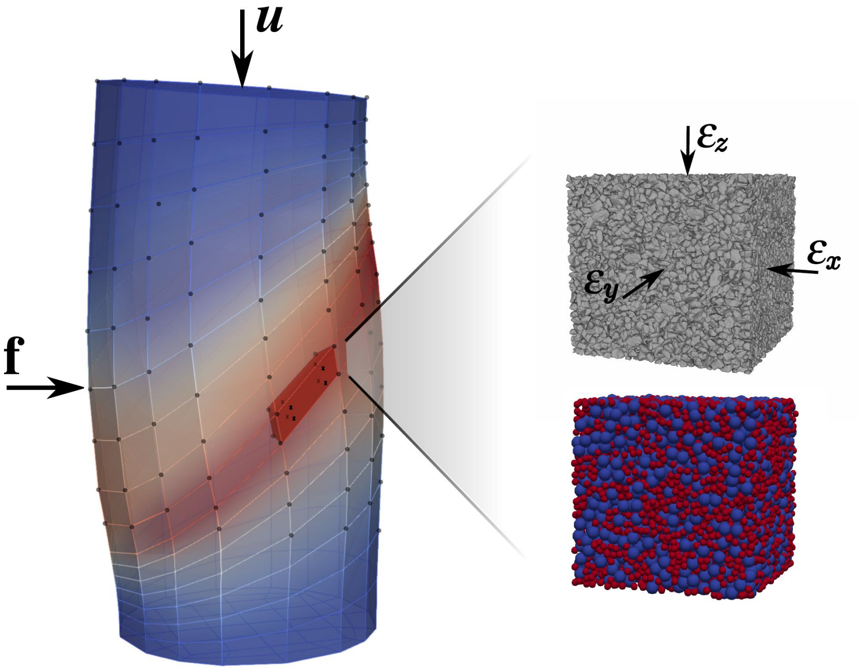


CIVIL-408 Multiscale Modeling in Mechanics

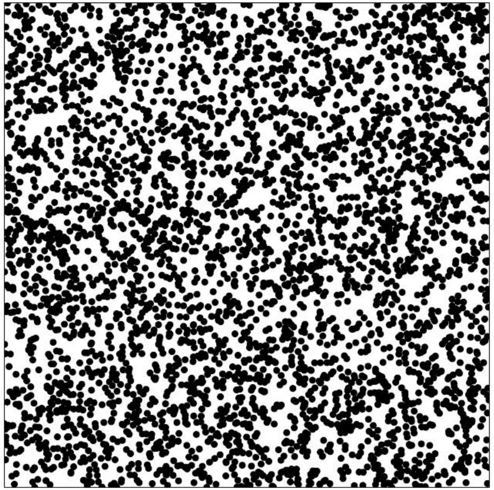
Prof. Kostas Karapiperis

Week 2

K.Karapiperis

Statistical homogeneity

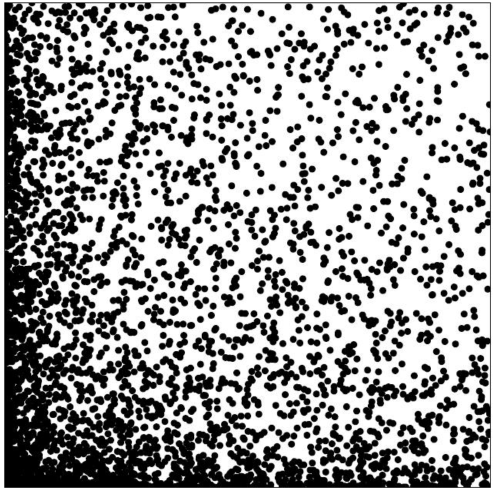
Statistically **homogeneous**



- Statistical *properties* of the microstructure do not change from point to point at the macroscale

Properties: volume fraction, spatial correlation, ..

Statistically **inhomogeneous**



- Otherwise, the material is statistically inhomogeneous (e.g. composite with a concentration gradient)

Effective response

We define **effective quantities** for a microstructure as spatial averages (with respect to the undeformed configuration)

$$\langle\cdot\rangle_\Omega = \frac{1}{V}\int_\Omega (\cdot)\,\mathrm{d}V \quad \neq \quad \langle\cdot\rangle_{\varphi(\Omega)} = \frac{1}{v}\int_{\varphi(\Omega)} (\cdot)\,\mathrm{d}v$$

