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On the necessity of accounting for second order terms in multiscale analyses

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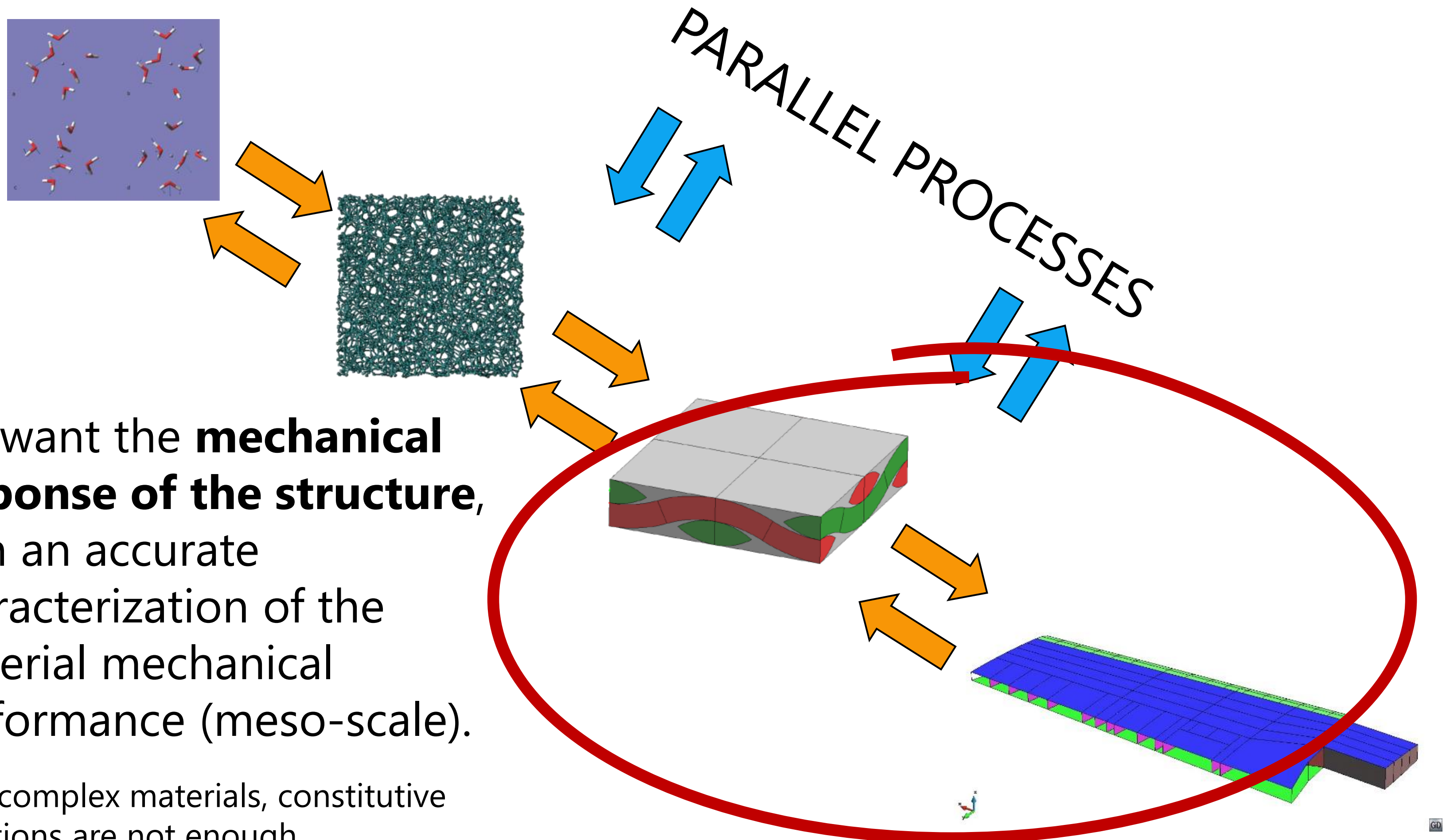
CIMNE International Center for Numerical Methods in Engineering
PLCd

Scope of this work



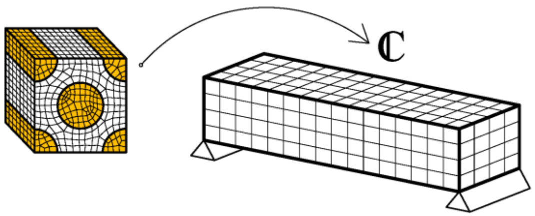
We want the **mechanical response of the structure**, with an accurate characterization of the material mechanical performance (meso-scale).

