Influence of Pore Morphology on Mechanical Properties of Second Gradient Materials

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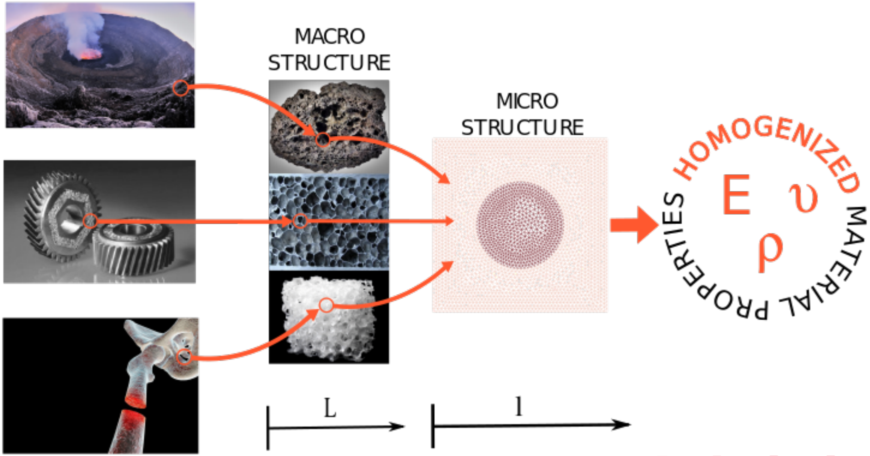
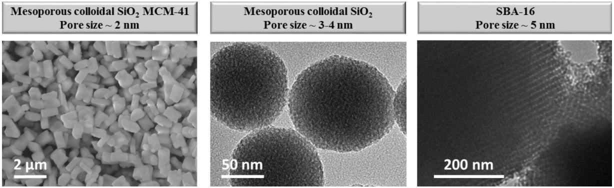
Homogenization translates behaviour of heterogeneous materials from the microscale level to the macroscale level. Most of the natural or man made materials are heterogeneous at some scale.



Knowledge Gap

- Homogenization methods typically account for volume fractions and do not consider microscopic morphology and their impact on material behaviour.
- Effects of higher-order parameters are still under investigation and experimentally are challenging to measure.
- Microscopic impact is usually more challenging for multi-physics problems.



Objectives

- Develop numerical framework capable of capturing higher-order homogenization parameters
- Investigate the role of pore/inclusion morphology (size, shape and distribution) on effective material properties

Methodology

Macroscale and microscale deformation energy of the RVE are equal:

$$\underbrace{\int_{\Omega^p} \Phi^m dV}_{\text{Microscale}} = \underbrace{\int_{\Omega^p} \Phi^M dV}_{\text{Macroscale}}$$

Φ^m is expressed with first-order theory and Φ^M with second-order theory:

$$\int_{\Omega^p} \frac{1}{2}(\overbrace{C^m_{ijkl} u^m_{i,j} u^m_{j,i}}^{\text{First-order}}) dV$$
$$=$$
$$\int_{\Omega^p} \frac{1}{2}(\underbrace{C^M_{ijkl} u^M_{i,j} u^M_{j,i} + 2G^M_{ijklm} u^M_{i,j} u^M_{k,lm} + D^M_{ijklmn} u^M_{i,jk} u^M_{l,mn}}_{\text{Second-order}}) dV$$

Methodology cont.

Macroscopic case is solved by evaluating deformation energy at the RVE's geometric center as $\overset{c}{X} = \frac{1}{V}\int_{\Omega^p} X dV$:

$$\int_{\Omega^p} \Phi^M dV =$$

$$\frac{V}{2}\left(C^M_{ijlm}\langle u^M_{i,j}\rangle\langle u^M_{l,m}\rangle + 2G^M_{ijklm}\langle u^M_{i,j}\rangle\langle u^M_{k,lm}\rangle\right) + \left(C^M_{ijlm}\bar{I}_{kn} + D^M_{ijklmn}\right)\langle u^M_{i,jk}\rangle\langle u^M_{l,mn}\rangle)$$

Microscopic case is solved through asymptotic homogenization method:

$$\boxed{\mathbf{u}^m(\boldsymbol{X}) = \overbrace{\overset{0}{\mathbf{u}}(\boldsymbol{X},\boldsymbol{y}) + \epsilon\overset{1}{\mathbf{u}}(\boldsymbol{X},\boldsymbol{y}) + \epsilon^2\overset{2}{\mathbf{u}}(\boldsymbol{X},\boldsymbol{y})}^{\text{Expanded microscale displacement field}}}$$

$$\underbrace{\epsilon = \frac{l}{L} = \frac{\text{microscale length}}{\text{macroscale length}}}_{\text{Homothetic ratio}} \qquad \underbrace{y_j = \frac{1}{\epsilon}(X_j - \overset{c}{X}_j)}_{\text{Local coordinate}}$$

Methodology cont.