e.g. **effective energy, effective stress,** etc

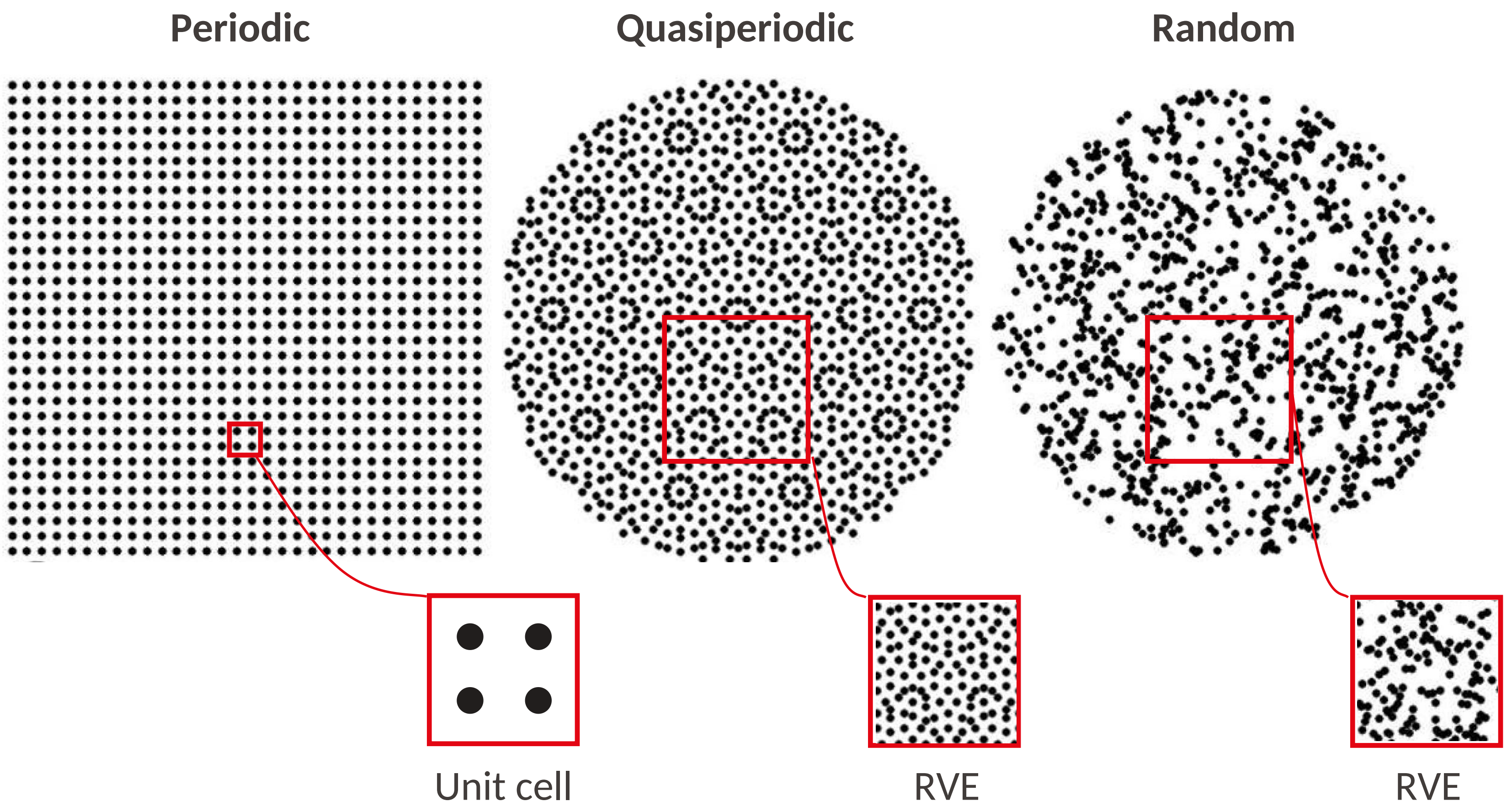
$$W_{\text{eff}} = \langle W \rangle$$

$$\boldsymbol{\sigma}_{\text{eff}} = \langle \boldsymbol{\sigma} \rangle$$

$$\ldots$$

How to choose the averaging volume?

Types of microstructures



Realizations and Ensemble Limit Theorem

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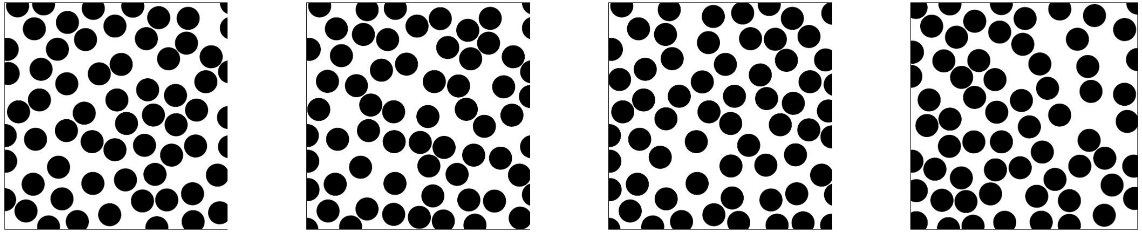
Configurations (or **realizations**):



Ensemble: a set of multiple realizations

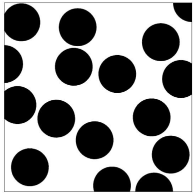
Assume that each configuration produces a **response** which generally differs between realizations (e.g., some averaged quantity).

