

# Mechanics of heterogeneous materials

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# Plan

- ① Representation of microstructures
  - Real microstructures
  - Random models
- ② Mechanics of microstructures
  - Boundary conditions for the unit cell
  - Bounds of effective properties
- ③ Representative volume elements
  - Numerical tools for the mechanics of microstructures
  - Apparent properties, effective properties
  - RVE for a two-phase material
- ④ Conclusions

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## ④ Conclusions

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## ② Mechanics of microstructures

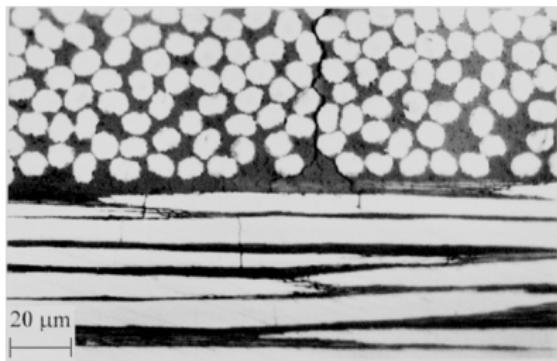
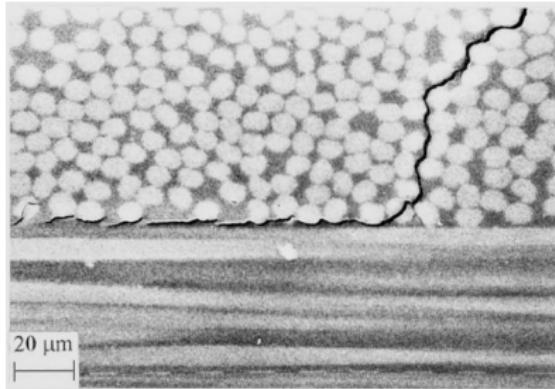
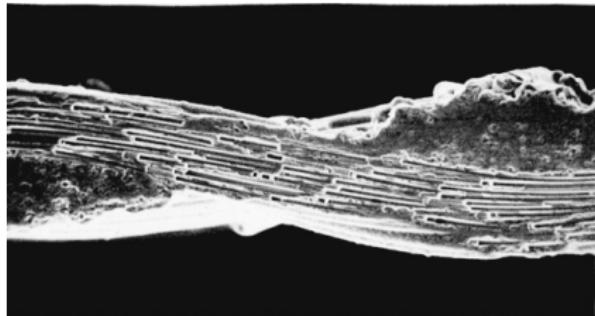
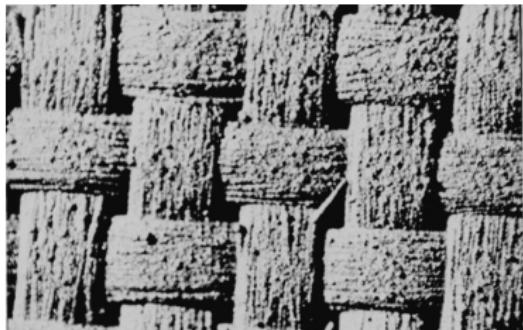
- Boundary conditions for the unit cell
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## ③ Representative volume elements

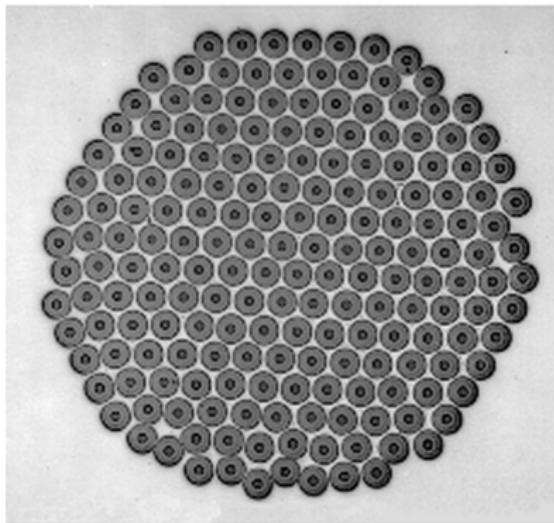
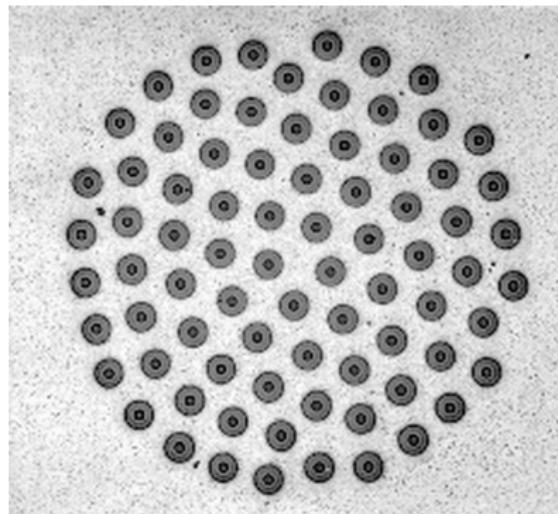
- Numerical tools for the mechanics of microstructures
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## ④ Conclusions

# Composite materials



## Metal matrix composites



Long fiber composites SiC-Ti (fiber diameter : 500  $\mu\text{m}$ )

