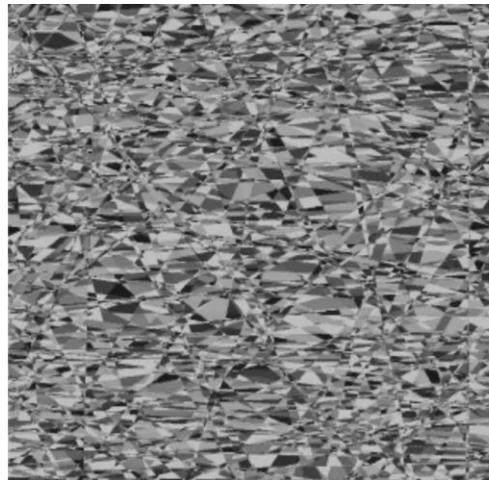
Isotropic



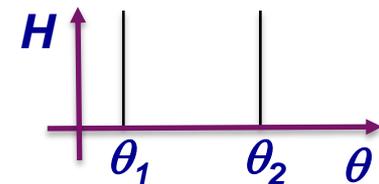
Quadratic



Histogram



« Box »



## □ Analysis by **Monte Carlo** methods

- Generate a large ensemble of Poisson tessellations
  - Compute the number of polyhedra
  - Compute the physical observables
- Estimate **moments & distributions**
- Compare to literature (when available!)

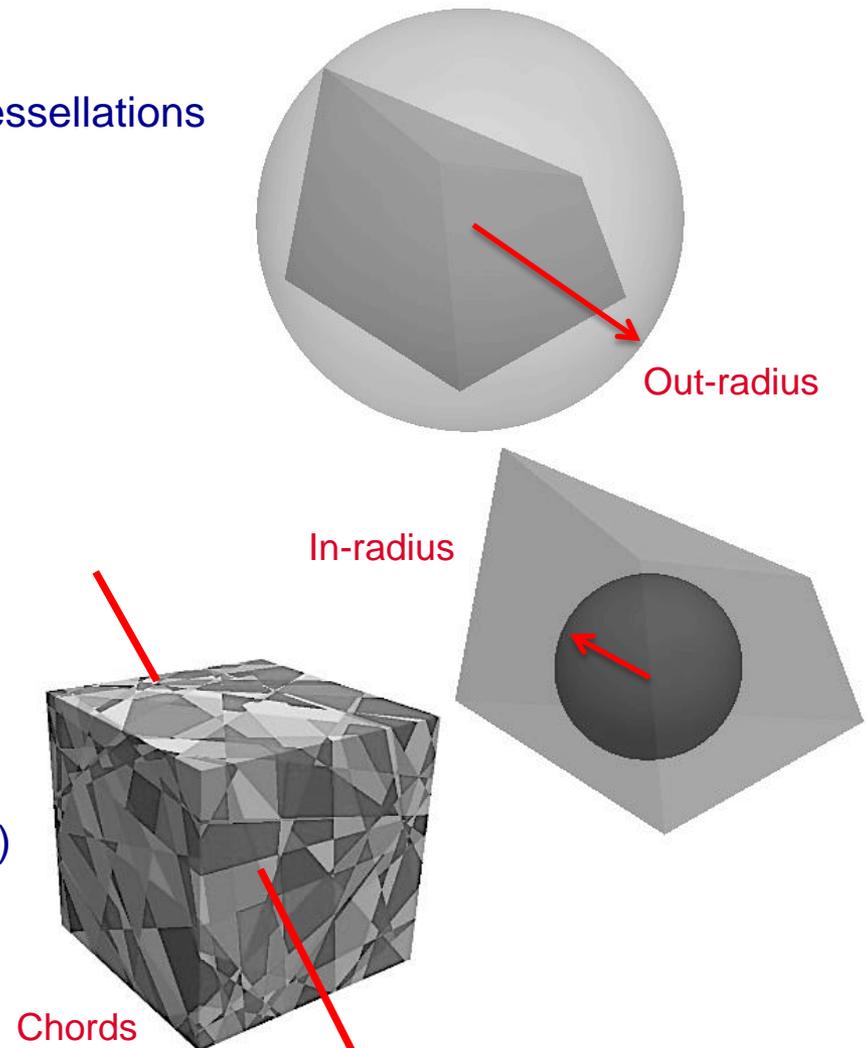
## □ Relevant observables:

### ➤ Polyhedral features

- **Volume** and **surface**
- Number of **faces** (connectivity)
- ***In-radius / out-radius*** (aspect ratio)

### ➤ Stereology

- **Chord length** distribution



# Polyhedral features [\*] of infinite tessellations with law H

□ Volume:  $\langle V_d \rangle = \frac{d!}{\zeta_d} \left( \frac{\alpha_d}{2\rho} \right)^d$

where

$$\zeta_d = \int_{\Omega_d^+} \cdots \int_{\Omega_d^+} \underbrace{[\mathbf{n}_1, \dots, \mathbf{n}_d]}_{\text{d-space determinant}} dH(\mathbf{n}_1) \cdots dH(\mathbf{n}_d)$$

[\*] Miles (1964); Schneider & Weil (2008)

□ Surface:  $\langle S_d \rangle = \alpha_d \rho \langle V_d \rangle$

□ Number of faces:  $\langle f_d \rangle = 2d$

□ In-radius: *exponentially* distributed, with  $\langle r_{\text{in},d} \rangle = \frac{1}{\alpha_d \rho}$

□ Out-radius: unknown

➤ Inequalities:  $\langle V_d^m \rangle \geq \langle V_d^m \rangle^{\text{iso}}$   
 $\langle S_d \rangle \geq \langle S_d \rangle^{\text{iso}}$

$$\alpha_d = 2\sqrt{\pi} \frac{\Gamma\left(\frac{d+1}{2}\right)}{\Gamma\left(\frac{d}{2}\right)}$$