With complex materials, constitutive equations are not enough.

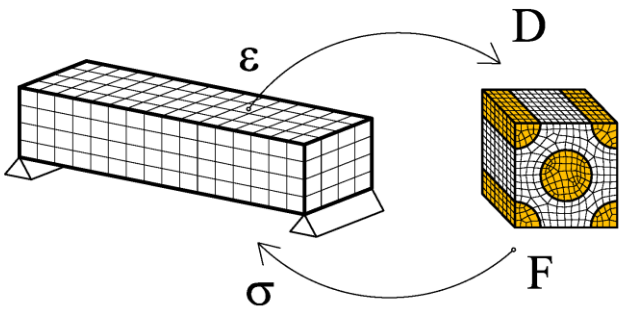
Information exchange between the models

Information can be exchanged in one direction or bi-directionaly:

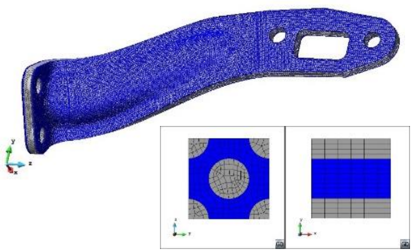
- Linear analysis and/or non-linear prediction



- Full non-linear analysis



In this last case, unless using some optimization procedure (*Otero et al. 2015*[1]) the computational cost can be extremely expensive



Core/Ext. laminae = 247261/108041 elements

FE^2	NLS
32d 14h 46′	11h 36′

1. **F. Otero** *et al.* "An efficient multi-scale method for non-linear analysis of composite structures" **Composite Structures 131**, 2015

Information exchange between the models

Current work is not focused on the amount of exchanges between the models, but on the amount of information shared in those exchanges.

In the macro-model, the material deformation in current configuration can be expressed as a Taylor series expansion around X_0:

$$\triangle \mathbf{x} = \mathbf{F}\left(\mathbf{X}_o\right) \cdot \triangle \mathbf{X} + \frac{1}{2}\mathbf{G}\left(\mathbf{X}_o\right) : \triangle \mathbf{X} \otimes \triangle \mathbf{X} + \mathcal{O}\left(\triangle \mathbf{X}_o^3\right)$$

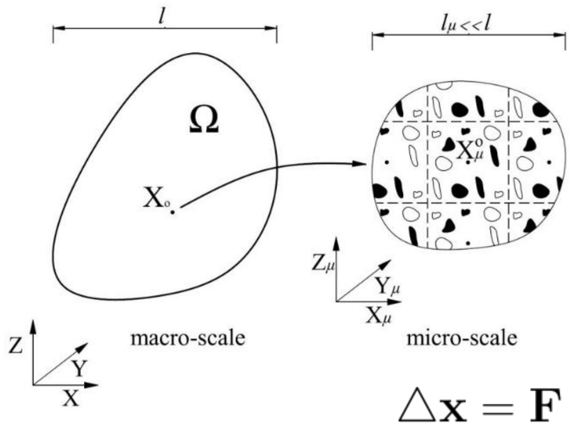
Depending on how many terms of the series we use, we will have a:

- First order theory
- Second order theory

This information can be also sent to the micro-model in order to improve its performance.