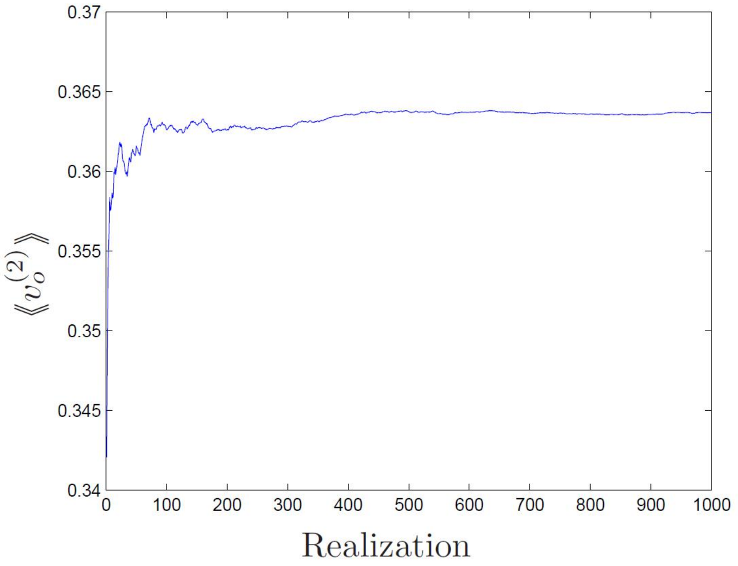
Ensemble average of a response over a set of *N* realizations: $\langle\!\langle \cdot \rangle\!\rangle_N = \frac{1}{N}\sum_{i=1}^{N}(\cdot)_i$

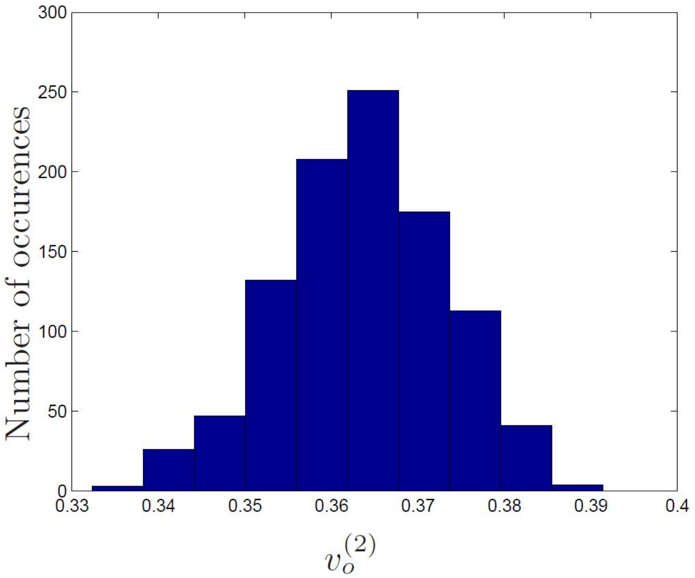
Central limit theorem: $\lim_{N\to\infty} \langle\!\langle \cdot \rangle\!\rangle_N = \langle\!\langle \cdot \rangle\!\rangle_\infty$

Ensemble enlargement

Example: volume fraction of particles for N = 1000 realizations of samples with a fixed number of particles (of uniform radii) randomly dispersed in a constant-size box.







$$\langle\langle v_2 \rangle\rangle_\infty = 0.3637$$

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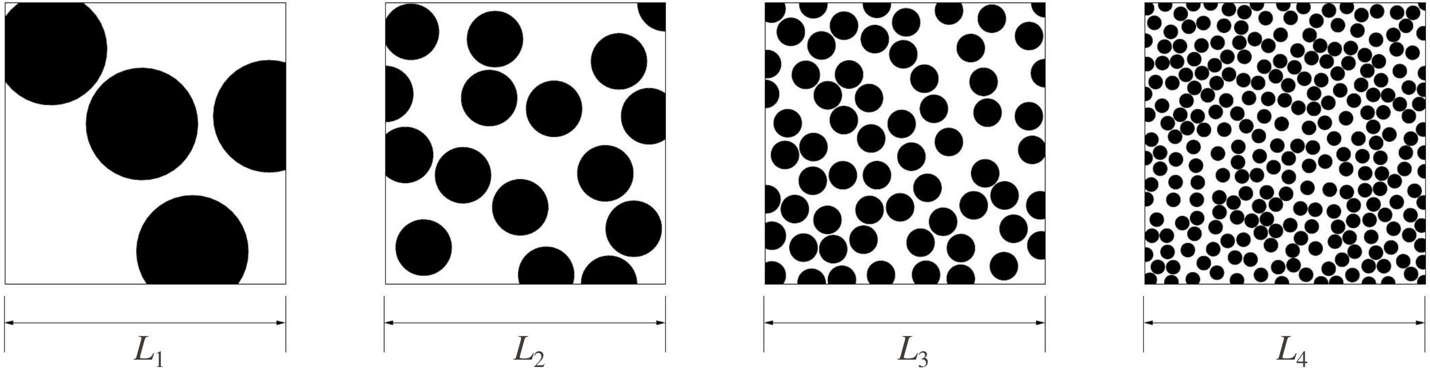
Sample enlargement

sample enlargement: increasing the size of the unit cell while keeping microstructural feature sizes constant



$l = \text{const.}$

$L_1 < L_2 < L_3 < \ldots$

sample enlargement: increasing the size of the unit cell while keeping microstructural feature sizes constant

limit: $\langle \cdot \rangle_\infty = \lim_{L/l \to \infty} \langle \cdot \rangle_{\Omega(L)}$ $\quad \langle \cdot \rangle_\infty = \langle\!\langle \langle \cdot \rangle_\infty \rangle\!\rangle_\infty$

convergence by sample enlargement vs. ensemble averaging at fixed size is not the same and not equally uniform (ensemble average leads to smoother convergence) but in the sample enlargement limit, a single realization is sufficient