[\*] Miles (1964); Schneider & Weil (2008)

- A straight line with orientation  $\mathbf{v}$  will encounter a number of hyper-planes having a *Poisson* distribution with density

$$\rho(\mathbf{v}) = \frac{\alpha_d}{2} \rho \int_{\Omega_d^+} |\mathbf{n} \cdot \mathbf{v}| dH(\mathbf{n})$$

$$\alpha_d = 2\sqrt{\pi} \frac{\Gamma\left(\frac{d+1}{2}\right)}{\Gamma\left(\frac{d}{2}\right)}$$

- The line  $\mathbf{v}$  will be cut into chords  $\ell$  *exponentially* distributed with average

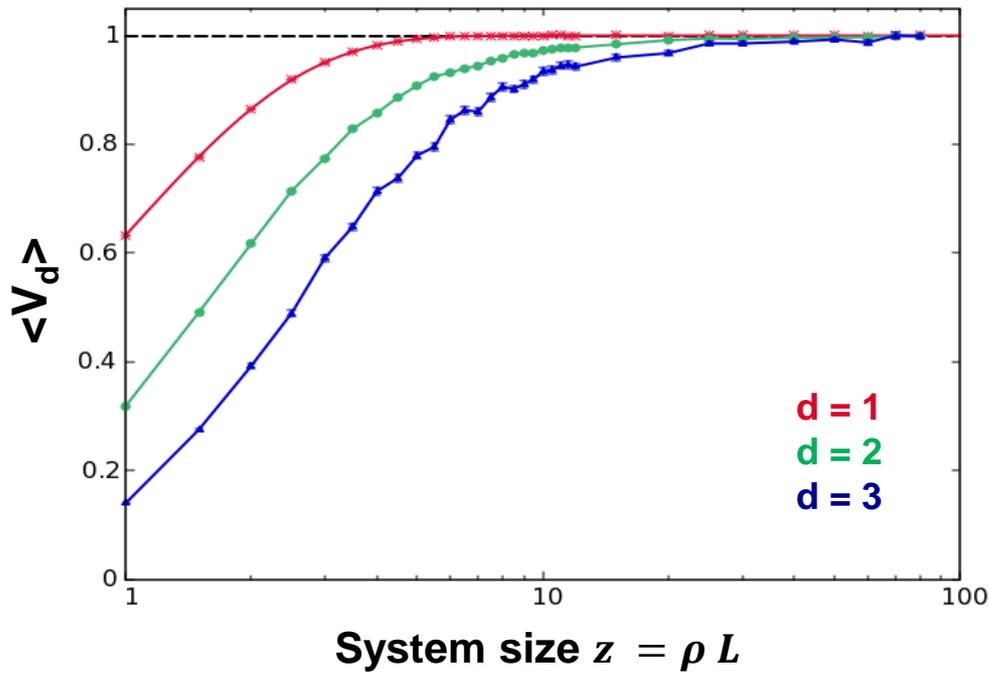
$$\langle \ell \rangle(\mathbf{v}) = 1/\rho(\mathbf{v})$$

- If the lines  $\mathbf{v}$  are *isotropic and homogeneous*, then

$$\Lambda \equiv \langle \ell \rangle = \alpha_d \frac{\langle V_d \rangle}{\langle S_d \rangle} = \frac{1}{\rho}$$

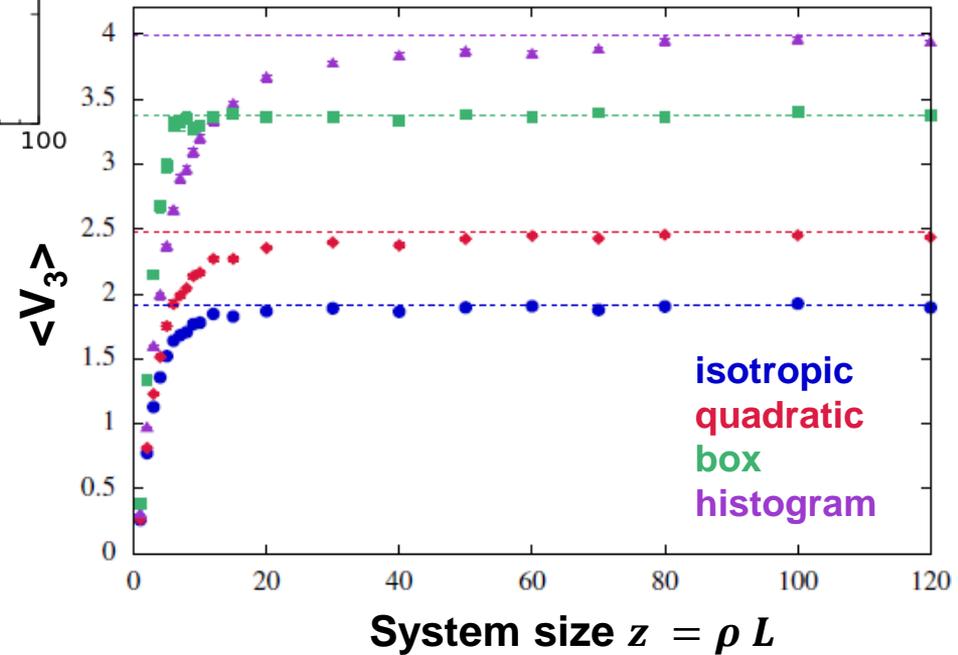
Correlation length of the tessellation

# Finite size effects: polyhedral features



- Monte Carlo results
- Asymptotic values for the moments:

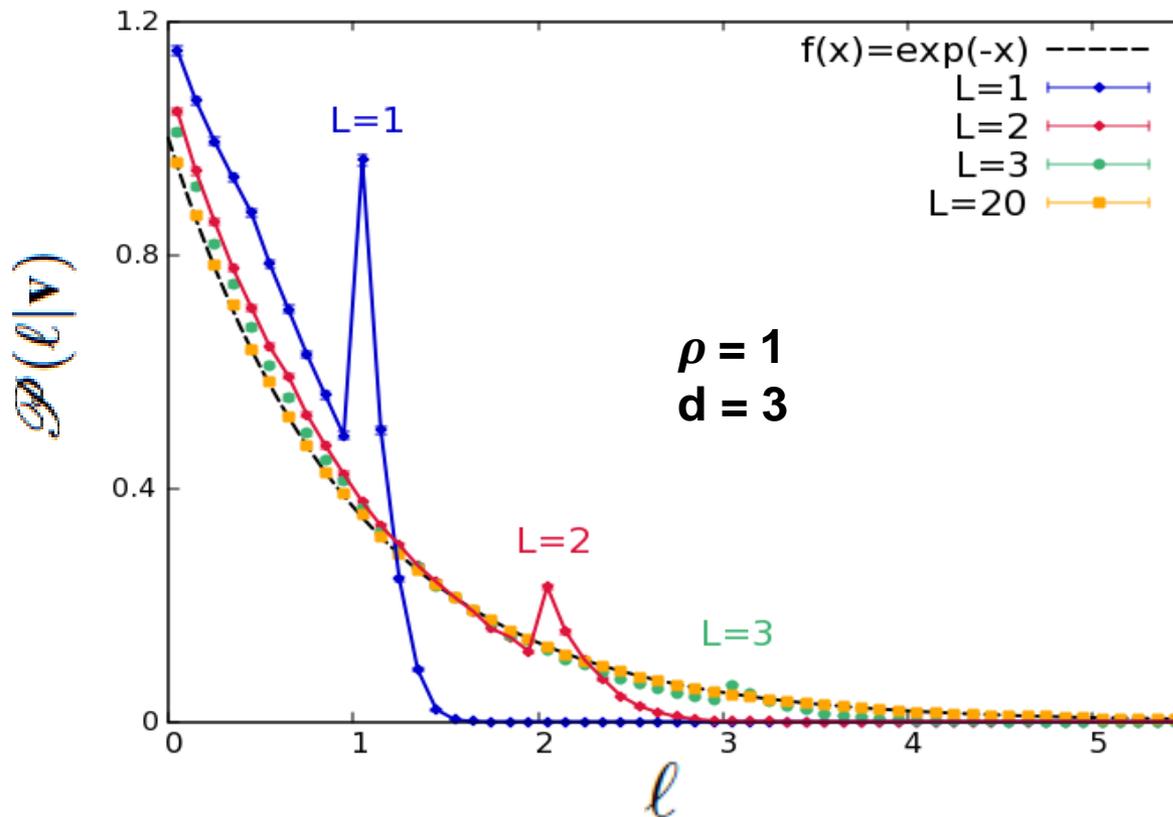
**Miles, Schneider & Weil**



# Finite size effects: chord length distribution

Sample lines with direction  $\mathbf{v}$ :  $\mathcal{P}(\ell|\mathbf{v}) = \rho(\mathbf{v})e^{-\ell\rho(\mathbf{v})}$

$$\rho(\mathbf{v}) = \frac{\alpha_d}{2} \rho \int_{\Omega_d^+} |\mathbf{n} \cdot \mathbf{v}| dH(\mathbf{n})$$

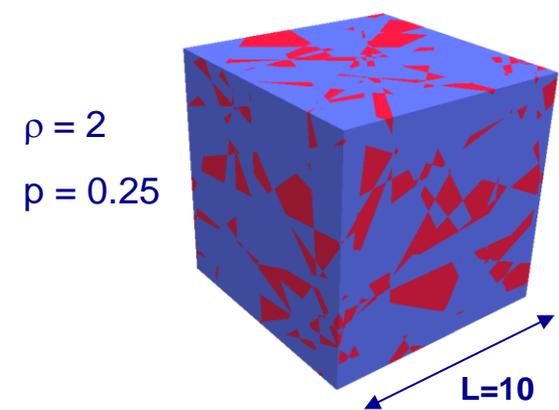
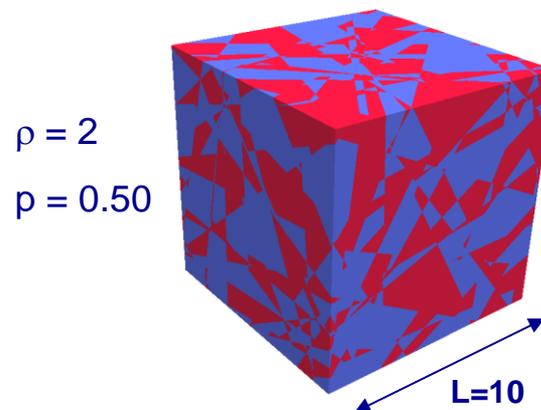
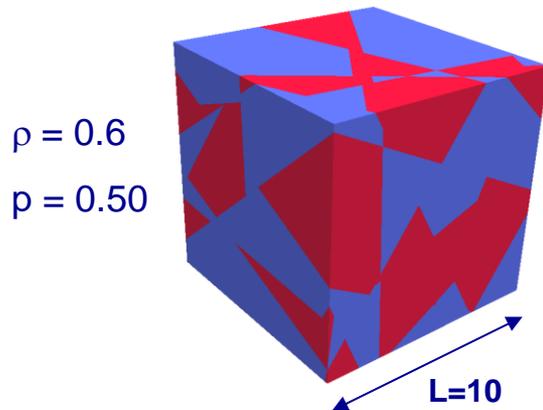


*Homogeneous and isotropic*  
lines:

$H$	$\langle \ell \rangle$	Monte Carlo
Isotropic	1	$0.999 \pm 1 \cdot 10^{-3}$
Linear	1	$0.993 \pm 9 \cdot 10^{-4}$
Parabolic	1	$0.993 \pm 1 \cdot 10^{-3}$
Box	1	$0.992 \pm 1 \cdot 10^{-3}$
Histogram	1	$0.993 \pm 1 \cdot 10^{-3}$

## □ Attribute **physical properties**:

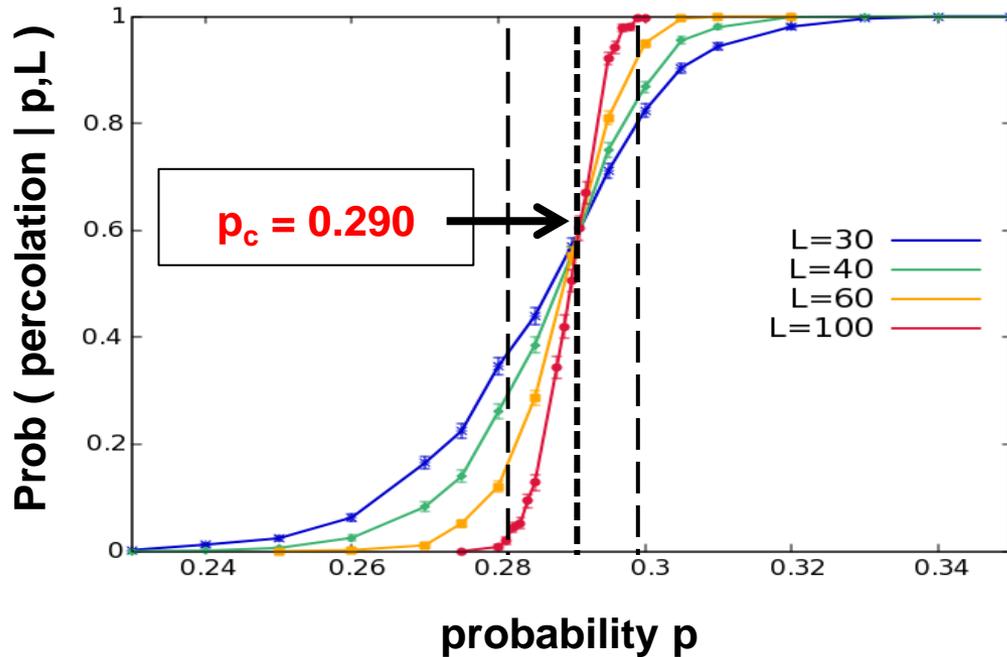
- Assign each polyhedron a « **label** »
- **Binary stochastic mixing**: red with probability  $p$ , blue with probability  $1 - p$
- Define a **cluster**: aggregate neighbouring polyhedra sharing the same colour



## □ Percolation threshold: $p_c$

- Value of  $p$  beyond which the red cluster spans **a.s.** the entire domain
- Rigorously defined for *infinite* tessellations
- Physical meaning: preferential paths

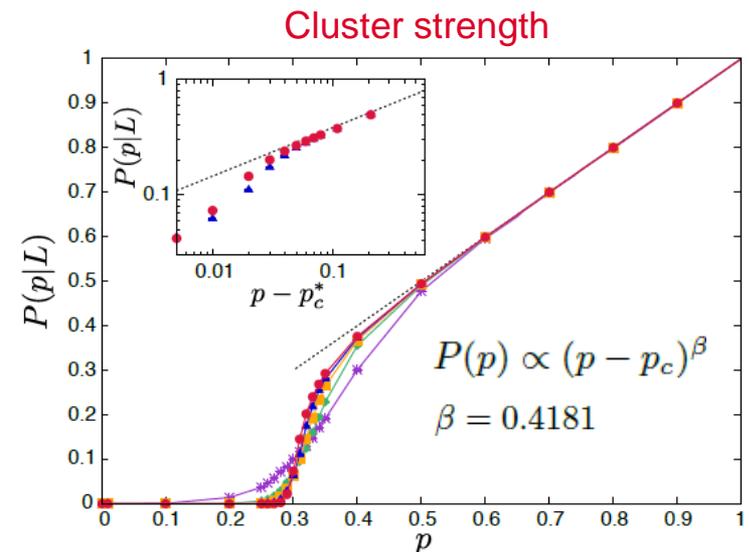
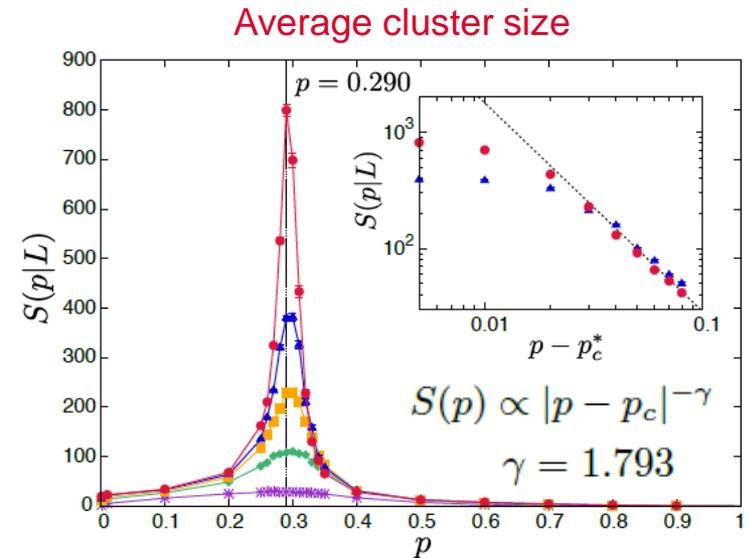
# Percolation properties for 3d Poisson geometries



3d Poisson :  $p_c = 0.290 \pm 0.007$  (Larmier et al., 2016)