2. Formulation

First Order and Enhanced First Order



$$\triangle \mathbf{x} = \mathbf{F}(\mathbf{X}_o) \cdot \triangle \mathbf{X} + \frac{1}{2}\mathbf{G}(\mathbf{X}_o) : \triangle \mathbf{X} \otimes \triangle \mathbf{X} + \mathcal{O}\left(\triangle \mathbf{X}_o^3\right)$$

Microscopic displacement field:

First Order:

$$\mathbf{u}_\mu(\mathbf{X}_o, \mathbf{X}_\mu) \cong [\mathbf{F}(\mathbf{X}_o) - \mathbf{I}] \cdot \mathbf{X}_\mu + \mathbf{w}(\mathbf{X}_\mu)$$

Enhanced First Order:

$$\mathbf{u}_\mu(\mathbf{X}_o, \mathbf{X}_\mu) \cong [\mathbf{F}(\mathbf{X}_o) - \mathbf{I}] \cdot \mathbf{X}_\mu + \frac{1}{2}\mathbf{G}(\mathbf{X}_o) : \mathbf{X}_\mu \otimes \mathbf{X}_\mu + \mathbf{w}(\mathbf{X}_\mu)$$

First Order homogenization

Admissible displacements and Boundary conditions:

$$\mathbf{F}\left(\mathbf{X}_o\right) = \frac{1}{V_\mu}\int_{\Omega_\mu} \mathbf{F}_\mu\left(\mathbf{X}_o, \mathbf{X}_\mu\right)\ dV - \frac{1}{V_\mu}\int_{\Omega_\mu} \nabla\mathbf{w}\left(\mathbf{X}_\mu\right)\ dV$$

The averaging equation states that: $\mathbf{F}\left(\mathbf{X}_o\right) = \frac{1}{V_\mu}\int_{\Omega_\mu} \mathbf{F}_\mu\left(\mathbf{X}_o, \mathbf{X}_\mu\right)\ dV$

Therefore: $\int_{\Omega_\mu} \nabla\mathbf{w}\left(\mathbf{X}_\mu\right)\ dV = \mathbf{0} \longrightarrow \int_{\partial\Omega_\mu} \mathbf{w}\left(\mathbf{X}_\mu\right) \otimes \mathbf{N}\ dA = \mathbf{0}$

The problem is solved applying periodic boundary fluctuations. This is, imposing $\mathbf{w}$ sufficiently regular so that:

$$\mathbf{w}\left(\mathbf{X}_\mu^+\right) = \mathbf{w}\left(\mathbf{X}_\mu^-\right),\ \forall\ pairs\ \left\{\mathbf{X}_\mu^+, \mathbf{X}_\mu^-\right\} \in \partial\Omega_\mu$$

First Order homogenization

Microscopic Strain Field:

$$\mathbf{E}_\mu(\mathbf{X}_o,\mathbf{X}_\mu)=\mathbf{E}(\mathbf{X}_o)+\mathbf{E}_\mu^w(\mathbf{X}_\mu) \quad , \quad \mathbf{E}_\mu^w=\frac{1}{2}\left(\nabla\mathbf{w}+(\nabla\mathbf{w})^T\right)=\nabla^s\mathbf{w}$$

Microscopic Boundary Value Problem:

$$\int_{\Omega_\mu}\mathbf{S}_\mu:\nabla^s\mathbf{w}\;dV=0 \qquad \forall\;\mathbf{w}\in\mathrm{V}_{\Omega_\mu}$$

$$\mathbf{E}_\mu=\frac{1}{2}\left(\mathbf{F}_\mu+\mathbf{F}_\mu^T\right)-\mathbf{I}=\nabla^s\mathbf{u}_\mu \;\; in \;\; \Omega_\mu$$

$$\mathbf{S}_\mu=\mathbf{S}_\mu(\mathbf{E}_\mu,\boldsymbol{\alpha})$$

Macroscopic Stress Tensor:

$$\mathbf{S}(\mathbf{X}_o,\mathbf{X}_\mu)\equiv\frac{1}{V_\mu}\int_{\Omega_\mu}\mathbf{S}_\mu(\mathbf{X}_o,\mathbf{X}_\mu)\;dV$$

$$\mathbf{S}(\mathbf{X}_o,\mathbf{X}_\mu)=\bar{\mathbf{C}}:\mathbf{E}(\mathbf{X}_o)+\frac{1}{V_\mu}\int_{\Omega_\mu}\mathbf{C}_\mu:\mathbf{E}_\mu^w(\mathbf{X}_\mu)\;dV \quad , \quad \bar{\mathbf{C}}\equiv\frac{1}{V_\mu}\int_{\Omega_\mu}\mathbf{C}_\mu\;dV$$