# Polycrystalline morphology



zinc coating

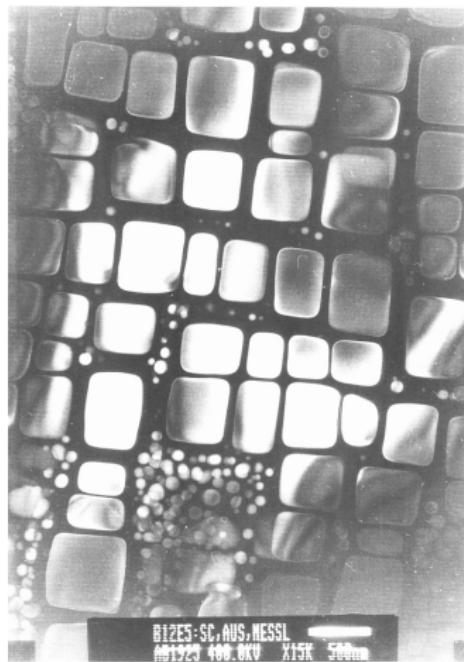


shape memory alloy Cu-Zn-Al

## Two-phase microstructures

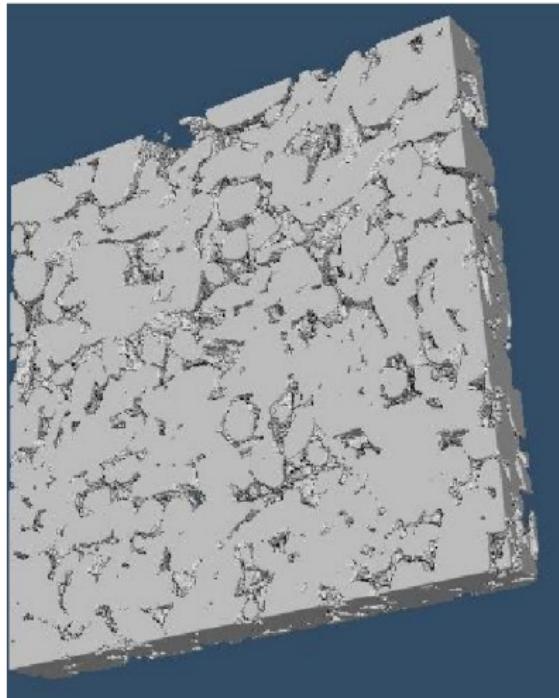


Titanium alloy Ti6242



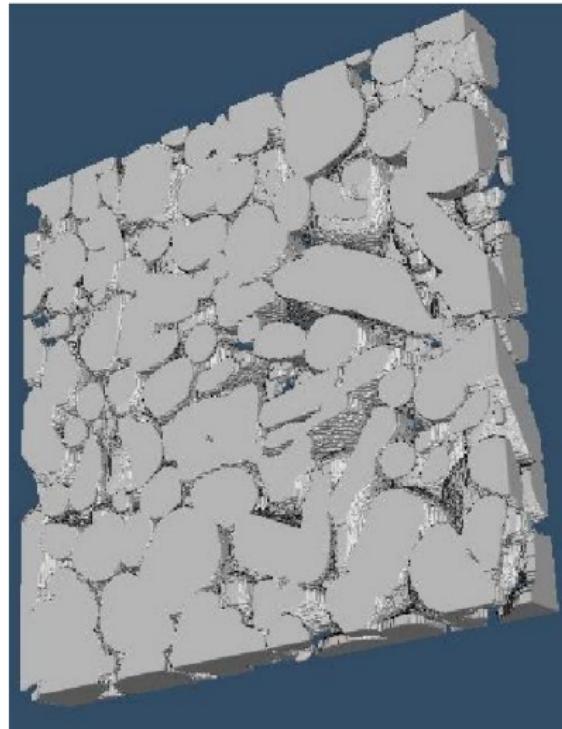
nickel-base single crystal superalloy

# Quasi-transparent materials



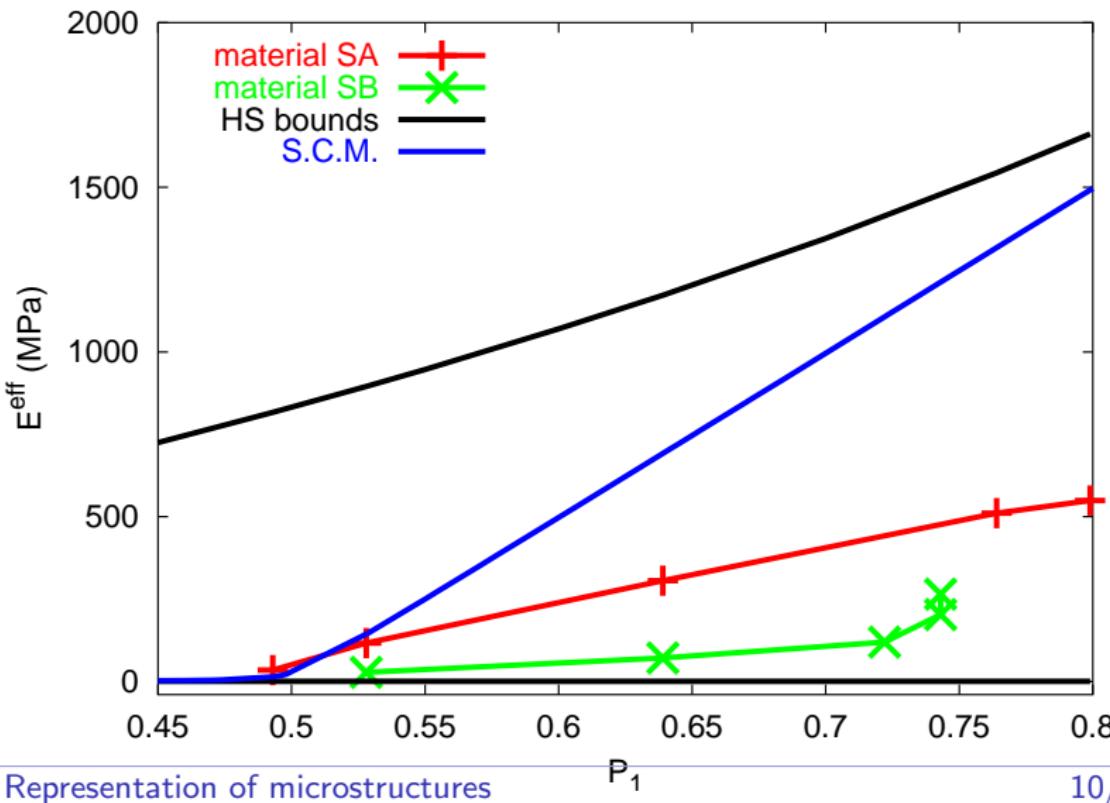
**Material A**

confocal microscopy  $250 \times 250 \times 30 \mu\text{m}^3$

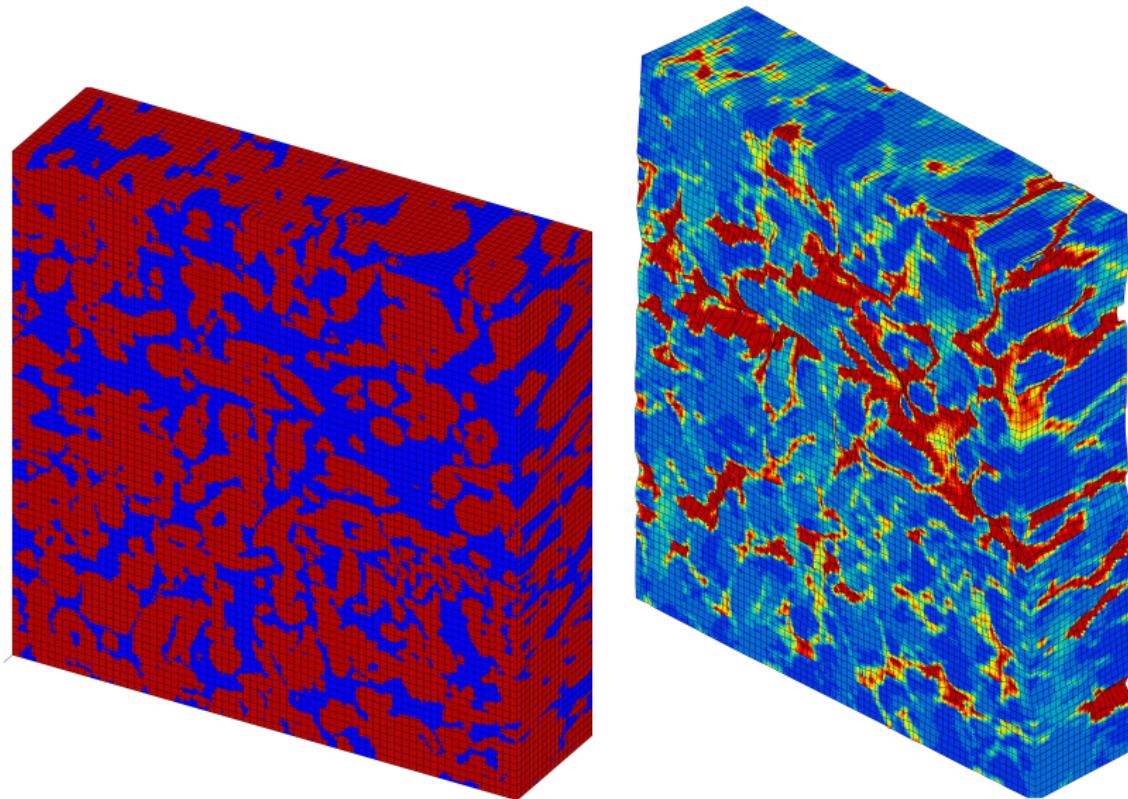


**Material B**

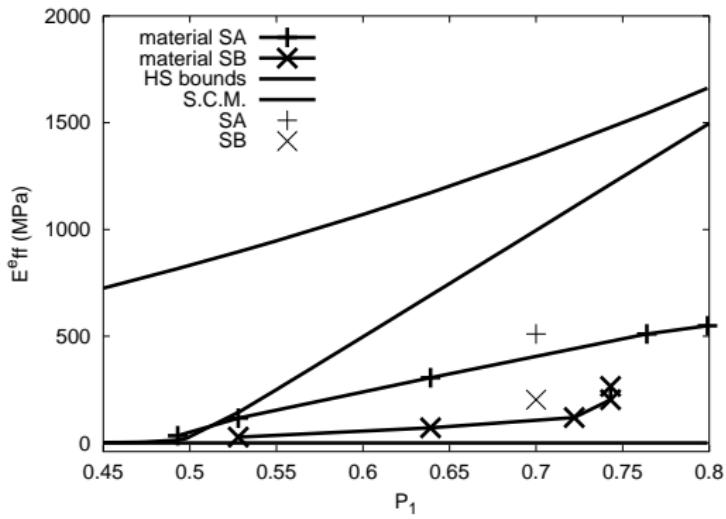
# Influence of morphology on elastic properties of ice creams!



