

Body-force enhanced second-order computational homogenisation for non-linear cellular materials and metamaterials



L. Wu, J. Segurado, M. Mustafa, & L. Noels University of Liege, Computational & Multiscale Mechanics of Materials Universidad Politécnica de Madrid, Department of Materials Science & IMDEA Materials Institute

ECCOMAS Thematic Conference: Computational Modeling of Complex Materials across the Scales (CMCS 2023), 10-13 October 2023



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 862015



- First vs. second order homogenisation •
 - First order homogenisation
 - Does not prevent spurious localisation •
 - No material length-scale
 - Second-order homogenisation
 - High order strain G_M and stress Q_M at macro-scale
 - Material length scale related to the RVE





- $\mathbf{F}_{\mathrm{M}}, \mathbf{G}_{\mathrm{M}} = \mathbf{F}_{\mathrm{M}} \otimes \nabla_{\mathrm{0M}}$ $\mathbf{P}_{\mathrm{M}}, \mathbf{Q}_{\mathrm{M}}$ Meso-scale BVP resolution
- Issue for metamaterial: RVE length is larger than unit cell because of patterning



change

CMCS2023

Second order homogenisation





- Account for patterning change
 - Micromorphic approach*
 - Constrains change of patterning modes
 - Developed in elasticity



 $\partial F_{\rm m}$

Body-force enhanced second

order homogenisation

- Enhanced second-order
 - homogenisation
 - Remove cell size dependency using a body-force
 - Arises from asymptotic homogenization in linear elasticity**
 - How to account for finite strain, elastoplasticity etc...?



*O. Rokoš, M. Ameen, R. Peerlings, M. Geers, J. Mech. Phys. Solids 123 (2019) **V. Monchiet, N. Auffray, J. Yvonnet, Mech. Mater. 143 (2020)

J. Yvonnet, N. Auffray, V. Monchiet, Int. J. Solids Struct. 191–192 (2020)

CMCS2023

 $\boldsymbol{b}_{\mathrm{m}}$



- Second order homogenisation with body force enhancement
 - Consider an equivalent homogeneous volume element
 - Cauchy homogenous Second order continuum $F_M(0), G_M$ $f_M(X), G_M$ $F_M(X), G_M$ $f_M(X), G_M$ 0 0 X $F_M(X), Q_M(X)$
 - Development of the (no-longer) homogeneous field



•





- Second order homogenisation with body force enhancement
 - Consider an equivalent homogeneous volume element
 - The equivalence of energy (Hill-Mandel condition) with introduction of body forces $\boldsymbol{b}_{\mathrm{m}}(\boldsymbol{X}_{\mathrm{m}})$:



• Is satisfied by the following introduction of micro-scale body forces and homogenised stresses

$$\mathbf{P}_{M} = \mathbf{P}_{M}(0) = \frac{1}{V_{0}} \int_{\Omega_{m0}} (\mathbf{P}_{m} - \boldsymbol{b}_{m} \otimes \boldsymbol{X}_{m}) d\Omega$$

$$\mathbf{Q}_{M} = \mathbf{Q}_{M}(0) = \frac{1}{2V_{0}} \int_{\Omega_{m0}} [\mathbf{P}_{m} \otimes \boldsymbol{X}_{m} + (\mathbf{P}_{m} \otimes \boldsymbol{X}_{m})^{T}] d\Omega + \frac{1}{2V_{0}} \int_{\Omega_{m0}} [\boldsymbol{b}_{m} \otimes \boldsymbol{X}_{m} \otimes \boldsymbol{X}_{m}] d\Omega - \frac{1}{2V_{0}} \left(\left[\frac{\partial \mathbf{P}_{M}(0)}{\partial \mathbf{F}_{M}} : \mathbf{G}_{M} \cdot \boldsymbol{J}_{M} + \left(\frac{\partial \mathbf{P}_{M}(0)}{\partial \mathbf{F}_{M}} : \mathbf{G}_{M} \cdot \boldsymbol{J}_{M} \right)^{T} \right] - \boldsymbol{B}_{M} \otimes \boldsymbol{J}_{M} \right)$$