Equilibrium condition at microscale: $(C^m_{ijkl} u^m_{k,l})_{,j} + f_i = 0$ leads to:

$$u^m_i(X, y) = u^M_i(X) + \epsilon\varphi_{abi} u^M_{a,b}(X) + \epsilon^2\psi_{abci} u^M_{a,bc}(X)$$

Recalculate microscopic deformation energy as follows:

$$\frac{V}{2}(\bar{C}_{abcd}\langle u^M_{a,b}\rangle\langle u^M_{c,d}\rangle + 2\bar{G}_{abcde}\langle u^M_{a,b}\rangle\langle u^M_{c,de}\rangle) + \bar{D}_{abcdef}\langle u^M_{a,bc}\rangle\langle u^M_{d,ef}\rangle)$$

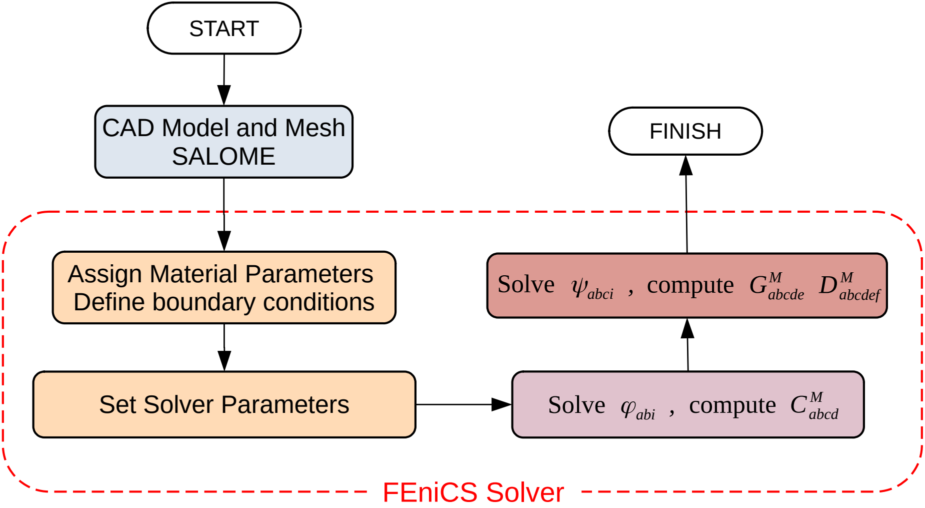
Compare macroscale and microscale energies to extract C^M, G^M and D^M leads to:

$$\boldsymbol{C^M_{abcd}} = \bar{C}_{abcd}$$

$$\boldsymbol{G^M_{abcde}} = \frac{1}{2}\bar{G}_{abcde}$$

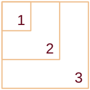
$$\boldsymbol{D^M_{abcdef}} = \bar{D}_{abcdef} - \frac{\epsilon^2}{V}\boldsymbol{C^M_{abcd}} \int_{\Omega^p} y_c y_j dV$$

Numerical Implementation in FEniCS



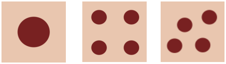
Problem Definition

- **Material**: concrete with $E_{concrete} = 40\,[GPa]$ and $\nu = 0.2$
- **Problem 1**: $E_{inclusion} = 0\,[GPa]$ and Volume Fraction $= 0 \rightarrow 50\%$
- **Problem 2**: Volume Fraction $= 20\%$ and $E_{inclusion} = 0 \rightarrow 40\,[GPa]$
- RVE size: square a x a; a = 1, 2, 3