# Mechanics of microstructures



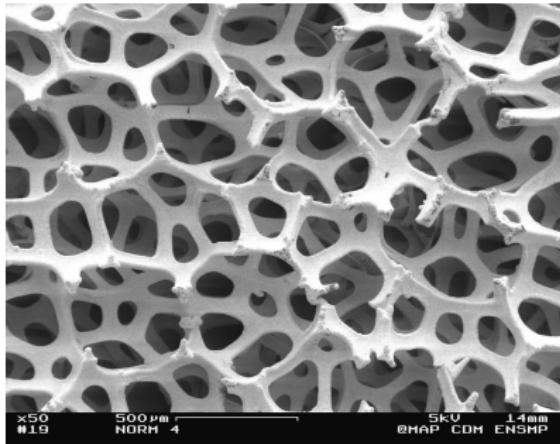
# Elastic properties of ice creams



# Materials with a high contrast in phase properties

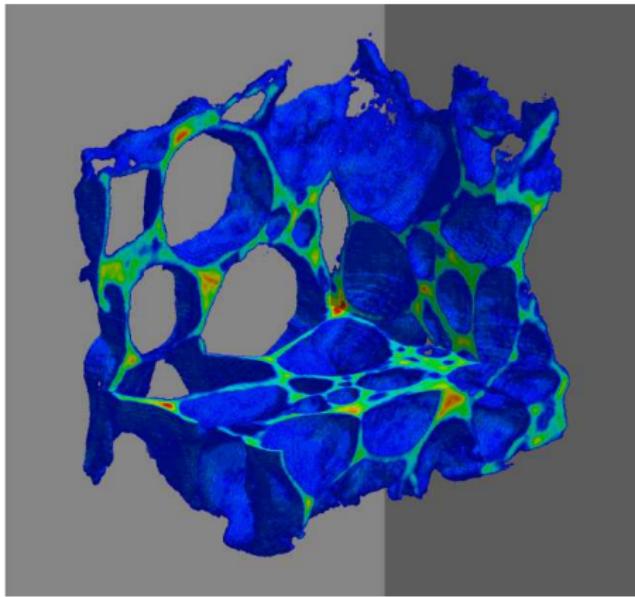


aluminum foam



nickel foam

# X-ray micro-tomography



experiment

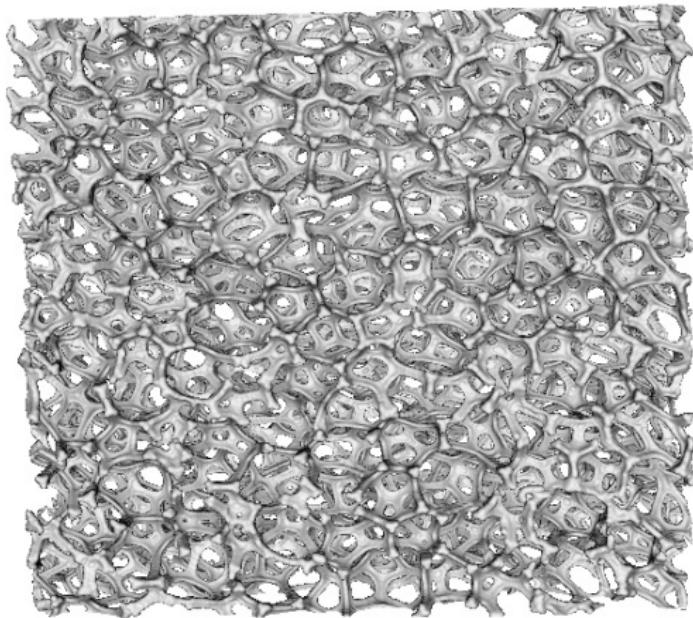
▶ animate

result

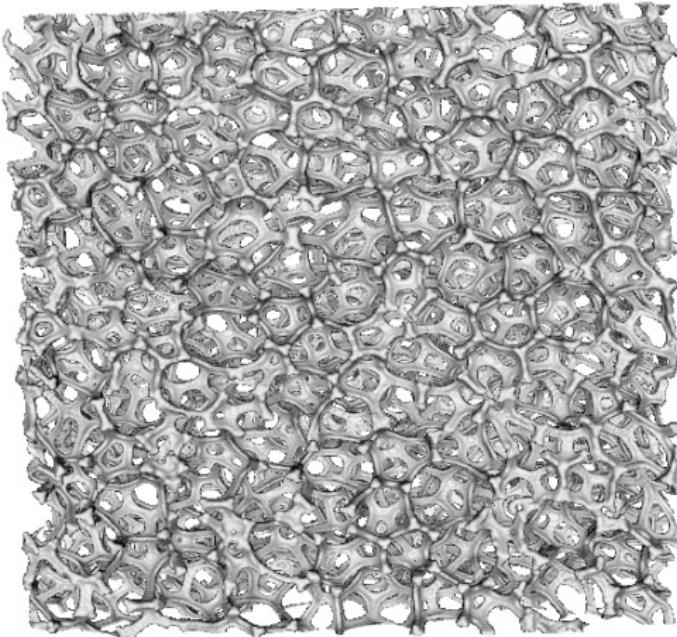
▶ animate

Representation of microstructures

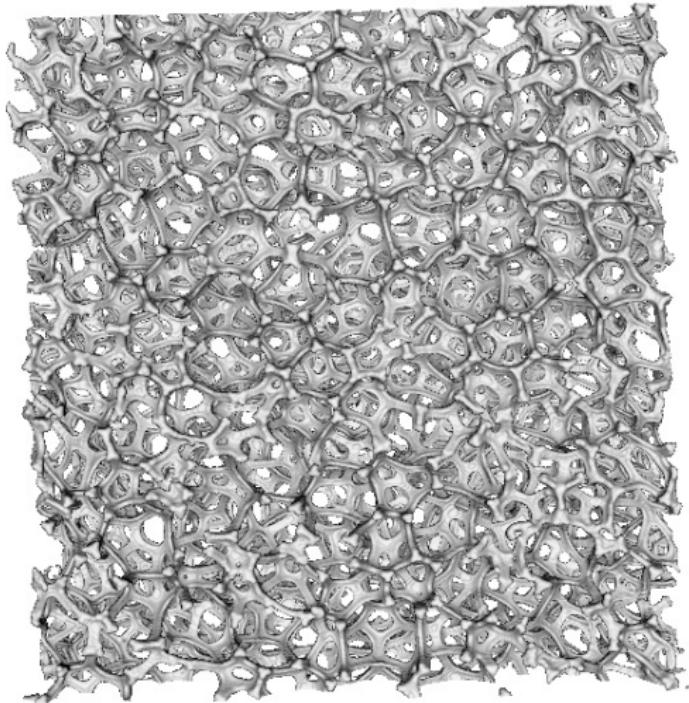
# In-situ X-ray micro-tomography



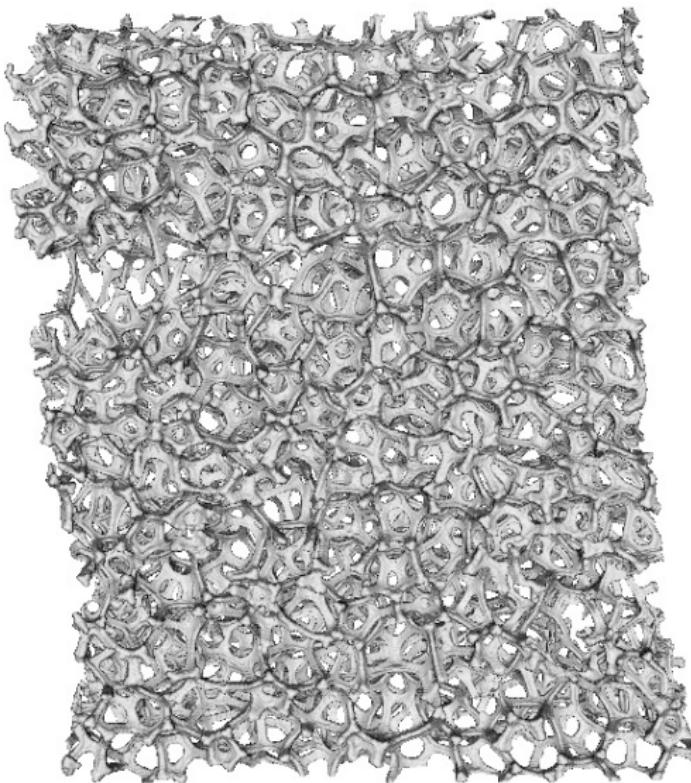
# In-situ X-ray micro-tomography



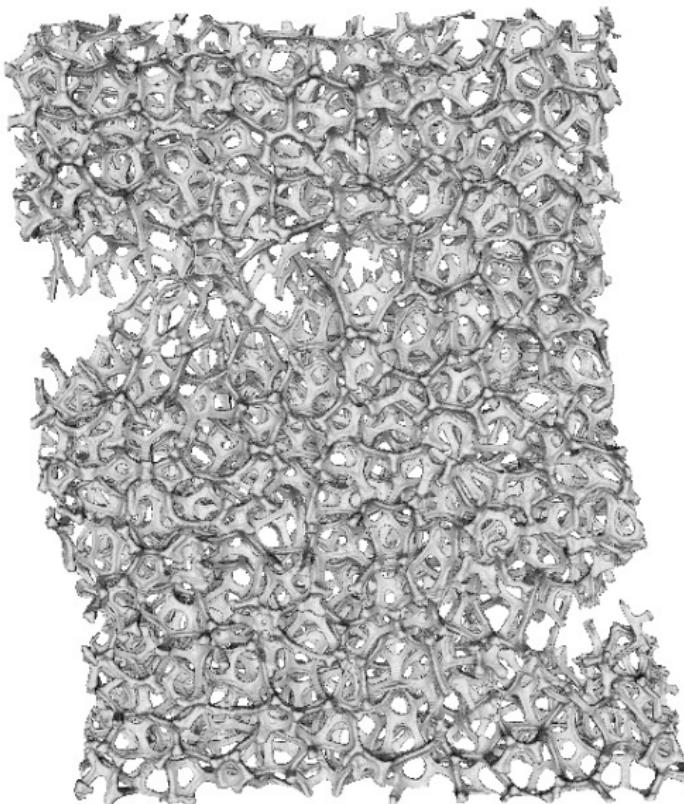
# In-situ X-ray micro-tomography



# In-situ X-ray micro-tomography



# In-situ X-ray micro-tomography



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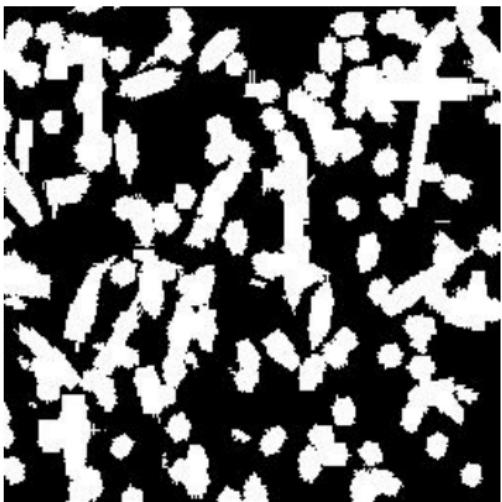
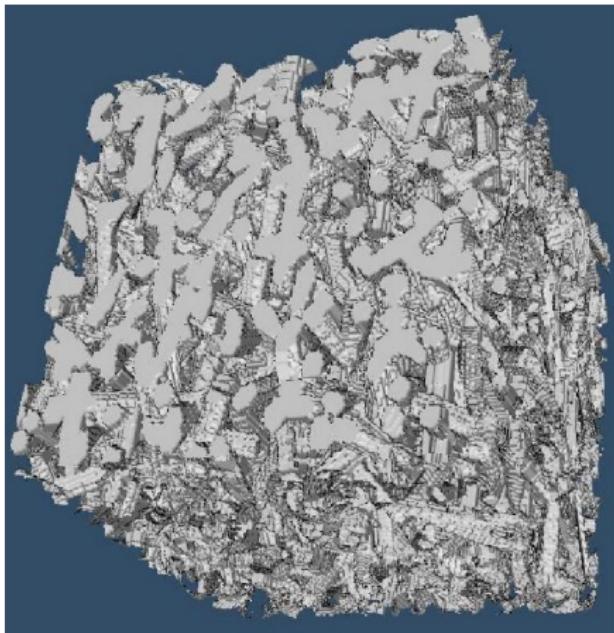
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## ③ Representative volume elements

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- RVE for a two-phase material

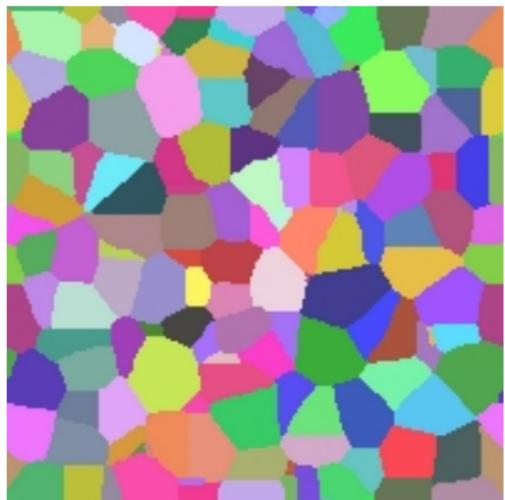
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# Random models for composite materials



Boolean schemes (mathematical morphology)

# Random models for polycrystalline microstructures



Voronoi mosaic

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# Objectives of microstructural mechanics

- **Mechanical behavior of heterogeneous materials**
  - ★ understanding deformation and fracture mechanisms
  - ★ influence of phase morphology: computation of RVE
  - ★ link to homogenization methods:
    - \* test available estimates
    - \* make predictions with a few assumptions and without violating bounds!
    - \* high contrast in phase properties
  - ★ additional information: variance of fields, dispersion, local heterogeneities
- **Computing small structures**
  - ★ mini-samples, thin films, coarse grain materials, MEMS
  - ★ stress concentration zones
- **Damage of materials** governed by maximal values, not by mean values

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# Notion of Homogeneous Equivalent Medium

- Local stress and strain

$$\tilde{\sigma}(\underline{x}) = \tilde{\mathbf{c}}(\underline{x}) : \tilde{\boldsymbol{\varepsilon}}(\underline{x})$$

- Global stress and strain

$$\Sigma = \frac{1}{V} \int_V \tilde{\sigma} dV = \langle \tilde{\sigma} \rangle, \quad \mathbf{E} = \frac{1}{V} \int_V \tilde{\boldsymbol{\varepsilon}} dV = \langle \tilde{\boldsymbol{\varepsilon}} \rangle$$

- Concentration tensor

imagine you can solve the BVP on  $V$  prescribed mean strain  
 $\mathbf{E}$ ,  $\exists \mathbf{A}$  such that

$$\tilde{\boldsymbol{\varepsilon}}(\underline{x}) = \tilde{\mathbf{A}}(\underline{x}) : \mathbf{E}$$

- Macroscopic constitutive law

$$\Sigma = \langle \tilde{\boldsymbol{\varepsilon}} : \tilde{\mathbf{c}} \rangle = \langle \tilde{\boldsymbol{\varepsilon}} : \tilde{\mathbf{A}} : \mathbf{E} \rangle = \tilde{\mathbf{C}}^{\text{eff}} : \mathbf{E}$$

$$\tilde{\mathbf{C}}^{\text{eff}} = \langle \tilde{\mathbf{c}} : \tilde{\mathbf{A}} \rangle$$

this is not the mean value of elastic moduli!