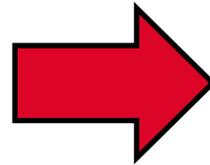
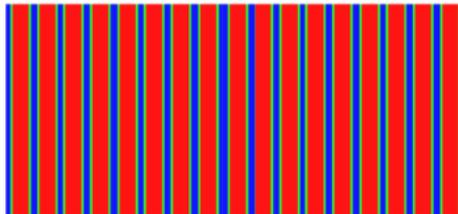
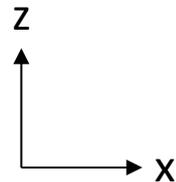
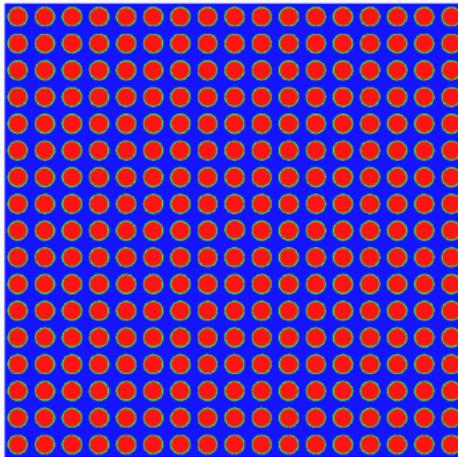
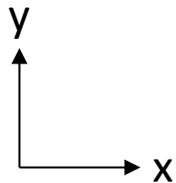
2d Poisson :  $p_c = 0.586 \pm 0.001$  (Lepage et al., 2010)

Cubic 3d lattice :  $p_c = 0.3126$  (Grassberger, 1992)

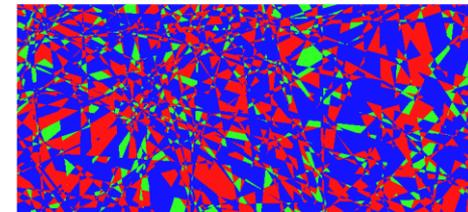
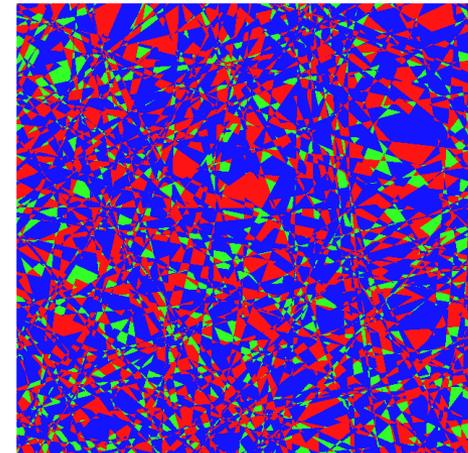


# Application to an eigenvalue problem

Intact assembly



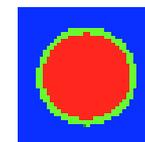
Damaged fuel



## Compositions:

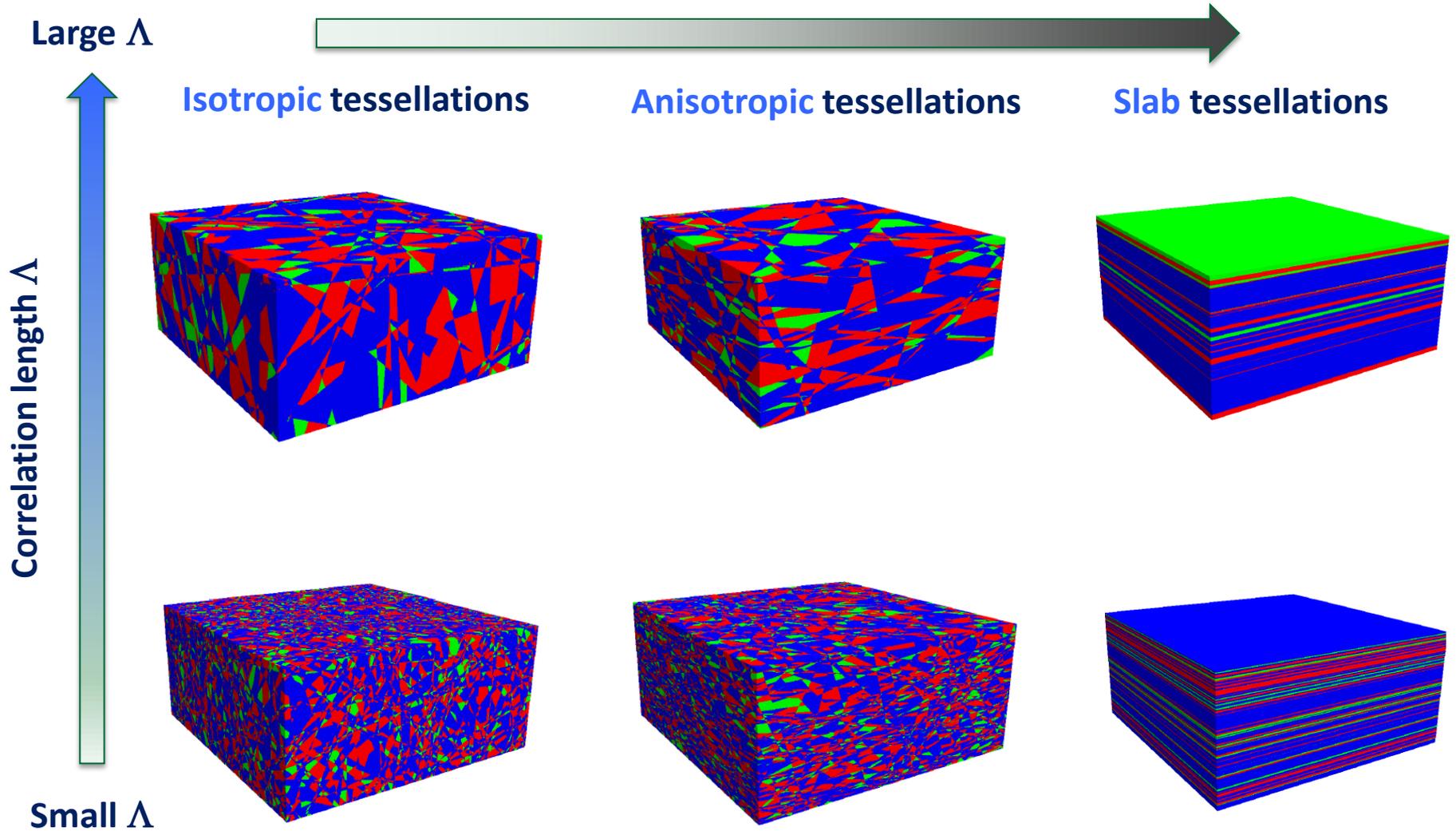
(ternary mixing,  
respecting volume  
fractions  $p$ )