Enhanced First Order homogenization

Admissible displacements and Boundary conditions:

$$\mathbf{F}\left(\mathbf{X}_o\right) = \frac{1}{V_\mu}\int_{\Omega_\mu} \mathbf{F}_\mu\left(\mathbf{X}_o, \mathbf{X}_\mu\right)\ dV - \mathbf{G}\left(\mathbf{X}_o\right)\cdot\frac{1}{V_\mu}\int_{\Omega_\mu}\mathbf{X}_\mu\ dV - \frac{1}{V_\mu}\int_{\Omega_\mu}\nabla\mathbf{w}\left(\mathbf{X}_\mu\right)\ dV$$

The first average theorem states that: $\mathbf{F}\left(\mathbf{X}_o\right) = \frac{1}{V_\mu}\int_{\Omega_\mu} \mathbf{F}_\mu\left(\mathbf{X}_o, \mathbf{X}_\mu\right)\ dV$

Choosing wisely the RVE (origin in its center): $\int_{\Omega_\mu}\mathbf{X}_\mu\ dV = \mathbf{0}$

Therefore, it is necessary to fulfil again: $\int_{\partial\Omega_\mu}\mathbf{w}\left(\mathbf{X}_\mu\right)\otimes\mathbf{N}\ dA = \mathbf{0}$

$$\mathbf{w}\left(\mathbf{X}_\mu^+\right) = \mathbf{w}\left(\mathbf{X}_\mu^-\right),\ \forall\ pairs\ \left\{\mathbf{X}_\mu^+, \mathbf{X}_\mu^-\right\}\in\partial\Omega_\mu$$

Enhanced First Order homogenization

Extra boundary condition:

As a natural extension of the first average theorem, the following relation between both scales must be fulfilled:

$$\mathbf{G}\left(\mathbf{X}_o\right) = \frac{1}{V_\mu}\int_{\Omega_\mu} \mathbf{G}_\mu\left(\mathbf{X}_o, \mathbf{X}_\mu\right)\ dV$$

Which can be achieved with this extra boundary condition:

$$\int_{\mathbf{N}_X^-} \mathbf{w}\ dA_{yz} = \mathbf{0} \quad , \quad \int_{\mathbf{N}_Y^-} \mathbf{w}\ dA_{xz} = \mathbf{0} \quad , \quad \int_{\mathbf{N}_Z^-} \mathbf{w}\ dA_{xy} = \mathbf{0}$$

Microscopic strain depends on the size of the RVE!

Microscopic strain field:

$$\mathbf{E}_\mu\left(\mathbf{X}_o, \mathbf{X}_\mu\right) = \mathbf{E}\left(\mathbf{X}_o\right) + \mathbf{E}_\mu^G\left(\mathbf{X}_o, \mathbf{X}_\mu\right) + \mathbf{E}_\mu^w\left(\mathbf{X}_\mu\right) \qquad \mathbf{E}_\mu^G = \frac{1}{2}\left(\mathbf{G}\cdot\mathbf{X}_\mu + \left(\mathbf{G}\cdot\mathbf{X}_\mu\right)^T\right)$$

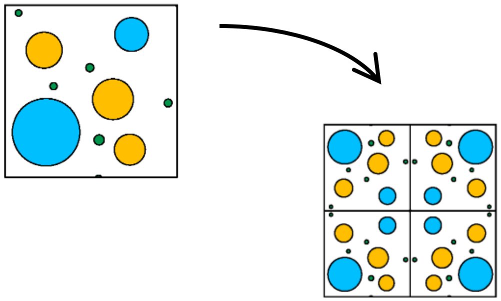
Enhanced First Order homogenization

Macroscopic Stress Tensor:

$$\hat{\mathbf{S}} = \bar{\mathbf{C}} : \mathbf{E}(\mathbf{X}_o) + \bar{\mathbf{B}} : \mathbf{G}(\mathbf{X}_o) + \frac{1}{V_\mu}\int_{\Omega_\mu} \mathbf{C}_\mu : \mathbf{E}_\mu^w(\mathbf{X}_\mu)\ dV \qquad \bar{\mathbf{B}} \equiv \frac{1}{V_\mu}\int_{\Omega_\mu} \mathbf{C}_\mu \otimes \mathbf{X}_\mu\ dV$$

$\bar{\mathrm{B}}$ is equivalent to the bending-extension coupling matrix in shells and beam elements. In order to use it, it is necessary to have these sort of elements.