# How to prescribe mean strain to a material volume element?

- Kinematic Uniform Boundary Conditions, KUBC
- Stress (Traction) Uniform Boundary Conditions, SUBC
- Periodicity Conditions
- Mixed conditions

## Kinematic Uniform Boundary Conditions (KUBC)

$$\underline{\mathbf{u}} = \underline{\mathbf{E}} \cdot \underline{\mathbf{x}}, \quad \forall \underline{\mathbf{x}} \in \partial V, \quad u_i = E_{ij} x_j$$

$$\langle \underline{\varepsilon} \rangle = \frac{1}{V} \int_V \underline{\varepsilon} dV = \underline{\mathbf{E}}$$

Proof (divergence theorem) :

$$\begin{aligned}\langle \varepsilon_{ij} \rangle &= \frac{1}{V} \int_V u_{(i,j)} dV = \frac{1}{V} \int_{\partial V} u_{(i)} n_j dS \\ &= E_{(ik)} \frac{1}{V} \int_{\partial V} x_k n_j dS = E_{(ik)} \frac{1}{V} \int_V x_{k,j} dV \\ &= E_{(ik)} \delta_{kj} = E_{ij}\end{aligned}$$

Mean work of internal forces:

$\underline{\sigma}^*$  a divergence free stress field

$\underline{\varepsilon}'$  a compatible strain field fulfilling KUBC boundary conditions

$$\langle \underline{\sigma}^* : \underline{\varepsilon}' \rangle = \underline{\Sigma} : \underline{\mathbf{E}}$$

where the macroscopic stress tensor is defined by  $\underline{\Sigma} = \langle \underline{\sigma}^* \rangle$

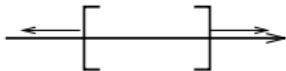
# Divergence theorem

Stokes, Gauss ...

$$\int_V u_{,i} dV = \int_{\partial V} u n_i dV$$

where  $u_{,i} = \frac{\partial u}{\partial x_i}$

$$1D : \int_a^b u'(x) dx = [u]_a^b$$



return

## Stress uniform boundary conditions (SUBC)

$$\underline{\mathbf{t}} = \underline{\boldsymbol{\sigma}} \cdot \underline{\mathbf{n}} = \underline{\boldsymbol{\Sigma}} \cdot \underline{\mathbf{n}}, \quad \forall \underline{\mathbf{x}} \in \partial V, \quad t_i = \sum_j \sigma_{ij} n_j$$

$$\langle \underline{\boldsymbol{\sigma}} \rangle = \frac{1}{V} \int_V \underline{\boldsymbol{\sigma}} \, dV = \underline{\boldsymbol{\Sigma}}$$

Proof (divergence theorem) :

$$\begin{aligned}\langle \sigma_{ij} \rangle &= \frac{1}{V} \int_V \sigma_{ij} \, dV = \frac{1}{V} \int_V \sigma_{ik} \delta_{kj} \, dV = \frac{1}{V} \int_V (\sigma_{ik} x_j)_{,k} \, dV \\ &= \frac{1}{V} \int_{\partial V} \sigma_{ik} x_j n_k \, dS = \frac{1}{V} \int_{\partial V} \sum_i x_j n_i \, dS = \sum_{ij}\end{aligned}$$

Mean work of internal forces:

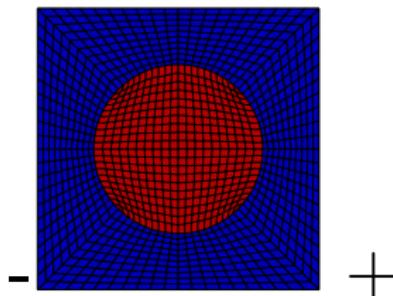
$\underline{\boldsymbol{\sigma}}^*$  a divergence free stress tensor fulfilling the KUBC boundary conditions  
 $\underline{\boldsymbol{\varepsilon}}'$  a compatible strain field

$$\langle \underline{\boldsymbol{\sigma}}^* : \underline{\boldsymbol{\varepsilon}}' \rangle = \underline{\boldsymbol{\Sigma}} : \underline{\mathbf{E}}$$

where macroscopic strain is defined by  $\underline{\mathbf{E}} = \langle \underline{\boldsymbol{\varepsilon}}' \rangle$

## Periodicity conditions

$\underline{u} = \tilde{\mathbf{E}} \cdot \underline{x} + \underline{v}$  where  $\underline{v}$  is a periodic fluctuation



$$\underline{v}(\underline{x}^+) = \underline{v}(\underline{x}^-), \quad \underline{u}(\underline{x}^+) - \underline{u}(\underline{x}^-) = \tilde{\mathbf{E}} \cdot (\underline{x}^+ - \underline{x}^-)$$

$\implies \underline{u}$  is not periodic!!!

$$\tilde{\sigma}(\underline{x}^-) \cdot \underline{n}^- = -\tilde{\sigma}(\underline{x}^+) \cdot \underline{n}^+, \quad (\underline{n}^- = -\underline{n}^+)$$

$$\langle \tilde{\varepsilon} \rangle = \tilde{\mathbf{E}}$$

$$\text{Proof : } \langle v_{i,j} \rangle = \frac{1}{V} \int_V v_{i,j} dV = \frac{1}{V} \int_{\partial V} v_i n_j dS = 0$$

Mean work of internal forces :

where macroscopic strain is defined by

$$\langle \tilde{\sigma} : \tilde{\varepsilon} \rangle = \tilde{\Sigma} : \tilde{\mathbf{E}}$$
$$\tilde{\Sigma} = \langle \sigma \rangle$$

## Example

compute the effective elastic properties of a composite within the periodic assumption...

local properties

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{12} \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 \\ c_{12} & c_{22} & c_{23} & 0 \\ c_{13} & c_{23} & c_{33} & 0 \\ 0 & 0 & 0 & c_{44} \end{bmatrix} \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{12} \end{bmatrix}$$

effective properties

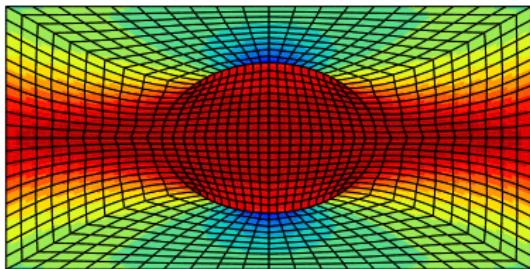
$$\begin{bmatrix} \Sigma_{11} \\ \Sigma_{22} \\ \Sigma_{33} \\ \Sigma_{12} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 \\ C_{12} & C_{22} & C_{23} & 0 \\ C_{13} & C_{23} & C_{33} & 0 \\ 0 & 0 & 0 & C_{44} \end{bmatrix} \begin{bmatrix} E_{11} \\ E_{22} \\ E_{33} \\ 2E_{12} \end{bmatrix}$$

# Simple extension

prescribe  $\langle \varepsilon \rangle$ , compute  $\langle \sigma \rangle \dots$

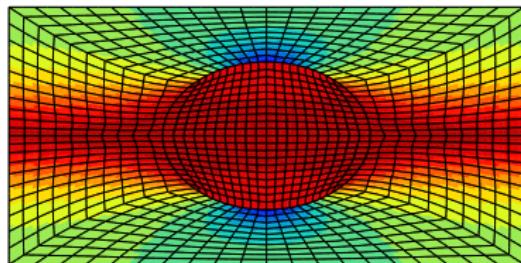
$$\mathbf{\tilde{E}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

KUBC



$$\begin{aligned}\Sigma_{11} &= C_{11} \\ \Sigma_{22} &= C_{12} \\ \Sigma_{33} &= C_{13} \\ \Sigma_{12} &= 0\end{aligned}$$

periodicity conditions

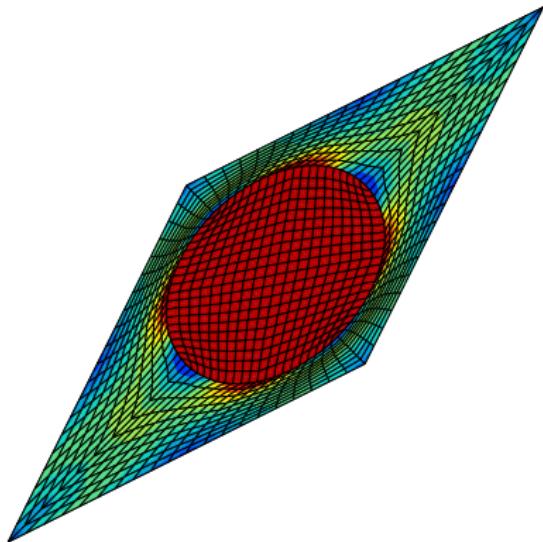


# Simple shear

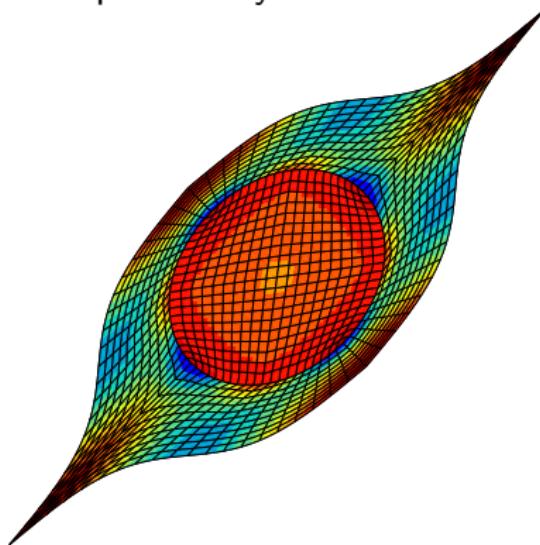
$$\mathbf{\Sigma} = \begin{bmatrix} 0 & 1/2 & 0 \\ 1/2 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\begin{aligned}\Sigma_{11} &= \Sigma_{22} = \Sigma_{33} = 0 \\ \Sigma_{12} &= C_{44}\end{aligned}$$

KUBC



periodicity conditions



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## 2 Mechanics of microstructures

- Boundary conditions for the unit cell
- **Bounds of effective properties**

## 3 Representative volume elements

- Numerical tools for the mechanics of microstructures
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## 4 Conclusions

# Nonlinear elasticity

- convex local elasticity potential

$$\underline{\sigma} = W'(\underline{\varepsilon}) = \frac{\partial W}{\partial \underline{\varepsilon}}$$

- convex global elasticity potential

$$\underline{\Sigma} = W^{\text{eff}'}(\underline{\varepsilon}) = \frac{\partial W^{\text{eff}}}{\partial \underline{\varepsilon}}$$