	<b>Fuel: UOX/MOX</b> : 35%
	<b>Cladding</b> : 10%
	<b>Moderator: H<sub>2</sub>O</b> : 55%

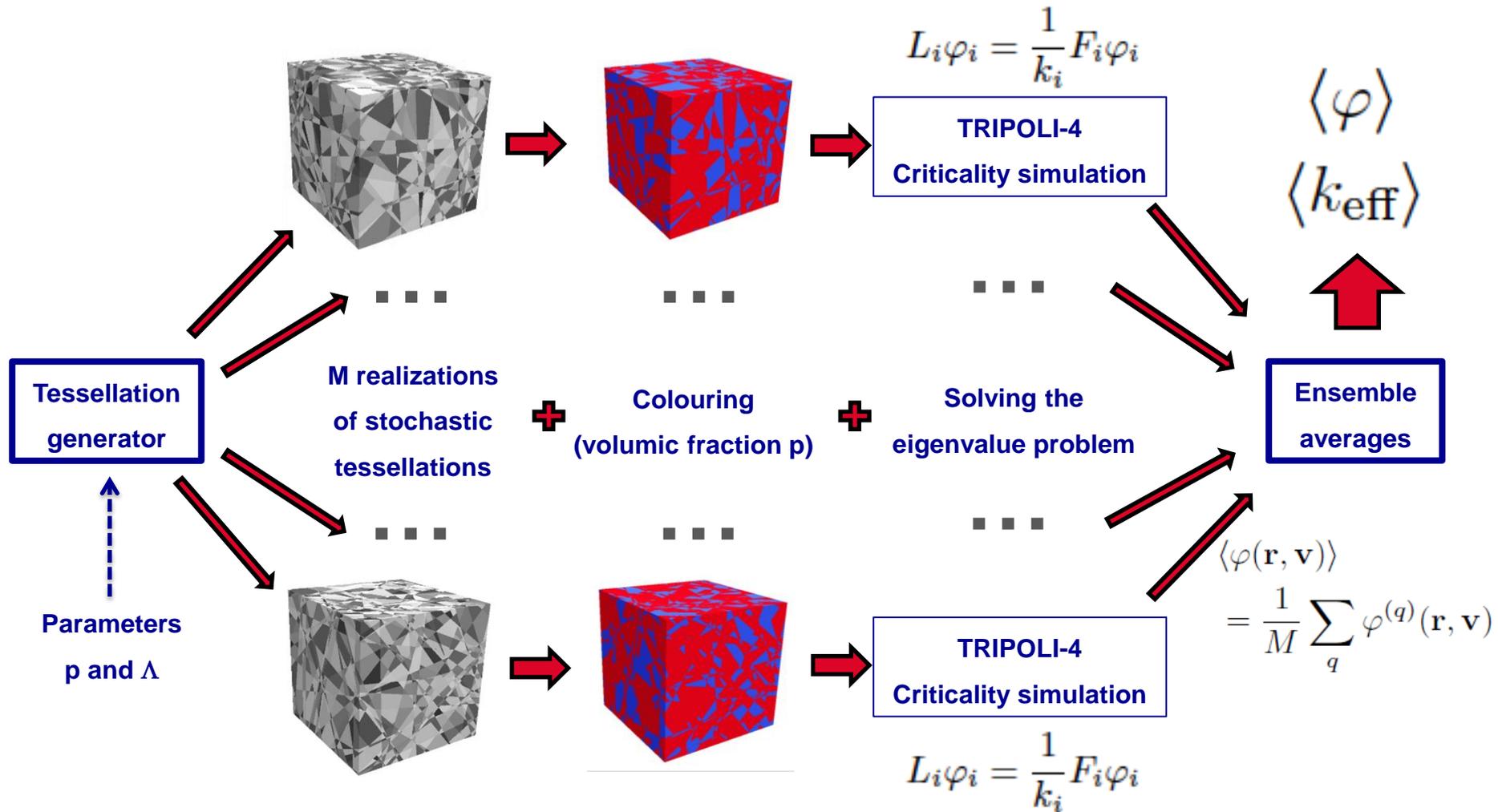


$\delta = 1.21$  cm

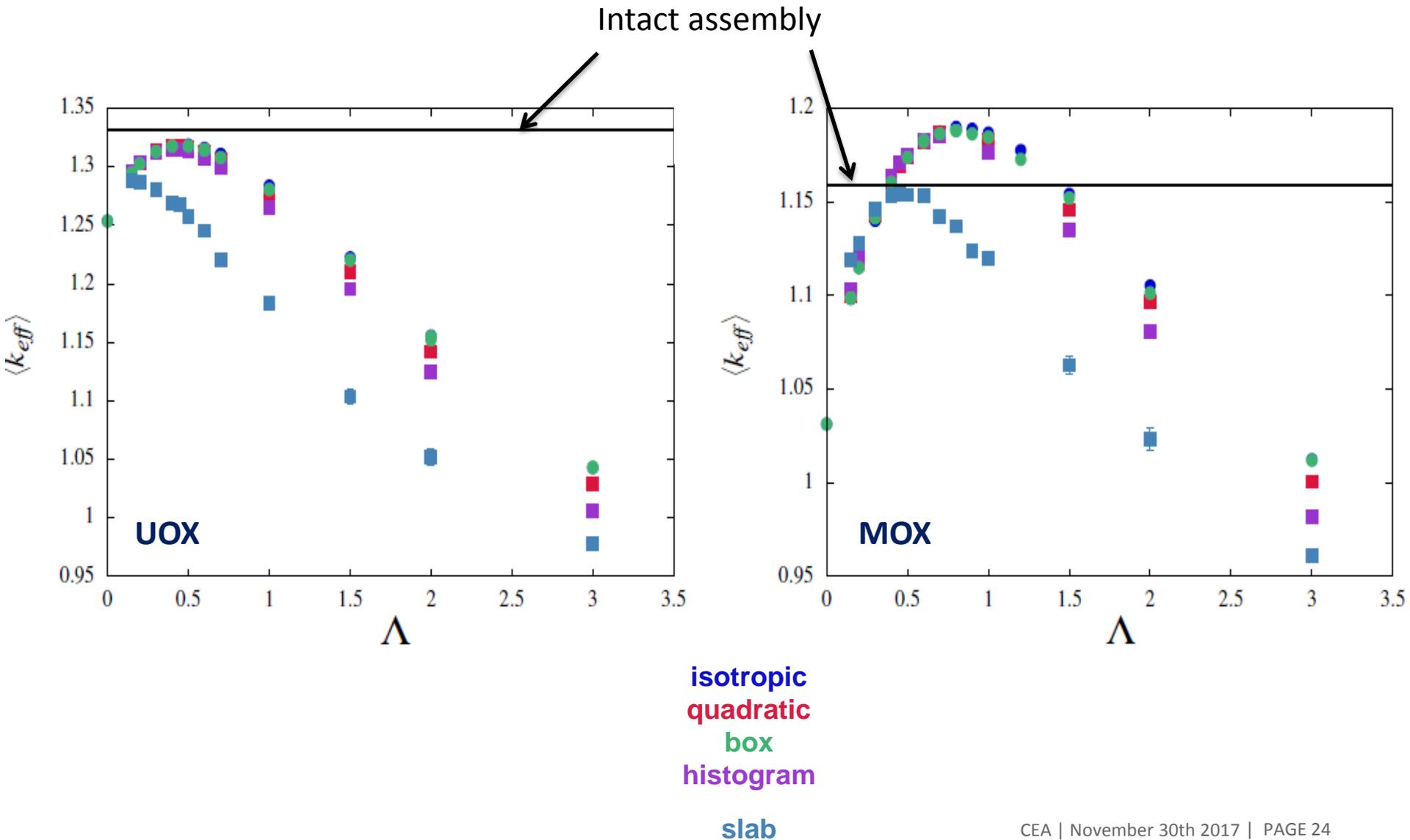
# BENCHMARK PARAMETERS



# REFERENCE SOLUTIONS BY MONTE CARLO METHODS



# AVERAGE EIGENVALUE $K_{EFF}$



# Thanks for your attention

## References

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- ❑ C. Larmier, E. Dumonteil, F. Malvagi, A. Mazzolo, A. Zoia, *Finite size effects and percolation properties of Poisson geometries*, *Phys. Rev. E* **94**, 012130 (2016)

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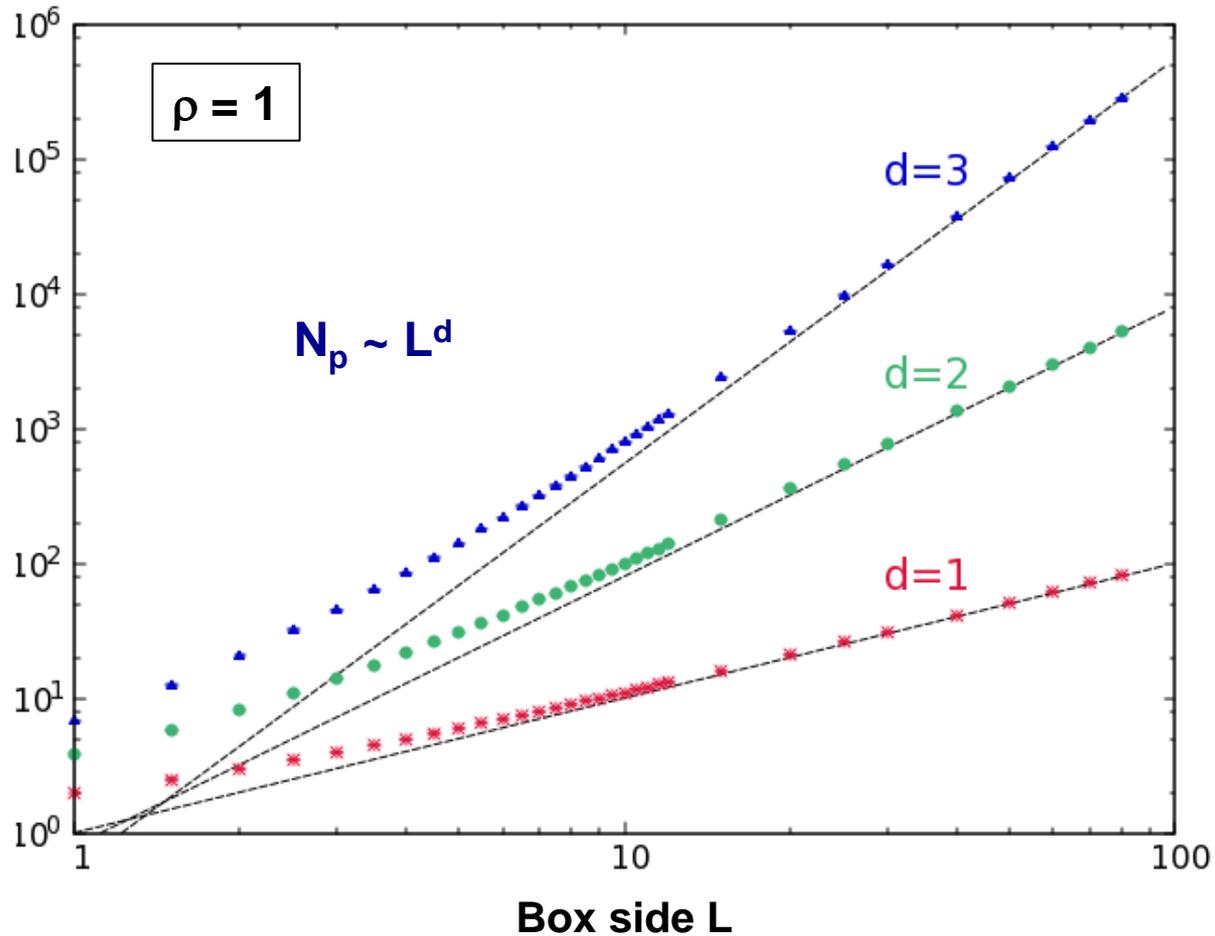
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# Effects of the tessellation density $\rho$