$$\int_{\Omega_{m0}} \mathbf{b}_{m} d\Omega = \int_{\Omega_{0}} \mathbf{B}_{M} d\Omega = - \int_{\Omega_{0}} \frac{\partial \mathbf{P}_{M}}{\partial \mathbf{F}_{M}} : \mathbf{G}_{M} : I d\Omega = - \int_{\Omega_{m0}} \left(\frac{\partial \mathbf{P}_{m}}{\partial \mathbf{F}_{M}} : \mathbf{G}_{M} \right) : I d\Omega$$

$$12-14 \text{ October 2023}$$



- Meso-scale problem
 - Micro-scale weak form

$$\int_{\Omega_{\mathrm{m}0}} \mathbf{P}_{\mathrm{m}}: (\delta \boldsymbol{w} \otimes \boldsymbol{\nabla}_{0}) - \mathbf{b}_{\mathrm{m}} \cdot \delta \boldsymbol{w} \mathrm{d}\Omega = 0$$



– Introduction of body forces $\boldsymbol{b}_m(\boldsymbol{X}_m)$:

 $\mathbf{b}_{m} = - \left(\begin{array}{c} \partial \mathbf{P}_{m} \\ \partial \mathbf{F}_{m} \end{array} \right) \begin{array}{c} \partial \mathbf{F}_{m} \\ \partial \mathbf{F}_{M} \end{array} : \begin{array}{c} \mathbf{G}_{M} \\ \mathbf{G}_{M} \end{array} : \mathbf{I} \end{array}$

Instantaneous tangent

Strain concentration tensor

Approximation

$$\mathbf{b}_{\mathrm{m}}^{n+1} = -\left(\left(\frac{\partial \mathbf{P}_{\mathrm{m}}}{\partial \mathbf{F}_{\mathrm{m}}}\right)^{n+1} : \left(\frac{\partial \mathbf{F}_{\mathrm{m}}}{\partial \mathbf{F}_{\mathrm{M}}}\right)^{n} : \mathbf{G}_{\mathrm{M}}^{n+1}\right) : \mathbf{I}$$





• Meso-scale problem resolution

Meso-scale FEM is a constrained problem

 $\begin{cases} \mathbf{f}_{m}(\mathbf{u}_{m}) - \mathbf{b}_{m}(\mathbf{u}_{m}) - \mathbf{C}^{T}\boldsymbol{\lambda} = -\mathbf{r} \to 0 & FE \\ \mathbf{C}\mathbf{u}_{m} - \mathbf{S}\begin{bmatrix} \mathbf{F}_{M}^{T} - \mathbf{I} \\ \mathbf{G}_{M}^{T} \end{bmatrix} = -\mathbf{r}_{c} \to 0 & \mathbf{C}, \end{cases}$

FE discretisation of weak form

 ${\cal C}$, ${\cal S}$ from boundary conditions, e.g. PBC

- Finite element resolution (F_M , G_M =cst)

$$\delta \mathbf{u}_{m} = -\widetilde{\mathbf{K}}^{-1} \left(\mathbf{Q}^{\mathrm{T}} \mathbf{r} + \left(\mathbf{C}^{\mathrm{T}} - \mathbf{Q}^{\mathrm{T}} \left(\frac{\partial \mathbf{f}_{m}}{\partial \mathbf{u}_{m}} - \frac{\partial \mathbf{b}_{m}}{\partial \mathbf{u}_{m}} \right) \mathbf{C}^{\mathrm{T}} (\mathbf{C} \mathbf{C}^{\mathrm{T}})^{-1} \right) \mathbf{r}_{c} \right)$$

with $\widetilde{\mathbf{K}} = \mathbf{C}^{\mathrm{T}} \mathbf{C} + \mathbf{Q}^{\mathrm{T}} \left(\frac{\partial \mathbf{f}_{m}}{\partial \mathbf{u}_{m}} - \frac{\partial \mathbf{b}_{m}}{\partial \mathbf{u}_{m}} \right) \mathbf{Q}$ & $\mathbf{Q} = \mathbf{I} - \mathbf{C}^{\mathrm{T}} (\mathbf{C} \mathbf{C}^{\mathrm{T}})^{-1} \mathbf{C}$