To simplify this formulation in solid elements, it is necessary to have a RVE with symmetry in the material distribution around its center.

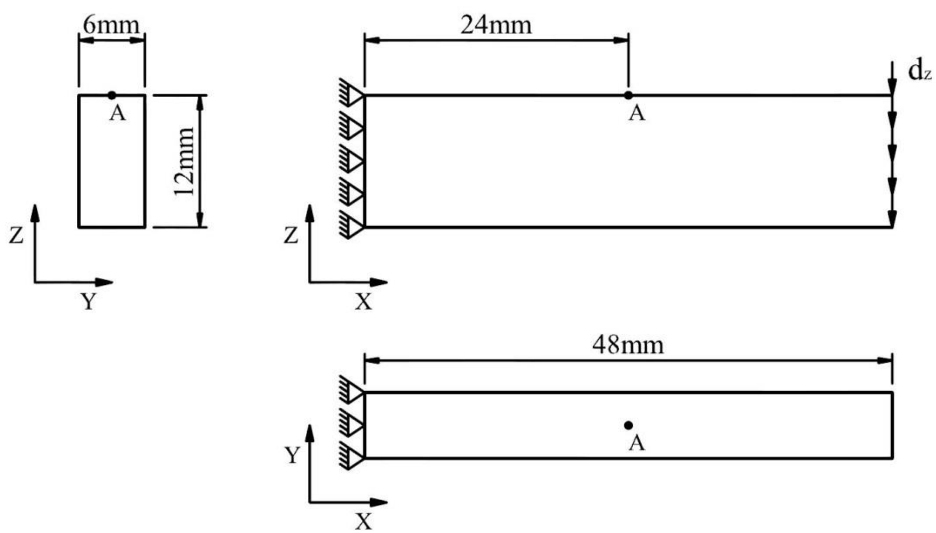


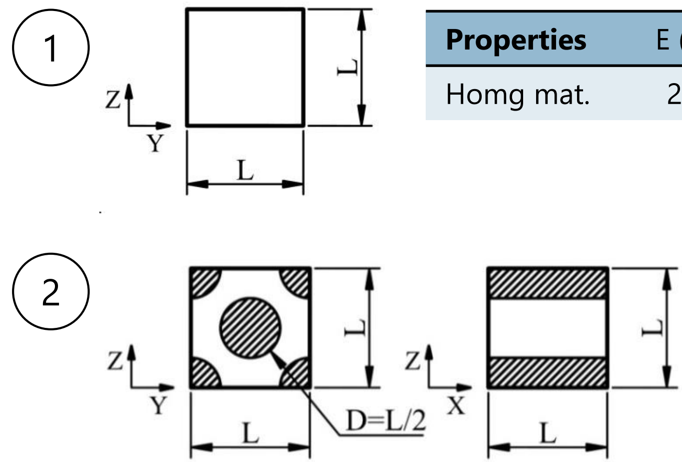
With this RVE, $\bar{\mathrm{B}} = \mathbf{0}$, and therefore:

$$\mathbf{S}(\mathbf{X}_o, \mathbf{X}_\mu) = \bar{\mathbf{C}} : \mathbf{E}(\mathbf{X}_o) + \frac{1}{V_\mu}\int_{\Omega_\mu} \mathbf{C}_\mu : \mathbf{E}_\mu^w(\mathbf{X}_\mu)\ dV$$