Ensemble and sample enlargement

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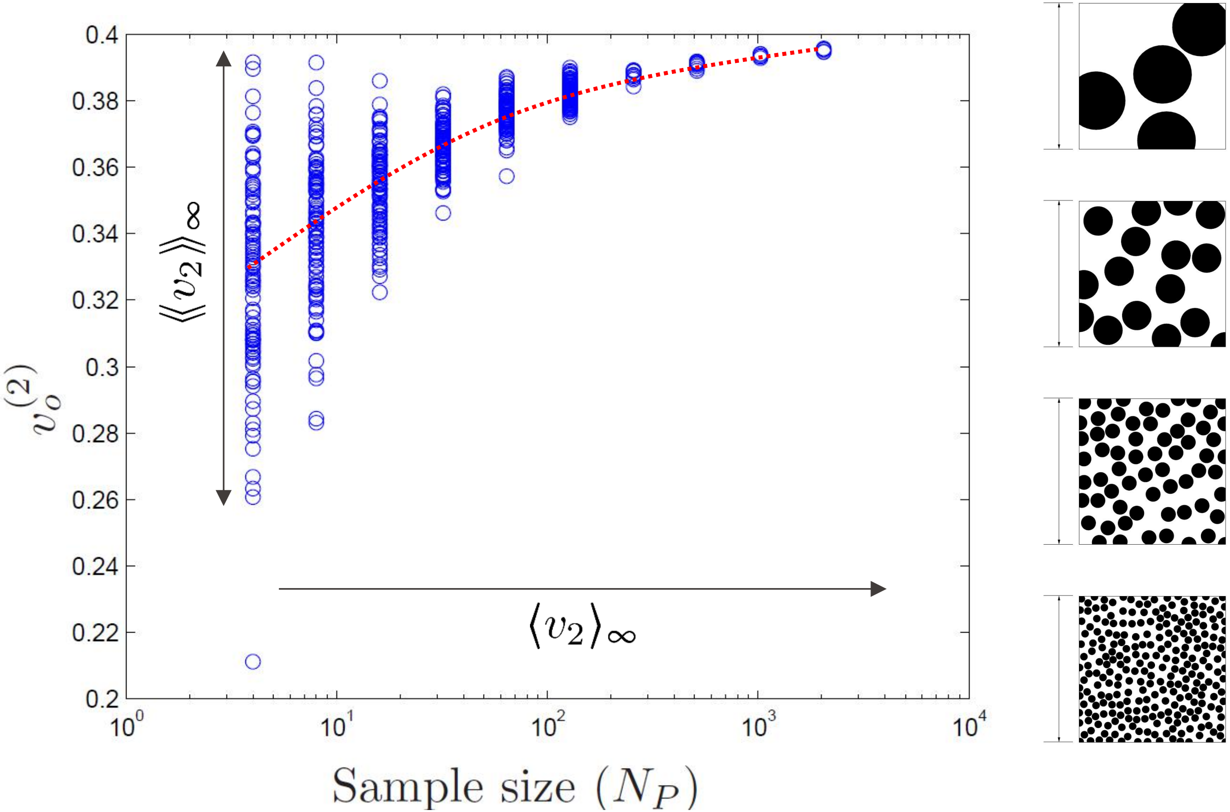
Example revisited: volume fraction of particles with constant radii



Representative volume element

Ideally, we seek an *infinitely large* sample, so averages do not differ between realizations. Such a sample is **statistically representative**, and a single analysis is sufficient to reveal the response.

For all practical purposes, we cannot work with infinite RVE sizes but will choose a **finite-size RVE** whose response is as close to the infinite limit as needed (even though, strictly speaking, it is not an **RVE**).

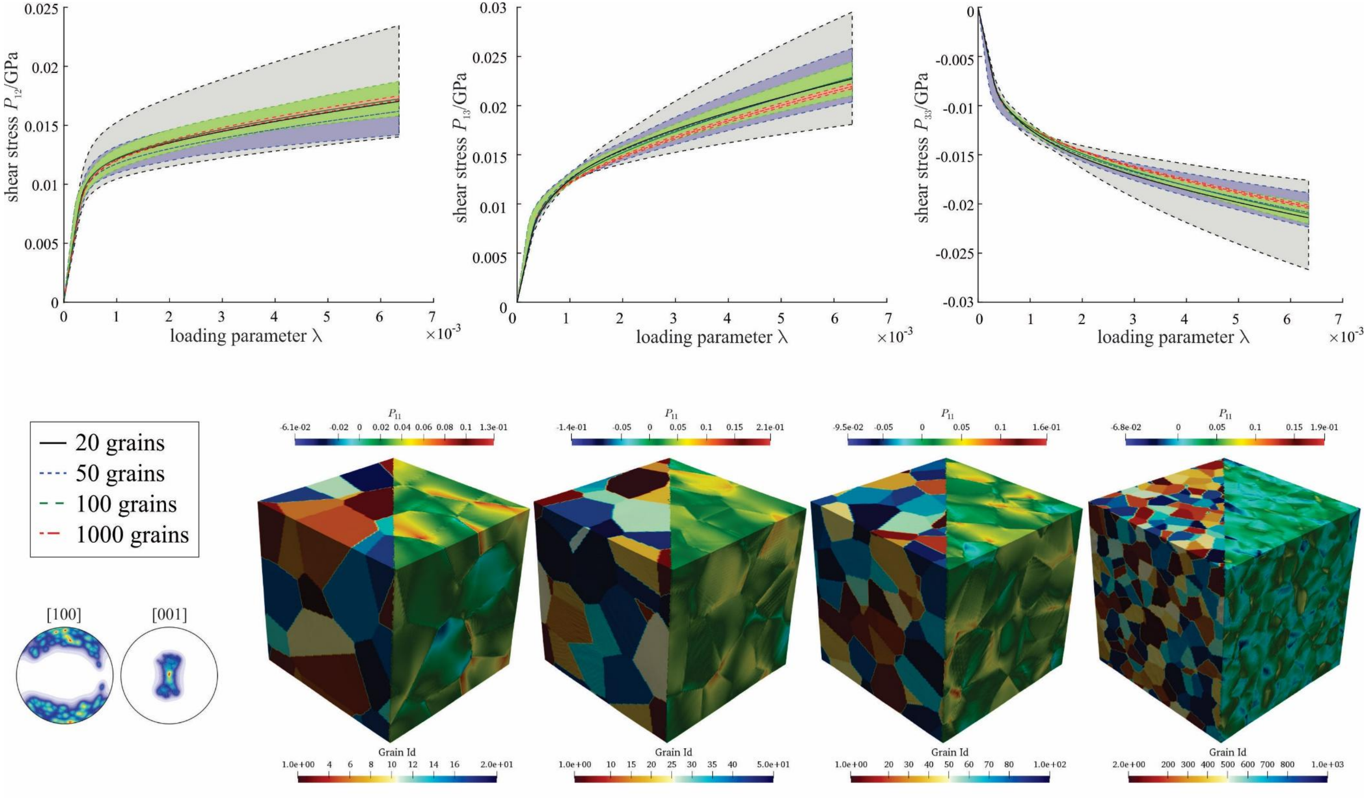
For example, we can find the required number of realizations *N* or the size *L* of an RVE by checking for a specific response if, e.g.,