- After convergence ($r = r_c = 0$)

$$\frac{\partial \mathbf{u}_{\mathrm{m}}}{\partial [\mathbf{F}_{\mathrm{M}}^{T} \ \mathbf{G}_{\mathrm{M}}^{T}]} = \widetilde{\mathbf{K}}^{-1} \left(\mathcal{C}^{\mathrm{T}} \mathcal{S} - \mathbf{Q}^{\mathrm{T}} \left(\frac{\partial \mathbf{f}_{\mathrm{m}}}{\partial \mathbf{u}_{\mathrm{m}}} - \frac{\partial \mathbf{b}_{\mathrm{m}}}{\partial \mathbf{u}_{\mathrm{m}}} \right) \mathcal{C}^{\mathrm{T}} (\mathcal{C} \mathcal{C}^{\mathrm{T}})^{-1} \mathcal{S} + \mathbf{Q}^{\mathrm{T}} \frac{\partial \mathbf{b}_{\mathrm{m}}}{\partial [\mathbf{F}_{\mathrm{M}}^{T} \ \mathbf{G}_{\mathrm{M}}^{T}]} \right)$$

$$One \ stiffness \ matrix \ \widetilde{\mathbf{K}} \ to \ "inverse"$$

$$\partial \mathbf{F} \qquad \partial \mathbf{u} \qquad (\partial \mathbf{P} \ \partial \mathbf{F} \qquad)$$

$$\frac{\partial \mathbf{F}_{\mathrm{m}}}{\partial \mathbf{F}_{\mathrm{M}}} = \nabla N \frac{\partial \mathbf{u}_{\mathrm{m}}}{\mathbf{F}_{\mathrm{M}}} \qquad \qquad \mathbf{b}_{\mathrm{m}} = -\left(\frac{\partial \mathbf{P}_{\mathrm{m}}}{\partial \mathbf{F}_{\mathrm{m}}}: \frac{\partial \mathbf{F}_{\mathrm{m}}}{\partial \mathbf{F}_{\mathrm{M}}}: \mathbf{G}_{\mathrm{M}}\right): \mathbf{I}$$











- Remove boundary effect
 - Linear elasticity
 - With the presented approach, the body forces are not uniform





 b_{m_1} [MPa · mm⁻¹] -2.35 -1.51 0.68

 $G_{M_{xxx}} = 0.4 / mm$





$$G_{M_{XYY}} = 0.4 / mm$$

0.23



9

- Remove boundary effect
 - Linear elasticity
 - Comparison with uniform body force*
 - Study of the higher-order operator: $\mathbb{L} = \frac{\partial \mathbf{Q}_{M}}{\partial \mathbf{G}_{M}}$







*J. Yvonnet, N. Auffray, V. Monchiet, Int. J. Solids Struct. 191–192 (2020)



-1

-2

-0.146

-1

0

 $\varepsilon_{m_{12}}[-]$

0.0039

1

2

0.138

Remove boundary effect

- Linear elasticity
- Comparison with no body force

















12-14 October 2023



Body-force enhanced second order homogenisation

A

В

D

С

0

X

- Remove boundary effect
 - Linear elasticity
 - Where does the size effect come from?
 - Study of the higher-order operators: $\mathbb{L} = \frac{\partial Q_M}{\partial G_M}$, $\mathbb{M}^{PG} = \frac{\partial P_M}{\partial G_M}$





*J. Yvonnet, N. Auffray, V. Monchiet, Int. J. Solids Struct. 191–192 (2020)





D

С

0

Х

A

• Convergence toward DNS ?















- Multiscale simulation on metastructures
 - Compression samples of different sizes
 - 6x34 holes plobal instability





19

Conclusions

- Effect of RVE size largely reduced
- Applicable to
 - Finite strain formulation
 - Elasto-plasticity
 - Local instabilities
 - Global instabilities

More on

 L. Wu, S. M. Mustafa, J. Segurado, and L. Noels. « Second-order computational homogenisation enhanced with non-uniform body forces for non-linear cellular materials and metamaterials. » Computer Methods in Applied Mechanics and Engineering, 407 (2023): 115931, doi: 10.1016/j.cma.2023.115931