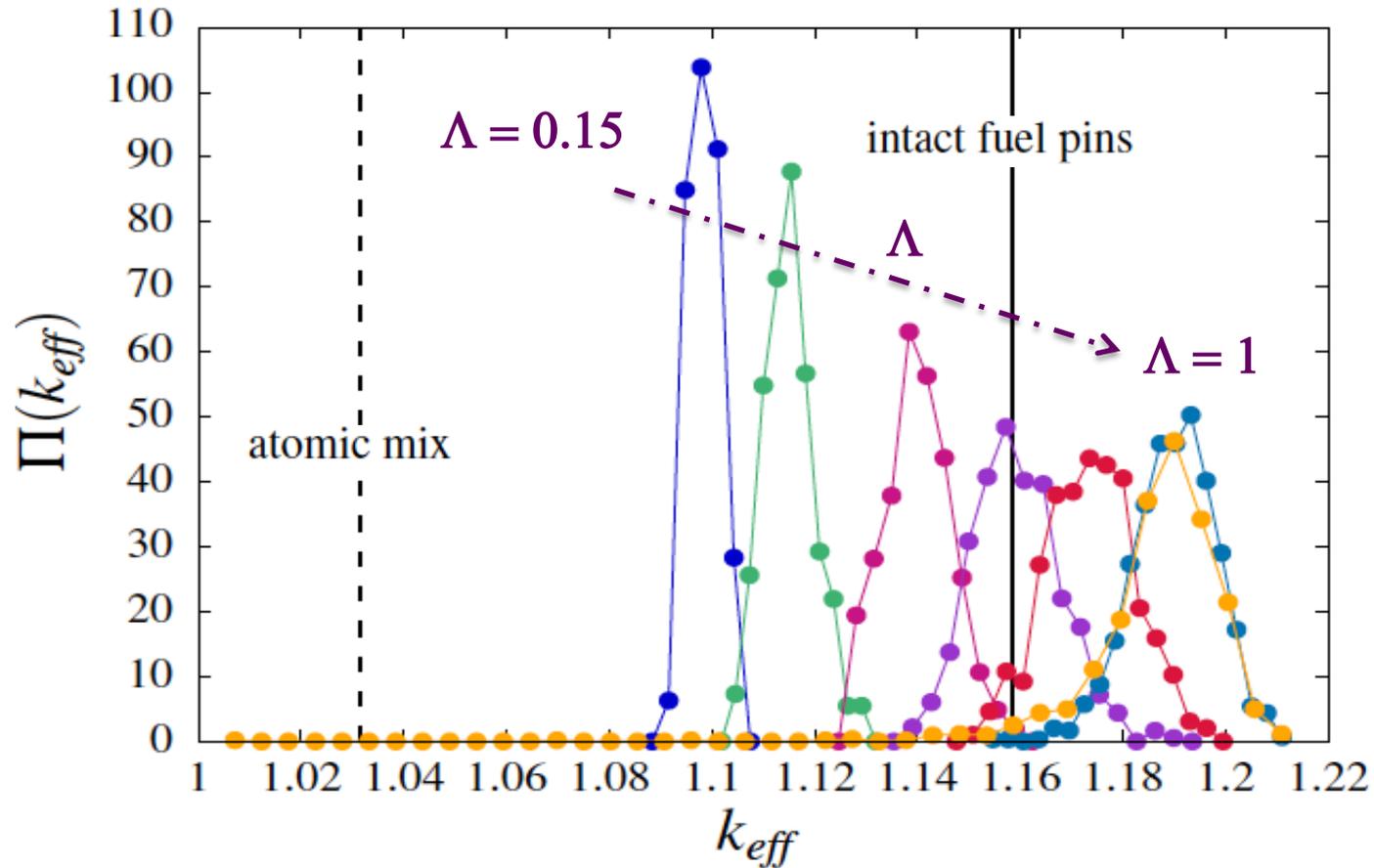
$N_p$  = average number of d-polyhedra



Dimensionless factor  $z = \rho L$  : system « size »

# DISTRIBUTION OF $k_{EFF}$ AS A FUNCTION OF $\Lambda$

MOX assembly with isotropic Poisson tessellation



## MOX assembly with $\Lambda = 1$