$$\frac{\langle\langle\cdot\rangle\rangle_{N+1} - \langle\langle\cdot\rangle\rangle_N}{\langle\langle\cdot\rangle\rangle_N} \leq \epsilon, \qquad \frac{\langle\cdot\rangle_{\Omega(L_{i+1})} - \langle\cdot\rangle_{\Omega(L_i)}}{\langle\cdot\rangle_{\Omega(L_i)}} \leq \epsilon$$

More accurate are *statistical measures* (e.g., check standard deviation, comparison to extrapolated values at infinity, etc.).

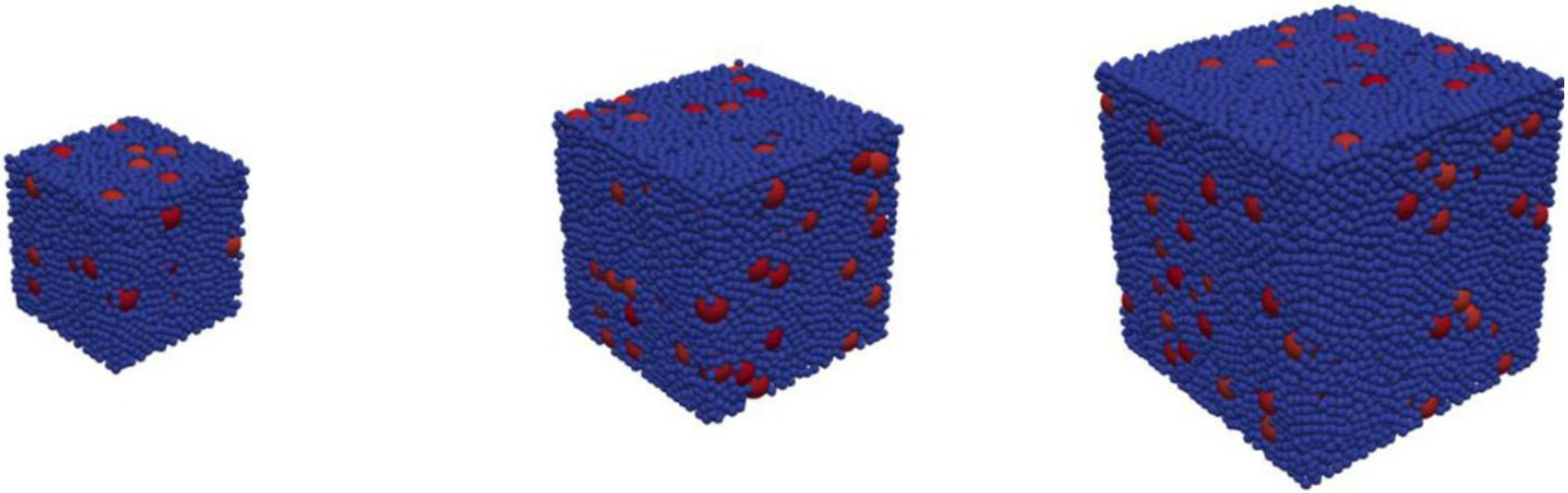
RVE - Magnesium alloy

Plastic deformation in a magnesium alloy



RVE - Granular materials

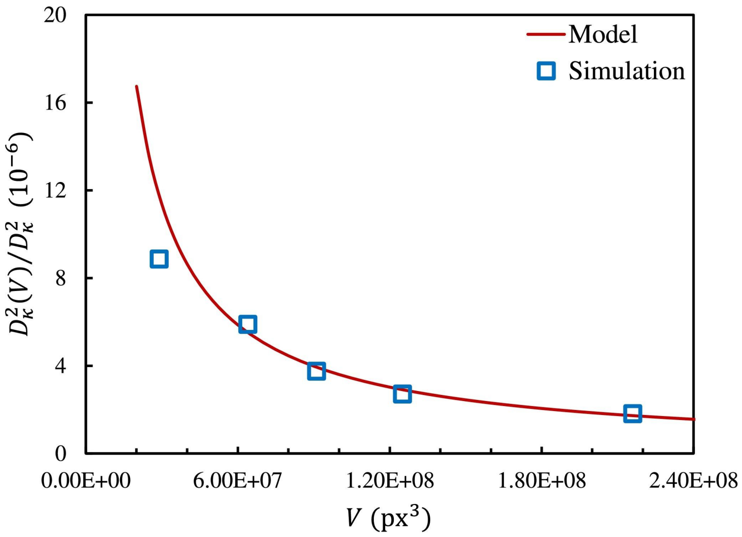
Mechanics behavior of bidisperse granular material

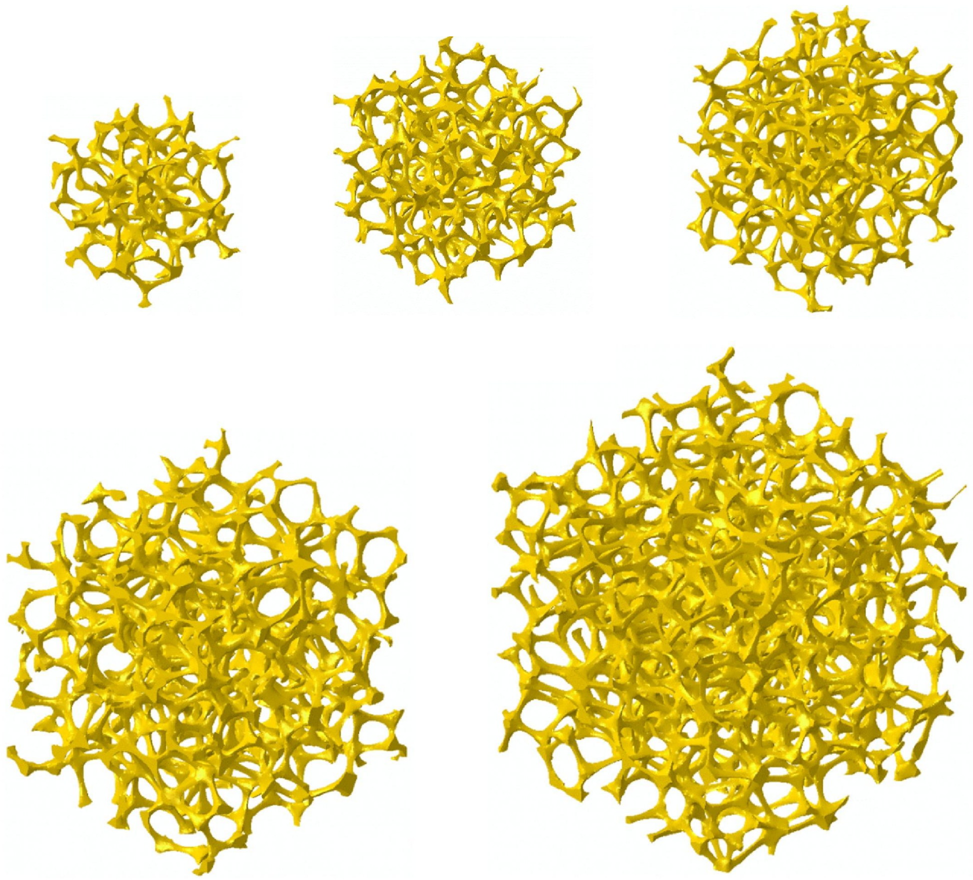


We generally choose the RVE size **as large as necessary**, **as small as possible**