- convex local dual potential

$$\underline{\varepsilon} = W^{*'}(\underline{\sigma}) = \frac{\partial W^*}{\partial \underline{\sigma}}$$

$$W^*(\underline{\sigma}) = \max_{\underline{\varepsilon}} (\underline{\sigma} : \underline{\varepsilon} - W(\underline{\varepsilon}))$$

- convex global dual potential

$$\underline{\Sigma} = \frac{\partial W^{\text{eff}*}}{\partial \underline{\sigma}}$$

# Theorem of potential energy

Boundary Value Problem

$$\begin{aligned}\operatorname{div} \underline{\sigma} + \underline{\mathbf{f}} &= 0 \\ \underline{\sigma} &= W'(\underline{\varepsilon}) \\ \underline{\mathbf{u}} &= \underline{\mathbf{u}}^d \quad \forall \underline{x} \in \partial V\end{aligned}$$

The potential energy theorem states that the solution  $\underline{\mathbf{u}}$  on  $V$  minimizes the potential energy  $\mathcal{F}$  :

$$\mathcal{F}(\underline{\mathbf{u}}') = \int_V (W(\underline{\varepsilon}') - \underline{\mathbf{f}} \cdot \underline{\mathbf{u}}') dV$$

with respect to kinematically admissible displacement fields  $\underline{\mathbf{u}}'$ .  $\underline{\mathbf{u}}'$  is kinematically admissible if it fulfills the boundary conditions  
 $\underline{\mathbf{u}} = \underline{\mathbf{u}}^d$  on  $\partial V$

## Consequence of the potential energy theorem

KUBC

$$\underline{\mathbf{u}}^d = \underline{\mathbf{E}} \cdot \underline{\mathbf{x}} \quad \forall \underline{\mathbf{x}} \in \partial V$$

$$\begin{aligned} \frac{1}{2} \int_V \underline{\varepsilon} : \underline{\mathbf{c}} : \underline{\varepsilon} dV &= \frac{1}{2} \int_V \underline{\sigma} : \underline{\varepsilon} dV = V \frac{1}{2} \underline{\Sigma} : \underline{\varepsilon} = \frac{1}{2} V \underline{\mathbf{E}} : \underline{\mathbf{C}} : \underline{\varepsilon} \\ &\leq \frac{1}{2} \int_V \underline{\varepsilon}' : \underline{\mathbf{c}} : \underline{\varepsilon}' dV \end{aligned}$$

test fonction

$$\underline{\mathbf{u}}' = \underline{\mathbf{E}} \cdot \underline{\mathbf{x}} \quad \forall \underline{\mathbf{x}} \in V$$

$$\underline{\mathbf{E}} : \underline{\mathbf{C}} : \underline{\mathbf{E}} \leq \underline{\mathbf{E}} : \langle \underline{\mathbf{c}} \rangle : \underline{\mathbf{E}}, \quad \forall \underline{\mathbf{E}}$$

Voigt upper bound for effective properties

# Theorem of complementary energy

BVP

$$\operatorname{div} \underline{\sigma} + \underline{\mathbf{f}} = 0$$

$$\underline{\varepsilon} = W^*(\underline{\sigma})$$

$$\underline{\mathbf{T}} = \underline{\sigma} \cdot \underline{\mathbf{n}} = \underline{\mathbf{T}}^d \quad \forall \underline{\mathbf{x}} \in \partial V$$

The stress solution  $\underline{\sigma}$  minimizes the functional:

$$\mathcal{F}^*(\underline{\sigma}^*) = \int_V W^*(\underline{\sigma}^*) dV$$

for any self-equilibrated stress field  $\underline{\sigma}^*$  and fulfilling the boundary conditions  $\underline{\sigma}^* \cdot \underline{\mathbf{n}} = \underline{\mathbf{T}}^d$

# Consequence of the complementary energy theorem

SUBC

$$\underline{\mathbf{T}}^d = \underline{\boldsymbol{\Sigma}} \cdot \underline{\mathbf{x}} \quad \forall \underline{\mathbf{x}} \in \partial V$$

$$\frac{1}{2} \int_V \underline{\sigma} : \underline{\mathbf{s}} : \underline{\sigma} dV = \frac{1}{2} V \underline{\boldsymbol{\Sigma}} : \underline{\mathbf{S}} : \underline{\boldsymbol{\Sigma}} \leq \frac{1}{2} \int_V \underline{\sigma}^* : \underline{\mathbf{s}} : \underline{\sigma}^* dV$$

test function

$$\underline{\sigma}^* = \underline{\boldsymbol{\Sigma}}$$

$$\underline{\boldsymbol{\Sigma}} : \underline{\mathbf{S}} : \underline{\boldsymbol{\Sigma}} \leq \underline{\boldsymbol{\Sigma}} : \langle \underline{\mathbf{s}} \rangle : \underline{\boldsymbol{\Sigma}}, \quad \forall \underline{\boldsymbol{\Sigma}}$$

Reuss lower bound

# Application to isotropic linear elasticity

- bounds for the shear modulus

$$\left\langle \frac{1}{\mu} \right\rangle^{-1} \leq \mu^{\text{eff}} \leq \langle \mu \rangle$$

$$\langle \mu \rangle = f\mu_1 + (1-f)\mu_2, \quad \left\langle \frac{1}{\mu} \right\rangle = f\frac{1}{\mu_1} + (1-f)\frac{1}{\mu_2}$$

- bounds for the bulk modulus

$$\left\langle \frac{1}{k} \right\rangle^{-1} \leq k^{\text{eff}} \leq \langle k \rangle$$

- non optimal bounds for Young's modulus

$$\langle E^{-1} \rangle^{-1} \leq E^h \leq \left( \frac{1}{3} \langle \mu \rangle^{-1} + \frac{1}{9} \langle k^{-1} \rangle \right)^{-1}$$

# Hashin/Shtrikman bounds in isotropic elasticity

additional microstructural information: isotropic distribution of phases

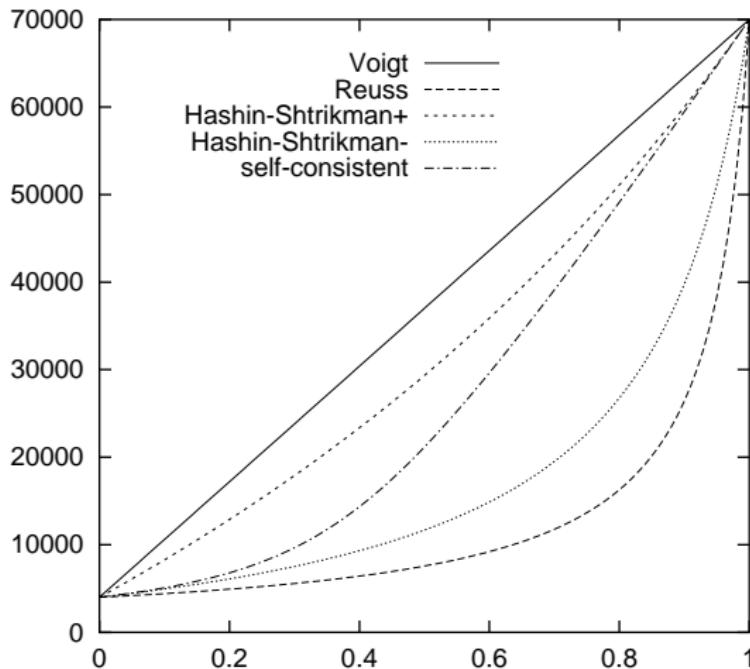
HS upper bounds

$$k^{HS+} = \left( f_1 k_1 + \frac{f_2 k_2}{1 + \alpha_1 \frac{k_2 - k_1}{k_1}} \right) \left( f_1 + \frac{f_2}{1 + \alpha_1 \frac{k_2 - k_1}{k_1}} \right)^{-1}$$

$$\mu^{HS+} = \left( f_1 \mu_1 + \frac{f_2 \mu_2}{1 + \beta_1 \frac{\mu_2 - \mu_1}{\mu_1}} \right) \left( f_1 + \frac{f_2}{1 + \beta_1 \frac{\mu_2 - \mu_1}{\mu_1}} \right)^{-1}$$

$$\alpha = \frac{3k}{3k + 4\mu}, \quad \beta = \frac{6(k + 2\mu)}{5(3k + 4\mu)}$$

# Hill's lens



isotropic mixture of two isotropic and incompressible phases  
( $\mu_1 = 70000\text{ MPa}$  et  $\mu_2 = 4000\text{ MPa}$ )

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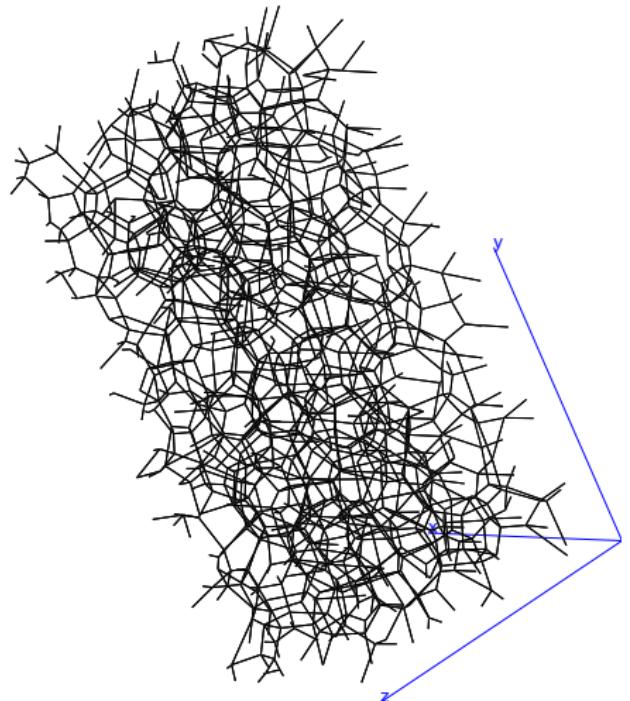
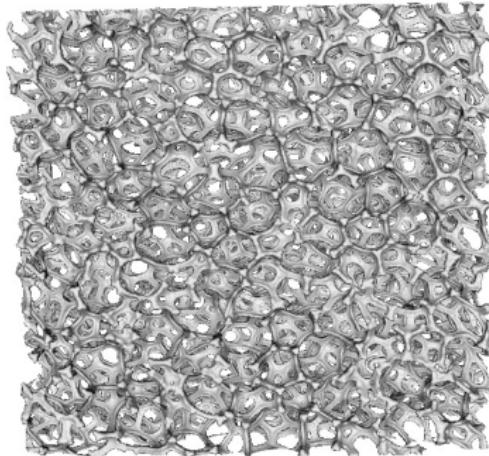
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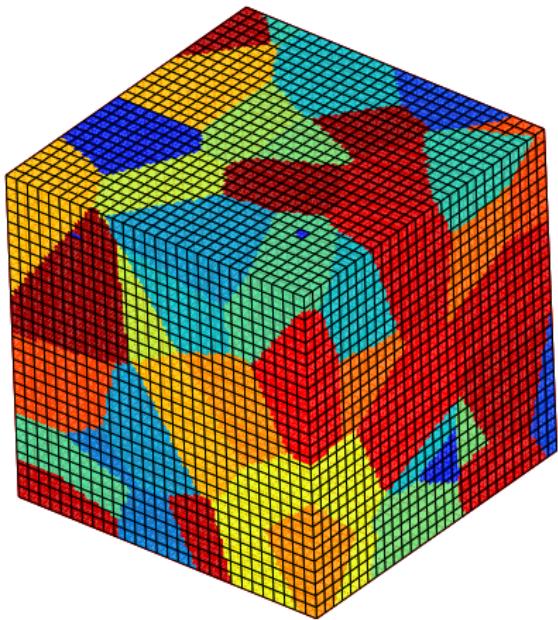
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# Meshing microstructures (1)