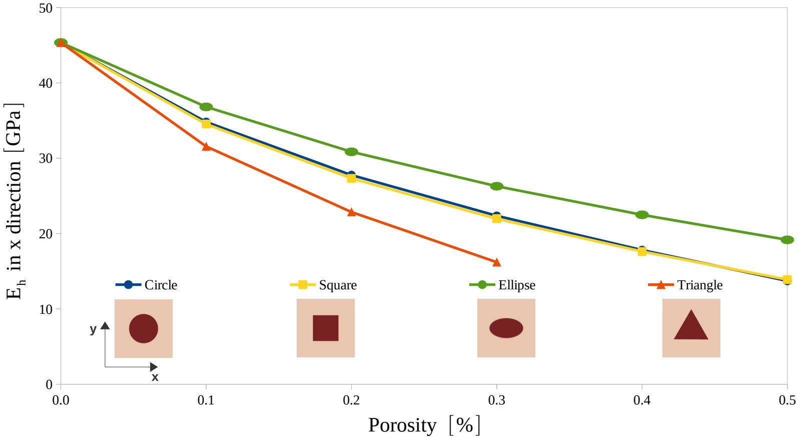


- Inclusion shape: circle, square, elipse and triangle

- Inclusion distribution: single, uniform and random



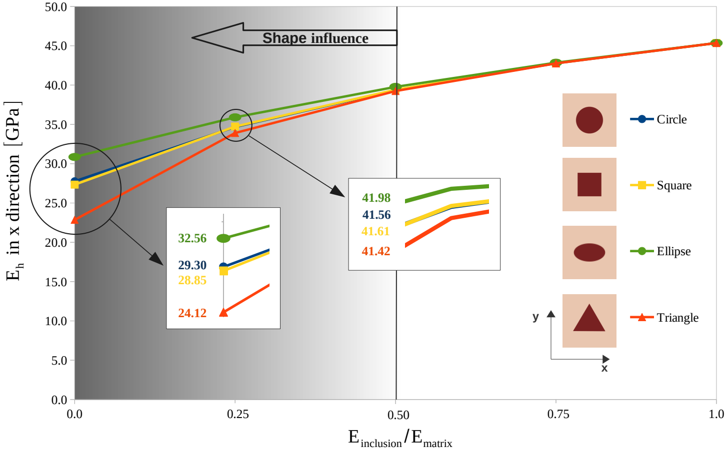
First-Order Parameters - Variation of Volume Fraction



Take away message

Obtained E_h is strongly influenced by the inclusion shape.

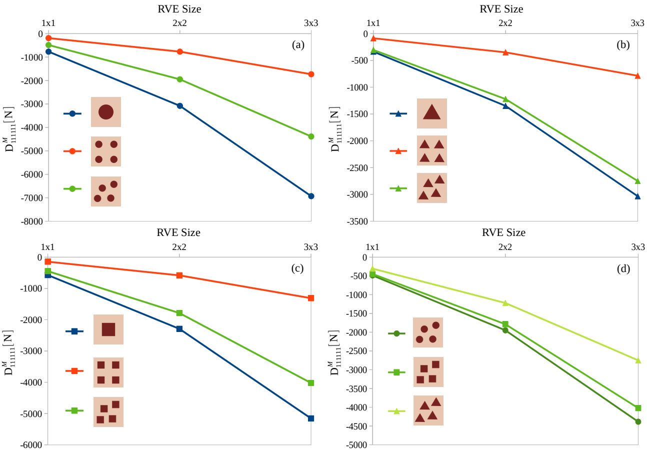
First-Order Parameters - Variation of $E_{inclusion}$



Take away message

Obtained E_h is influenced by inclusion shape influence once $E_{void} < 0.5E_{matrix}$ and obtained stiffness matrix C^M is cubic/orthotropic.

Higher-Order Parameters - Variation of D^M_{111111}



Take away message

Obtained D^M_{111111} is influenced by pore shape and distribution.

Conclusions

1. First order parameter C^M is strongly influenced by pore/inclusion shape and difference between properties of matrix and pore/inlusion.
2. Second order parameters $\boldsymbol{D}^{\boldsymbol{M}}$ and $\boldsymbol{G}^{\boldsymbol{M}}$ are influenced by size, shape and distribution of pores/inclusions.
3. Due to the sensibility of C^M to the inclusion's shape and property, tailored materials with specific microstrcuture can be designed for various engineering and scientific applications.

Acknowledgement

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Thank You for Your Attention!

- Vazic B., Abali E., Yang H., and **Newell P.***, Mechanical Analysis of Heterogeneous Materials with Higher-Order Parameters *Engineering with Computers*, 2021, https://doi.org/10.1007/s00366-021-01555-9.

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InterPore