3. Numerical Example

Numerical example – Cantilever beam





Properties	E (GPa)
Homg mat.	26.56

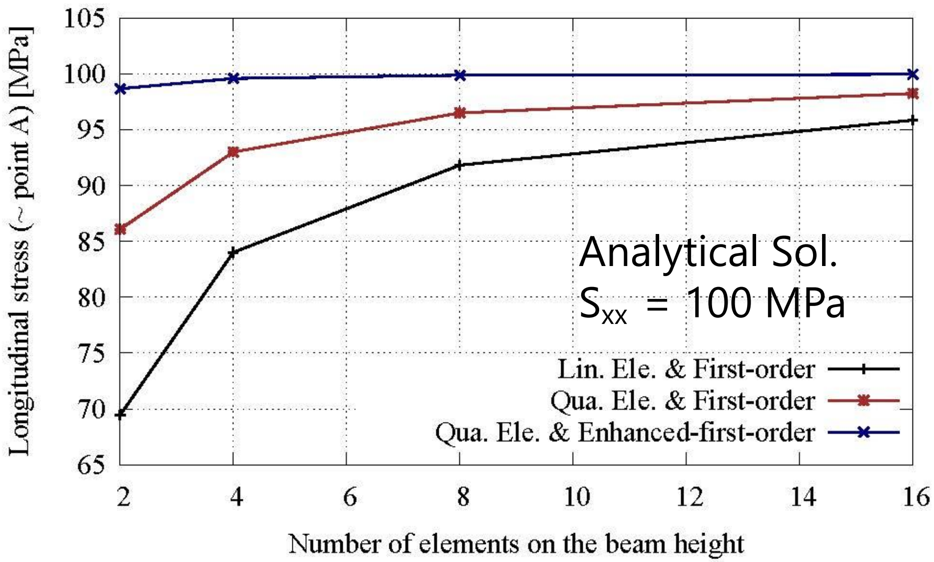
Properties	E (GPa)	v
Matrix	4,52	0,36
Long. Fiber (40%)	235	0,21

Model	Elements	Theory
LE&FO	Linear	First-order
QE&FO	Quadratic	First-order
QE&EFO	Quadratic	Enhanced-first-order

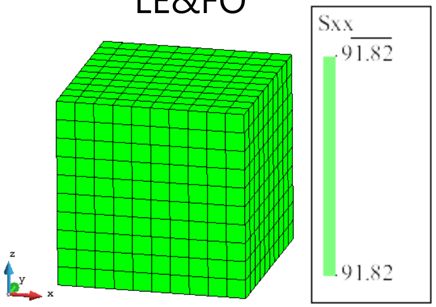
Mesh	Elements	L (mm)
Macro1	8x1x2	1,3525
Macro2	16x2x4	0,6762
Macro3	32x4x8	0,3381
Macro4	64x8x16	0,1691