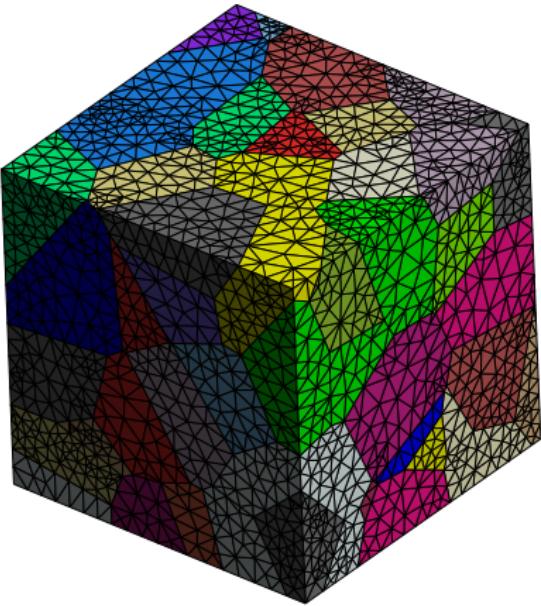


beam network

## Mesning microstructures (2)



multiphase elements

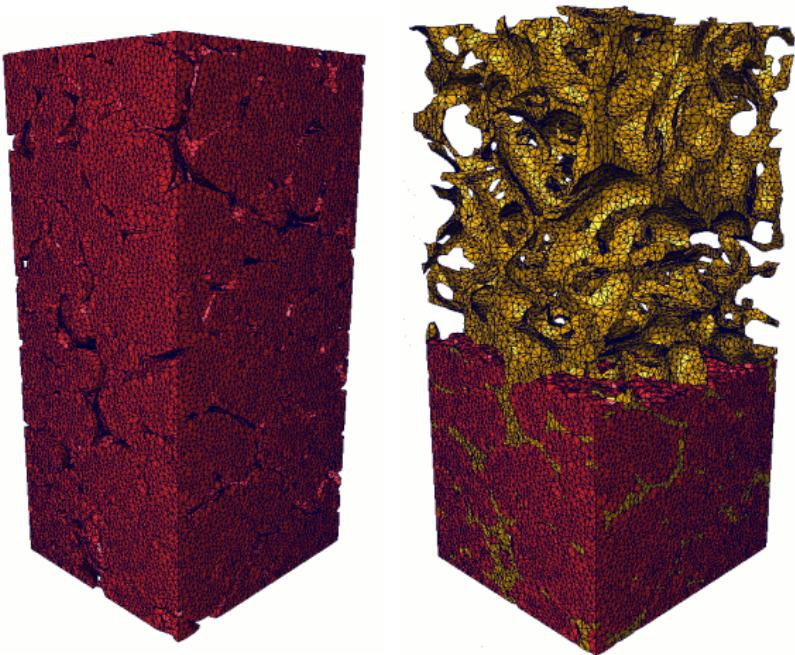


free meshing

# Zirconia–glass composites (Saint–Gobain)

elasticity        at  
600°C  
 $E_{Zr} = 230$  GPa  
 $E_{verre} = 73$  GPa

1500000 dof  
25 processors  
1/2 hour

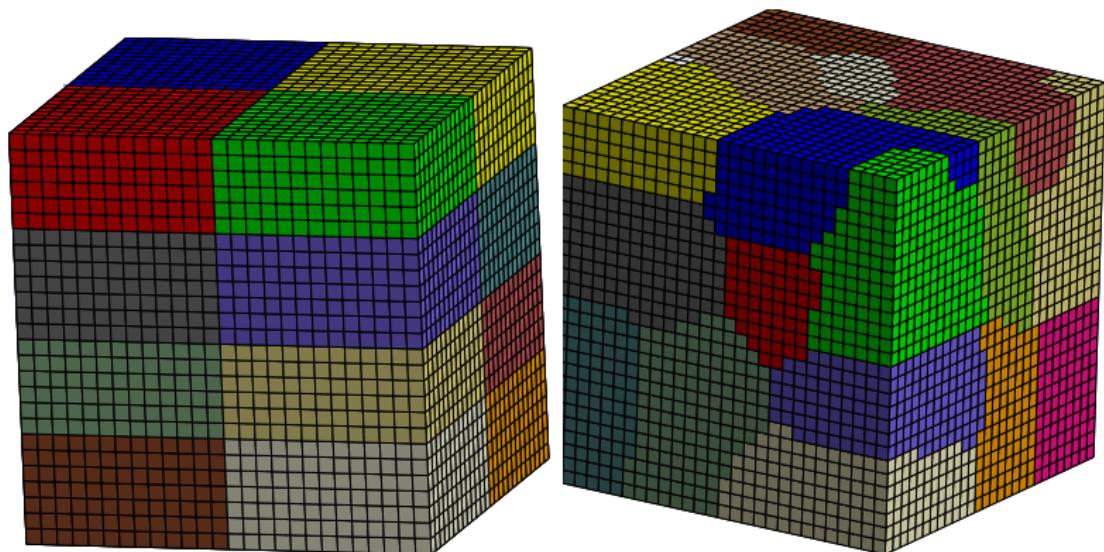


# Parallel computing



cluster of 160 processors

## Parallel computing (2)



subdomain decomposition method

# Plan

## 1 Representation of microstructures

- Real microstructures
- Random models

## 2 Mechanics of microstructures

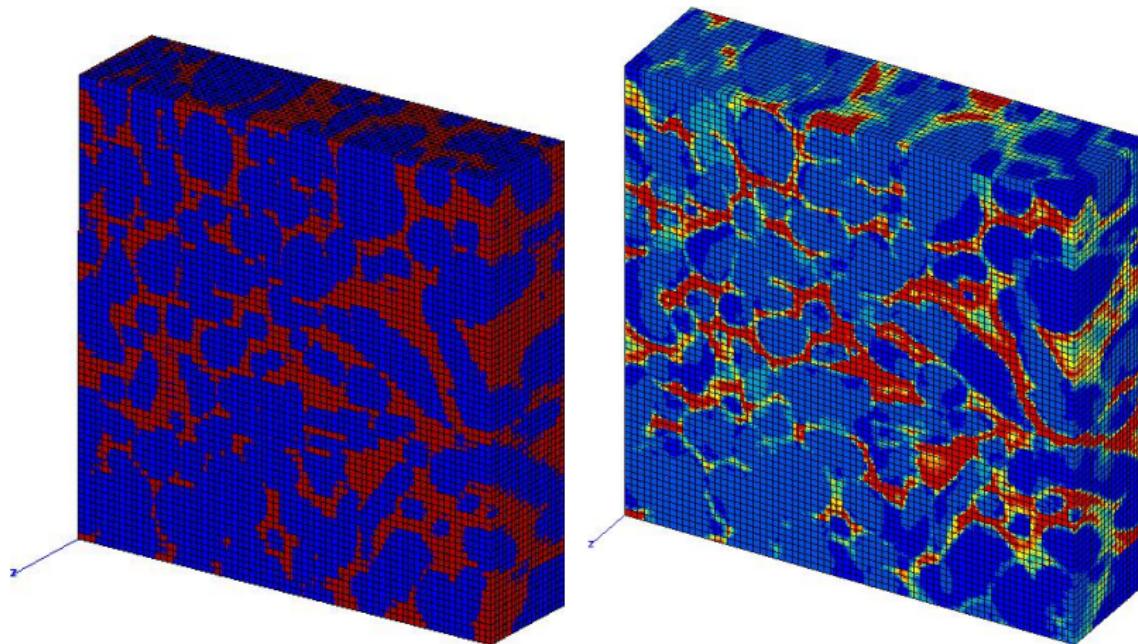
- Boundary conditions for the unit cell
- Bounds of effective properties

## 3 Representative volume elements

- Numerical tools for the mechanics of microstructures
- Apparent properties, effective properties**
- RVE for a two-phase material

## 4 Conclusions

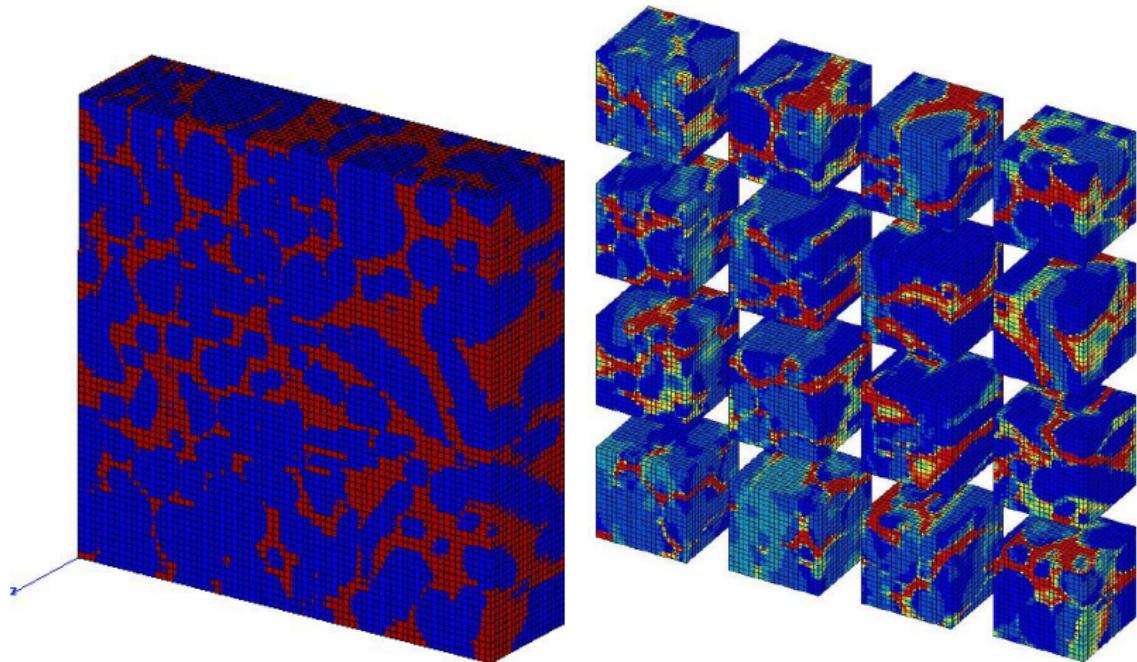
# Apparent properties, effective properties (1)