RVE - Metallic foams

Mechanical behavior of open cell random metallic foams





Variance of elastic moduli as a function of RVE size

RVEs for periodic microstructures

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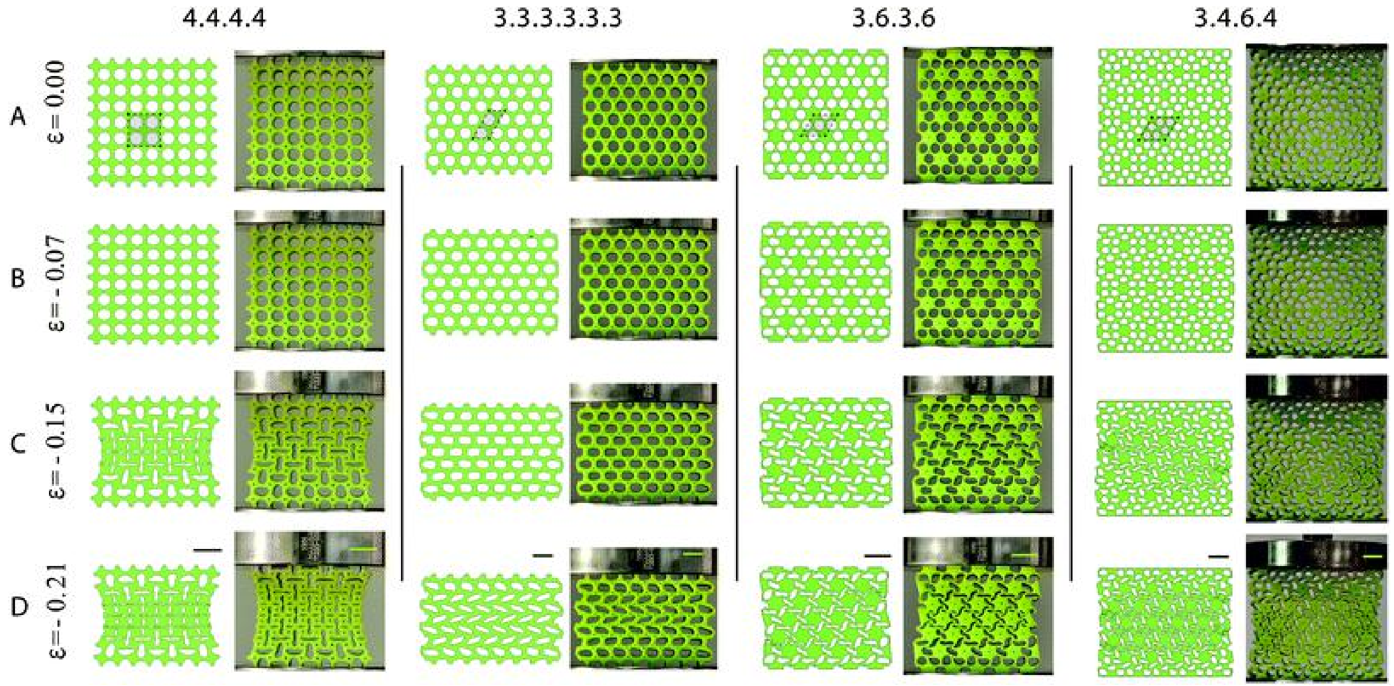
For **periodic** microstructures, the RVE is identical to the **unit cell (UC)**, i.e., the smallest unit whose periodic tiling results in the complete microstructure. It is generally ***not unique***. It also ***depends on the problem***.



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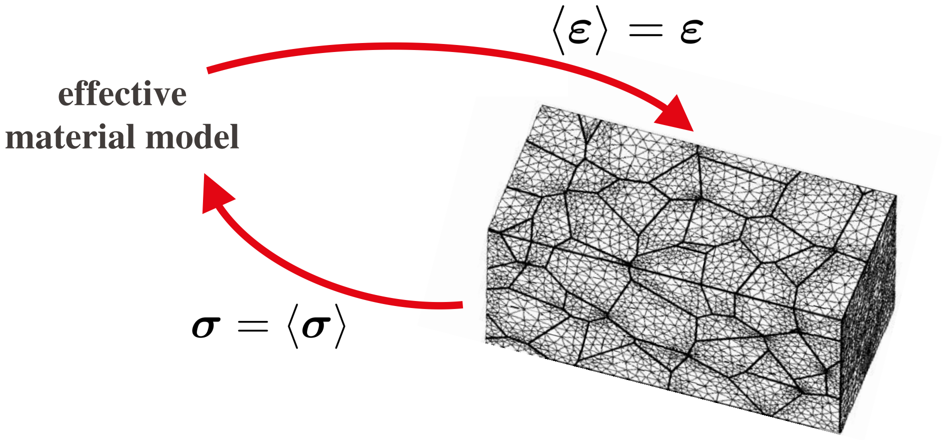
Computational homogenization

Homogenization strategy:

Compute the effective constitutive response of the material by solving a lower-scale boundary value problem from an RVE.



Questions:

How do we impose an effective macroscale strain tensor at the microscale?
How do we return an effective stress tensor from the microscale to the macroscale?

Note: Calculating averages is simple, imposing averages is not.

Averaging Theorems - *Average strain*

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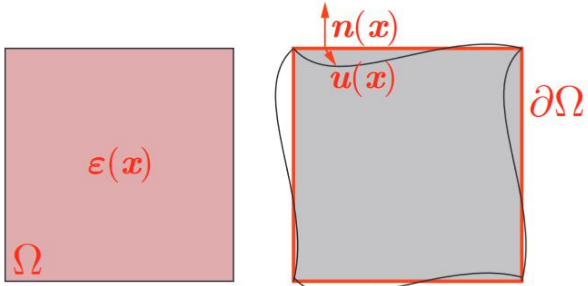
Consider a RVE Ω with volume $V = |\Omega|$

We can compute the volume-averaged strain tensor by using the divergence theorem to obtain (assuming smooth a displacement field)

$$\langle \varepsilon_{ij} \rangle = \frac{1}{V} \int_{\Omega} \varepsilon_{ij} dV = \frac{1}{2V} \int_{\Omega} (u_{i,j} + u_{j,i}) dV = \frac{1}{2V} \int_{\partial\Omega} (u_i n_j + u_j n_i) dS$$

Or in tensor notation:

$$\langle \boldsymbol{\varepsilon} \rangle = \frac{1}{V} \int_{\partial\Omega} \mathrm{sym}(\boldsymbol{u} \otimes \boldsymbol{n}) dS$$



average strain calculation

Averaging Theorems - *Average stress*

Analogously the average stress tensor is derived by exploiting the relation:

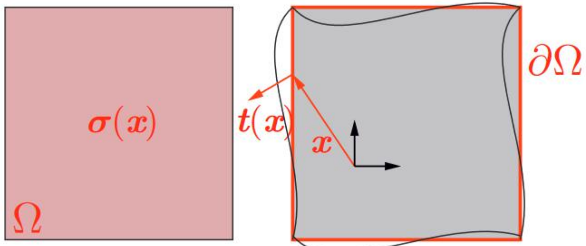
$$\sigma_{ij} = \sigma_{ik}\delta_{jk} = \sigma_{ik}x_{j,k}$$

Taking into consideration the balance of linear momentum and the definition of traction:

$$\begin{aligned}\langle\sigma_{ij}\rangle =& \frac{1}{V}\int_{\Omega}\sigma_{ij}dV = \frac{1}{V}\int_{\Omega}\sigma_{ik}x_{j,k}dV = \frac{1}{V}\left[\int_{\partial\Omega}\sigma_{ik}x_j n_k dS - \int_{\Omega}\sigma_{ij,k}x_j dV\right] \\ &= \frac{1}{V}\left[\int_{\partial\Omega}t_i x_j dS - \int_{\Omega}\rho(a_i - b_i)x_j dV\right]\end{aligned}$$

Or in tensor notation in the quasistatic case (with b=0):

$$\langle\boldsymbol{\sigma}\rangle = \frac{1}{V}\int_{\partial\Omega}\boldsymbol{t}\otimes\boldsymbol{x}\; dS$$



average stress calculation

Averaging Theorems - *Numerical evaluation*

Practically, in a finite element setting:

Strain:

$$\langle \boldsymbol{\varepsilon}^h \rangle = \frac{1}{V} \sum_{\alpha=1}^{n} \mathrm{sym}(\boldsymbol{u}^\alpha \otimes \tilde{\boldsymbol{n}}^\alpha)$$

where:

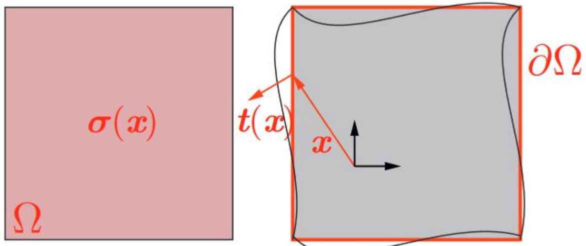
$$\tilde{\boldsymbol{n}}^\alpha = \frac{1}{d} \sum_{e} \boldsymbol{n}_e^\alpha A^\alpha$$

Stress:

$$\langle \boldsymbol{\sigma}^h \rangle = \frac{1}{V} \sum_{\alpha=1}^{n} \mathrm{sym}(\boldsymbol{F}^\alpha \otimes \boldsymbol{x}^\alpha)$$

where:

$$\boldsymbol{F}^\alpha = \sum_{e} \sum_{\alpha} \int_{\partial\Omega_e} \boldsymbol{t} N_e^\alpha \, dS$$



average stress calculation

Outlook: Computational homogenization

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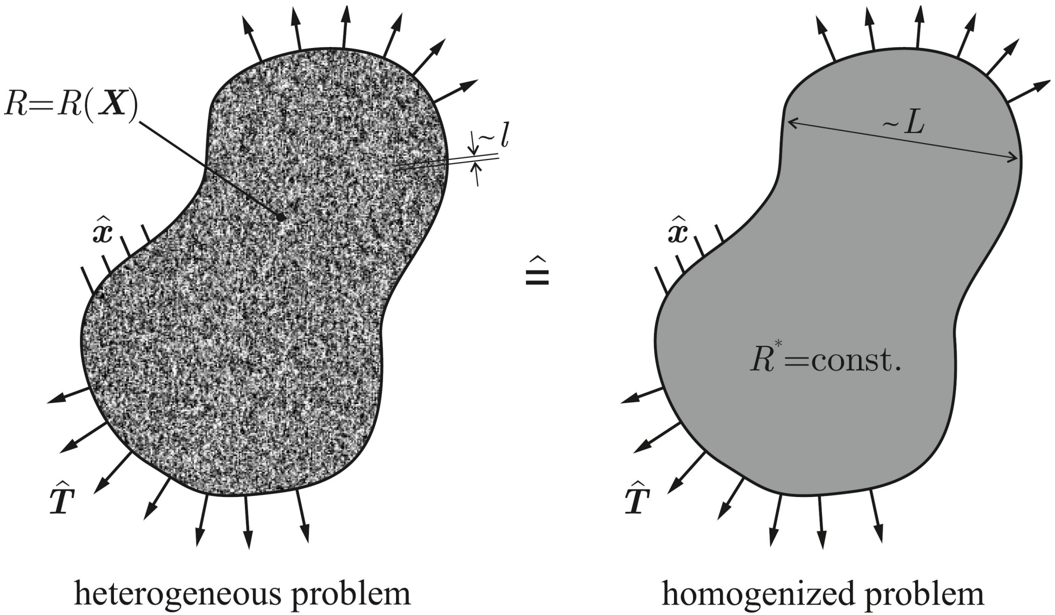
A sneak peek into the formal homogenization problem:



Discussion

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That's what I prepared for you today.

What would you like to discuss?

Reading for next class:

Multiscale Modeling, D.M. Kochmann

Chapters 4-5