Cantilever beam – Homogeneous material

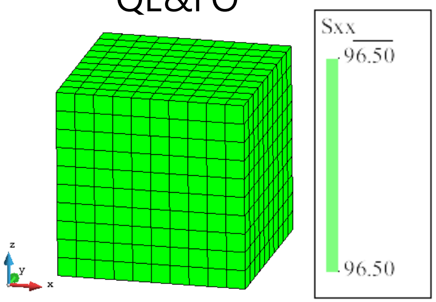
Microstructure Results



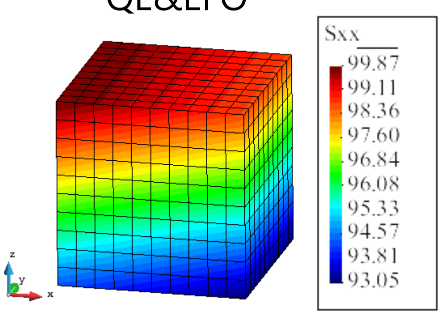
LE&FO



QE&FO



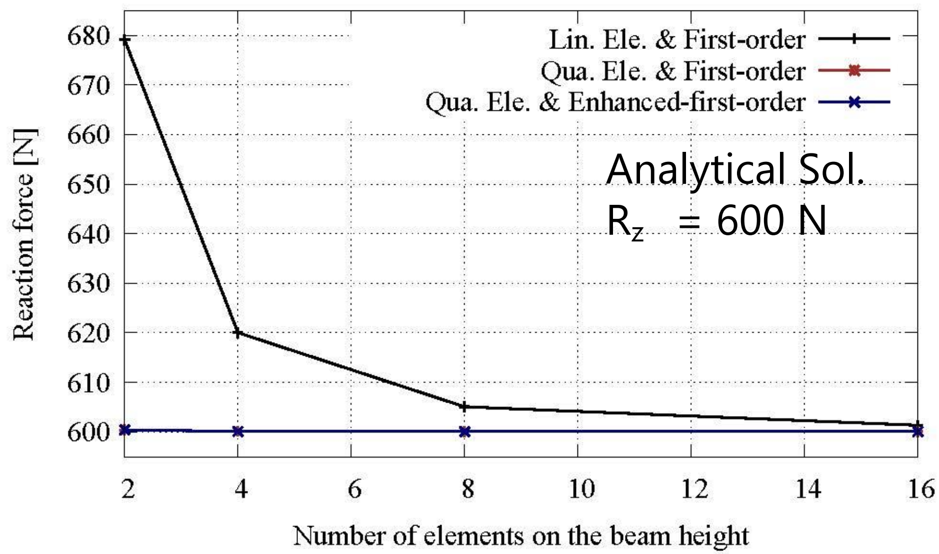
QE&EFO



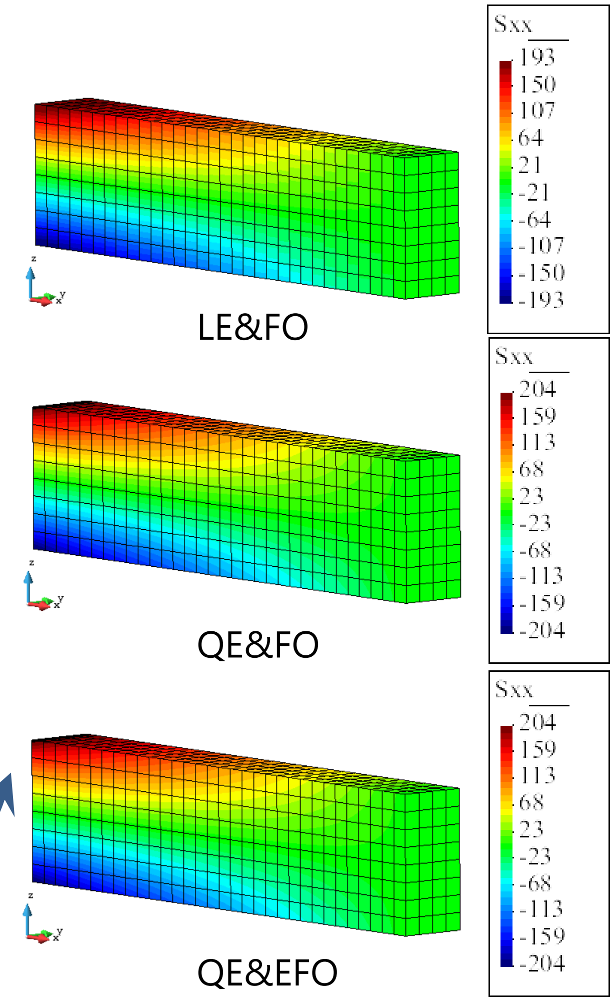
Sxx (MPa)	LE&FO	%	QE&FO	%	QE&EFO	%
Macro1	69,43	30,57	86,08	13,92	98,66	1,34
Macro2	84,02	15,98	93,00	7,00	99,59	0,41
Macro3	91,82	8,18	96,50	3,50	99,87	0,14
Macro4	95,86	4,14	98,25	1,75	99,96	0,04