Apparent Young's modulus for a material volume element with SUBC:

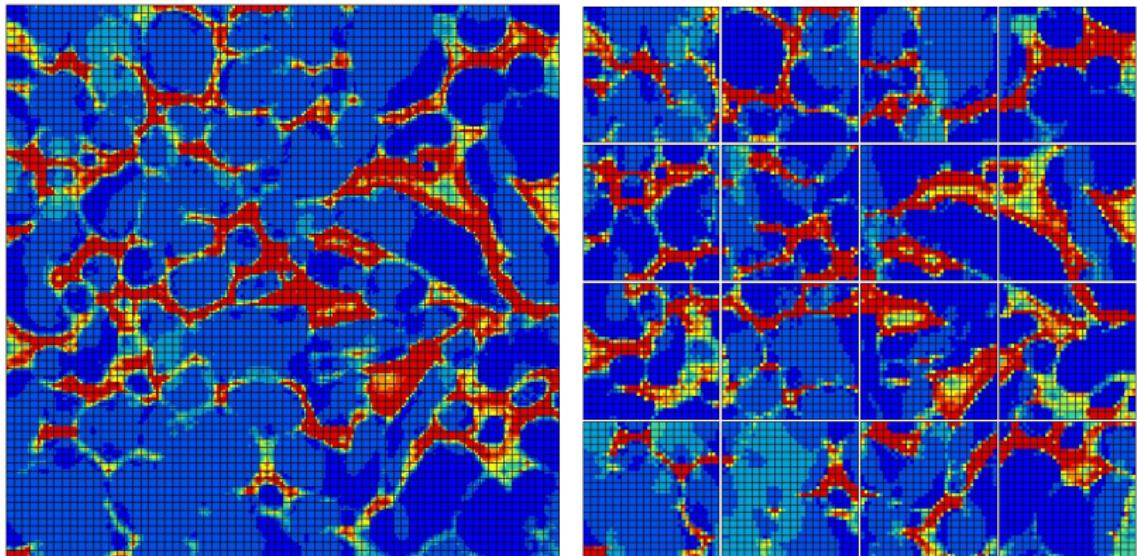
$$\mathbf{C}_{\approx \text{SUBC}}^{\text{app}}$$

## Apparent properties, effective properties (2)



Apparent Young's modulus (SUBC) for material volume element and a partition of it into 16 sub-volumes

## Apparent properties, effective properties (3)



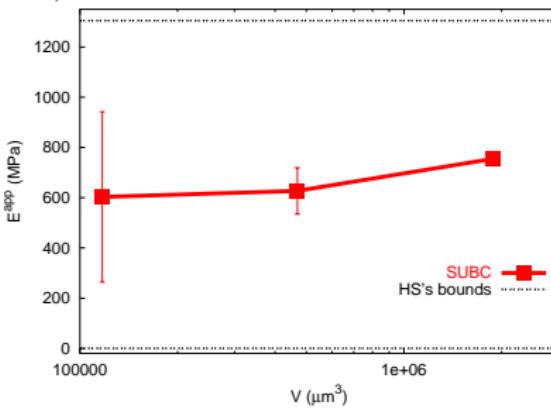
Apparent Young's modulus (SUBC) for material volume element and a partition of it into 16 sub-volumes

# Apparent properties, effective properties (4)

First Huet's theorem:

$$\overline{\mathbf{C}_{\approx \text{SUBC}}^{\text{app}}} \leq \mathbf{C}_{\approx \text{SUBC}}^{\text{app}}$$

with  $\overline{\mathbf{C}_{\approx \text{SUBC}}^{\text{app}}} = \frac{1}{n} \sum_{i=1,n} \mathbf{C}_{\approx \text{SUBC}}^{\text{app},i}$



## Apparent properties, effective properties (5)

First Huet's theorem:

$$\overline{\mathbf{C}_{SUBC}^{app}} \leq \mathbf{C}_{SUBC}^{app} \leq \mathbf{C}_{KUBC}^{app} \leq \overline{\mathbf{C}_{KUBC}^{app}}$$

with  $\overline{\mathbf{C}_{SUBC}^{app}} = \frac{1}{n} \sum_{i=1,n} \mathbf{C}_{SUBC}^{app,i}$

## Apparent properties, effective properties (6)

First Huet's theorem:

$$\overline{\mathbf{C}_{\approx \text{SUBC}}^{\text{app}}} \leq \mathbf{C}_{\approx \text{SUBC}}^{\text{app}} \leq \mathbf{C}_{\approx \text{KUBC}}^{\text{app}} \leq \overline{\mathbf{C}_{\approx \text{KUBC}}^{\text{app}}}$$

with  $\overline{\mathbf{C}_{\approx \text{SUBC}}^{\text{app}}} = \frac{1}{n} \sum_{i=1,n} \mathbf{C}_{\approx \text{SUBC}}^{\text{app},i}$

Second Huet's theorem:

$$\overline{\mathbf{C}_{\approx \text{SUBC}}^{\text{app}}} \leq \mathbf{C}_{\approx}^{\text{eff}} \leq \overline{\mathbf{C}_{\approx \text{KUBC}}^{\text{app}}}$$

# Towards a definition of the Representative volume element size

- ① “sufficiently large, sufficiently small...”       $I \ll I_{RVE} \ll L_\omega$
- ② the apparent properties are independent from boundary condition type (deterministic definition)      [Sab, 1992]
- ③ “the smallest material volume element of the composite for which the usual spatially constant “overall modulus” macroscopic constitutive representation is a sufficiently accurate model to represent the mean constitutive response”  
[Drugan, Willis, 1996]
- ④ practical question: can you estimate the effective properties by testing volume elements smaller than the deterministic RVE size?  
⇒ yes, statistical approach      [Kanit et al., 2003]

# Plan

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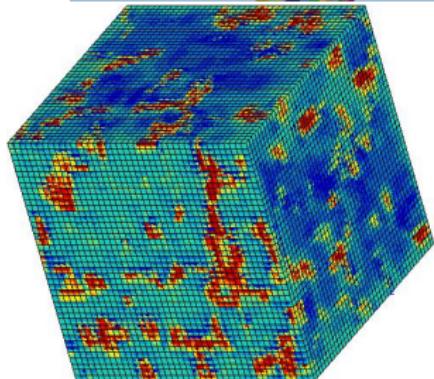
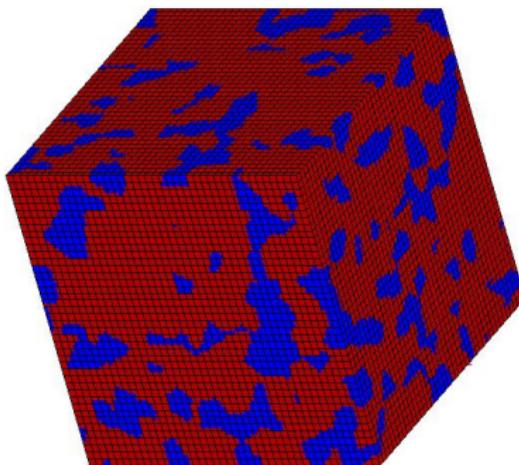
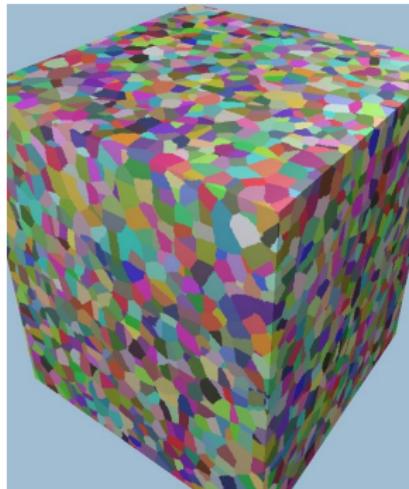
- Boundary conditions for the unit cell
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## 3 Representative volume elements

- Numerical tools for the mechanics of microstructures
- Apparent properties, effective properties
- RVE for a two-phase material

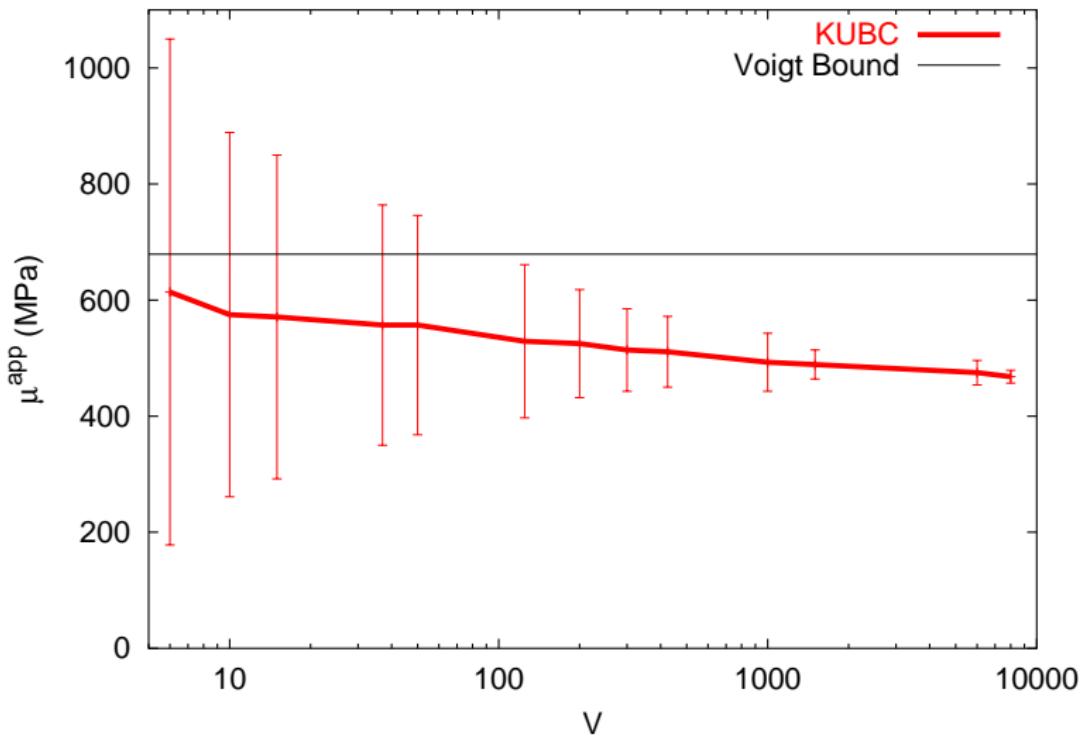
## 4 Conclusions

## Voronoi mosaic

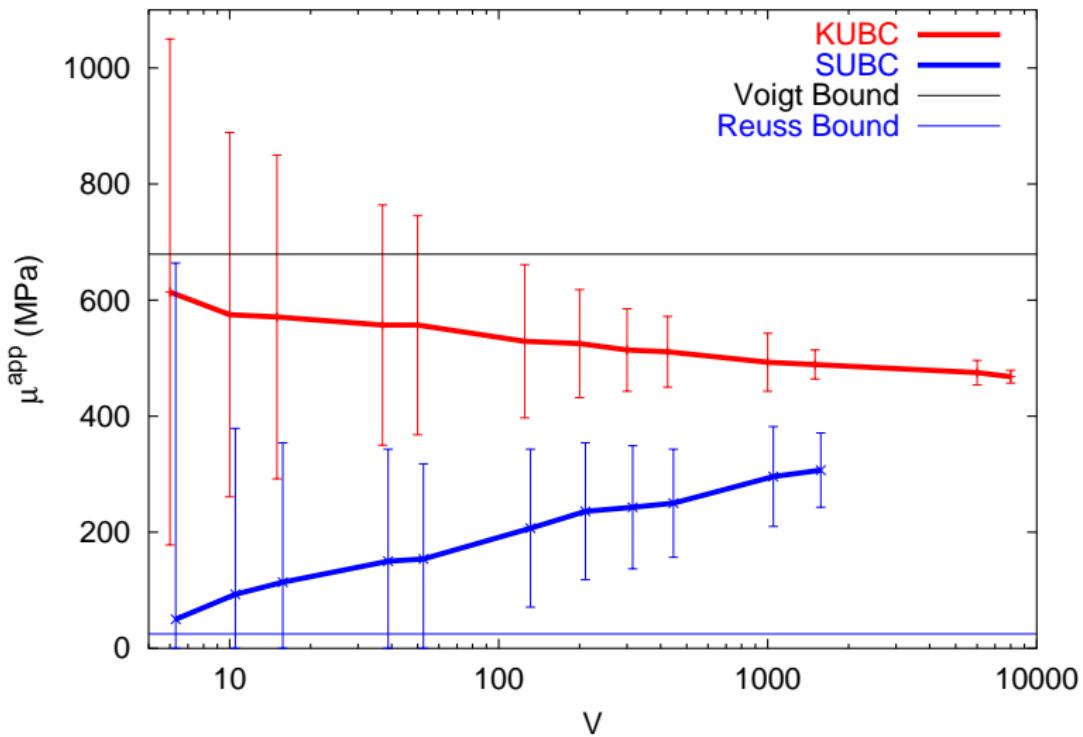


hard phase:  $E = 2500 \text{ MPa}$ ,  $\nu = 0.3$   
 $\lambda = 2.44 \text{ W/mK}$ ,  
soft phase:  $E = 25 \text{ MPa}$ ,  $\nu = 0.49$   
 $\lambda = 0.0244 \text{ W/mK}$ ,

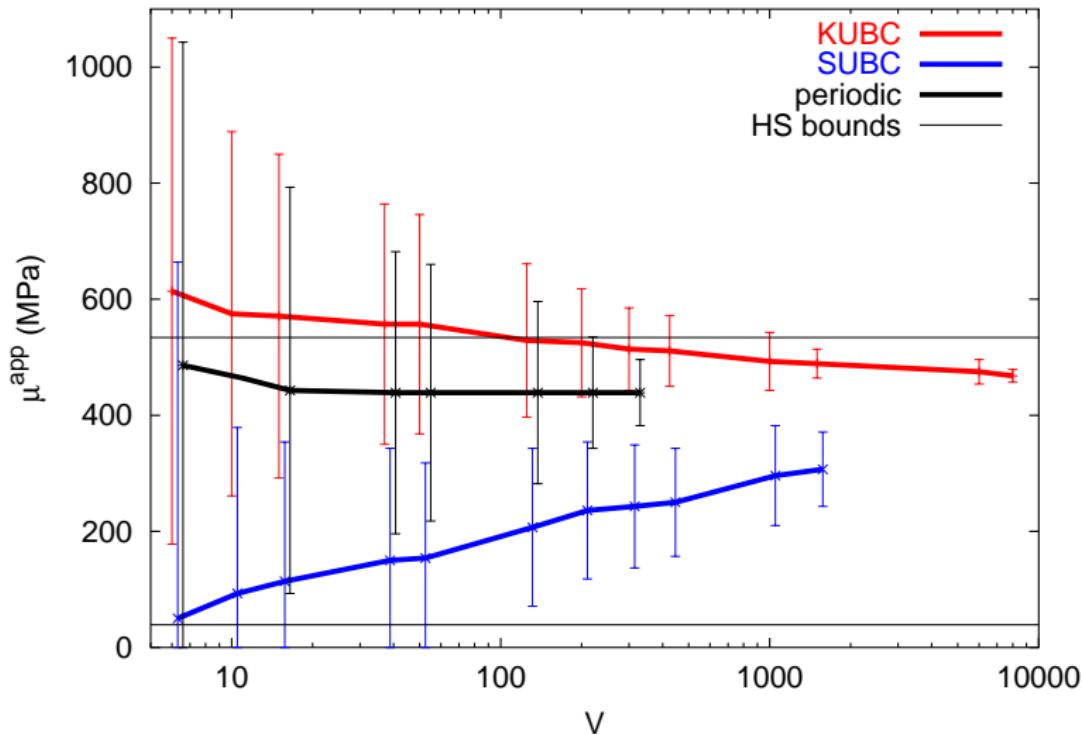
# Shear modulus



# Shear modulus



# Shear modulus



## RVE and integral range

$Z(x)$  a random variable (volume fraction, Young's modulus...)

The variance  $D_Z^2(V)$  of apparent property  $Z$  in a volume  $V$  takes the asymptotic form

$$D_Z^2(V) = D_Z^2 \frac{A_3}{V}$$

where  $D_Z^2$  is the point variance of  $Z$  :

$$D_Z^2 = P(1 - P) \text{ for volume fraction } (Z = P)$$

$$D_\mu^2 = P(1 - P)(\mu_1 - \mu_2)^2 \text{ for a two-phase material}$$

$A_3$  is called *integral range*

For volume fraction ( $Z = P$ ) and Voronoi mosaics,  $A_3 = 1.18$

[Gilbert, 1962]

## Statistical definition of the RVE

For a sufficient number of realizations  $n$ , the mean apparent property  $\bar{Z}$  lies within the interval of confidence

$$Z^{\text{eff}} \pm \frac{2D_Z(V)}{\sqrt{n}}$$

The relative precision in the estimation of the mean is:

$$\epsilon_{\text{rel}} = \frac{2D_Z(V)}{\sqrt{n}Z^{\text{eff}}} = \frac{2D_Z \sqrt{\left(\frac{A_3}{V}\right)^\alpha}}{\sqrt{n}Z^{\text{eff}}}$$

For given precision  $\epsilon$  and number of realization  $n$ , the RVE size is defined by

$$V_{\text{RVE}} = A_3 \left( \frac{4D_Z^2}{n\epsilon_{\text{rel}}^2 Z^{\text{eff}}} \right)$$

## RVE size for Voronoi mosaics

$\epsilon_{rel}$ (%)	$\mu$	$k$	$\lambda$	$P$
1	71253	13340	5504	2000
5	2850	534	220	80

$V_{RVE}$  for  $n = 10$ , periodic boundary conditions  
 $V_{RVE}(\mu) > V_{RVE}(k) > V_{RVE}(\lambda) > V_{RVE}(P)$

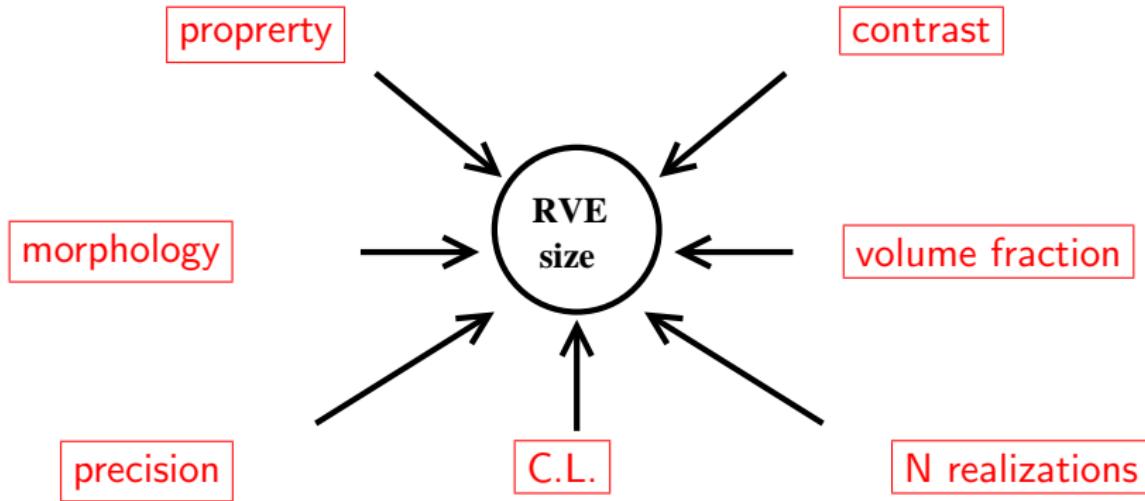
$$V_{RVE}(1\%) > V_{RVE}(5\%)$$

$\epsilon_{rel}$ (%)	$\mu$	$\lambda$	$k$	$P$
1	1300	765	400	150
5	52	30	16	6

Number of realizations for  $V$  (*sans biais*) = 125, periodic boundary conditions

$$n_\mu > n_\lambda > n_k > n_P$$

# RVE size depends on...



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# Conclusions

- **RVE size** : 1 large computation = N smaller + periodic BC
- **simplified homogenization models** for designing composites (lineair, non lineair)
- **optimization** of the microstructure for a target property, difficult in 3D!  
3D images + mathematical morphology
- **size effects** in materials and structures (perforated structures...)
- **damage, fracture** lifing techniques for heterogeneous materials