Cantilever beam – Homogeneous material

Macrostructure Results

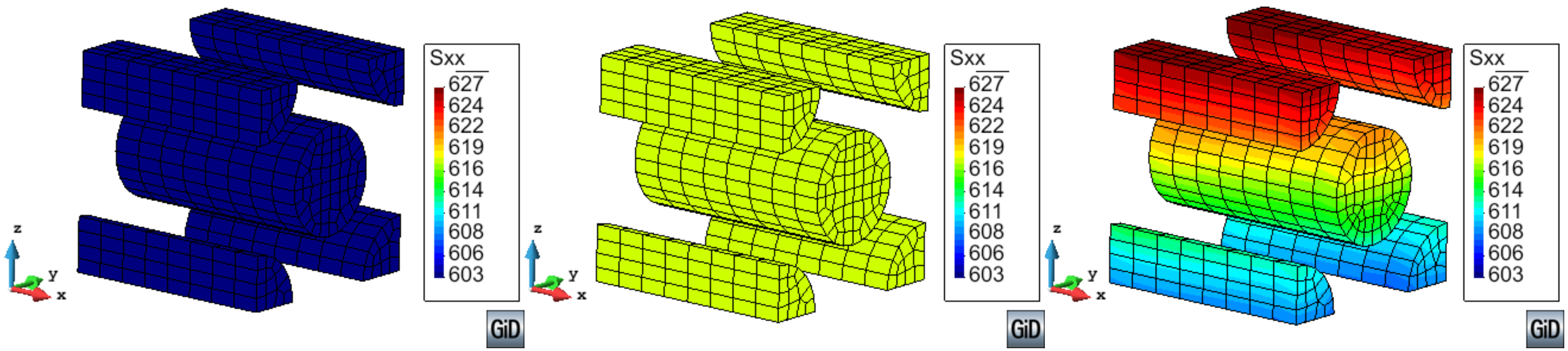


Rz (N)	LE&FO	%	QE&FO	%	QE&EFO	%
Macro1	679,09	13,18	600,43	0,07	600,43	0,07
Macro2	620,03	3,34	600,12	0,02	600,12	0,02
Macro3	605,09	0,85	600,09	0,01	600,09	0,01
Macro4	601,34	0,22	600,08	0,01	600,08	0,01



Cantilever meam – Composite material

Microstructure Results



LE&FO QE&FO QE&EFO

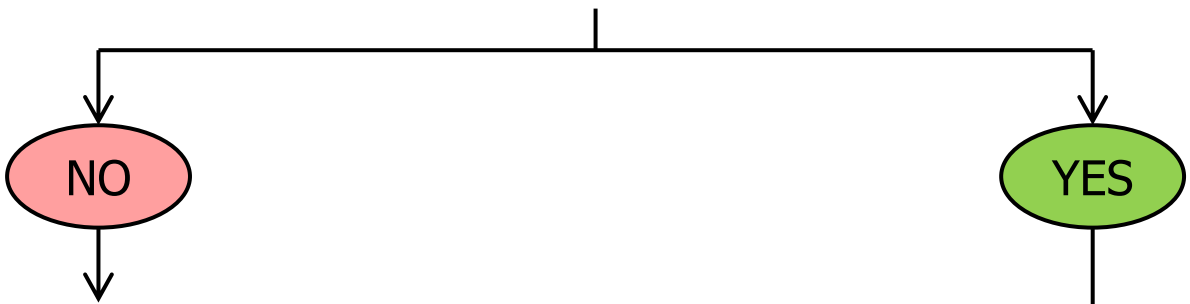
Sxx (MPa)	Fiber			Matrix		
	LE&FO	QE&FO	QE&EFO	LE&FO	QE&FO	QE&EFO
Macro1	454,56	543,31	616,13	11,11	11,18	14,10
Macro2	534,71	584,90	622,41	11,69	12,01	13,67
Macro3	578,97	606,60	625,56	12,23	12,46	13,25
Macro4	603,02	617,54	627,07	12,53	12,68	12,98

4. Discussion

Are second order terms really needed?

Homogenization methods are an improved procedure to characterize the material response.

- Do we need to know the failure mechanism of the material?
- Do we need to characterize the material non-linear behavior of the structure?



2^{nd} order terms are NOT NEEDED

They increase the computational cost of the numerical analysis and they do not improve it.

Are second order terms really needed?

YES

Is the main aim of the simulation to characterize the micro-structure or the macro-structure?

Including 2nd order terms will provide a better characterization of the material failure mode, however, not always this improved characterization is required.

In most cases, it is more useful to improve the discretization of the macro-structure than to have a detailed prediction of the material performance.

Are second order terms really needed?

micro-structure

↓

In this case the 2nd order terms can become a requirement for the correct prediction of material failure.

Taking into account 2nd order terms allows considering loading cases that cannot be taken into account with a first order approach (i.e. bending modes).

Therefore, there will be some failure modes that will not be characterized unless these terms are used.

There are some drawbacks

- Non-linear analysis using multi-scale methods are really expensive.
- Including 2nd order terms:
    - Increases also the computational cost of the analysis.
    - Makes necessary to account for the size of the microstructure Representative Volume Element.
    - Requires a RVE with a symmetric material distribution around its center.

Acknowledgements

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