Multiscale homogenization methods for the numerical analysis of composite materials

Xavier Martinez
Sergio Oller – Fermín Otero
Presentation of the Institution

UPC and CIMNE

and the Research Group

CIMNE Composites – PLCd Group
Location

BARCELONA
Although its main campus is located in Barcelona, it has also campuses in four other cities close to Barcelona.

The UPC was founded in 1965 when several architectural and engineering schools where gathered together. Some of them existed from mid XIX century.

In 1990 the Faculty of Nautical Studies joins the UPC. It is the oldest nautical school in Spain as it was founded in 1769.
CIMNE is a research center associated to the UPC. It was founded in 1987 as a partnership between the regional government and the UPC. The aim of CIMNE is the development of numerical methods and computational techniques for advancing knowledge and technology in engineering in applied sciences.

It has more than 200 research scientists working in several disciplines. It has 8 branches and more than 30 classrooms spread around the globe.
The research areas that are covered by CIMNE can be summarized in the following:

**Bio-Medical Engineering Area**
- Bio-mechanics Group

**Computational and Information Technologies Area**
- Information and Communication Technology Group
- Large-scale Scientific Computing Group
- Mathematical and Computational Modelling Group
- Pre and Post-Processing

**Transport Area**
- Aerospace Engineering Group
- Naval and Marine Engineering Group

**Civil and Mechanical Engineering Area**
- Fluid Mechanics Group
- Geomechanics Group
- Industrial Forming Processes Group

**Energy and Environment Area**
- Building, Energy and Environmental Group
- Nature Group
- Risk Analysis Group

**Structural Mechanics Group**
CIMNE Composites or PLCd group is composed by the following people:

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<th>Dr. Sergio Oller Martínez</th>
<th>Dr. Xavier Martínez</th>
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<tr>
<td>M.Sc. Fermin Otero</td>
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<td>M. Sc. Vicent Alemany Mari</td>
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+ The Salta (Argentina) team:
  Dr. Bibiana Luccioni
  Dr. Facundo Bellomo
  Dr. Rita Rango
Some of the research lines in which the group has worked or is working are:

- **Constitutive modelling of biological tissues**
  - Constitutive equations describe the macroscopic behavior resulting from the internal constitution of a material. They represent, through a mathematical model, the real behavior of a material. However...

- **Inverse methods for the determination of material parameters using optimization techniques**
  - A common difficulty encountered when modelling biological tissues is determining the correct material parameters for the constitutive models used to represent their behavior. Unlike inert tissues, b...

- **Numerical Simulation of Fatigue**
  - The fatigue phenomenon is defined more generally in the ASTM E1823 standard as: "the process of permanent, progressive and localized structural change which occurs to a material point subjected to st...

- **Inflatable Structures**
  - This research line is linked with a project developed for West Virginia University. This project consisted in the numerical simulation of an inflatable structure designed to stop a high pressure fluid...
Some of the research lines in which the group has worked or is working are:

- Phenomenological homogenization methods
- Multi-scale homogenization methods
- Delamination of composites
- Fiber buckling of composite laminates

A more detailed description of these research lines can be obtained from www.cimne.com/PLCd

All the developments are implemented in an in-house FEM code: PLCd
Xavier Martinez

- Civil Engineer by the Polytechnic University of Catalonia (2001)
- Researcher at CIMNE since 2004
- Professor at the UPC since 2009
  - Teaching at the Faculty of Nautical and Naval Studies (FNB)
  - Teaching at the Civil Engineering School
  - Vice-Dean of academic affairs at the FNB
- Member of the board committee of the Spanish Association of Composite Materials (AEMAC) since 2015

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Course Outline

1. Introduction to Multiscale Methods
   1.1. Need for multiscale methods
   1.2. Some examples of multiscale procedures

2. First Order Computational Homogenization (FOCH)
   2.1. Basic Principles
   2.2. Formulation
   2.3. Implementation
   2.4. Numerical examples
3. Enhanced First Order Computational Homogenization (EFOCH)
   3.1. Formulation
   3.2. Implementation
   3.3. Numerical examples – Comparison FOCH vs. EFOCH
   3.4. Discussion

4. Non-Linear Analyses Using Multiscale Methods
   4.1. Different approaches to conduct non-linear analyses
   4.2. Proposal of a Non-Linear Strategy (NLS + SFS)
   4.3. Mesh objectivity – Fracture length
   4.4. Numerical implementation
   4.5. Numerical Examples
1. Introduction to Multiscale Methods
**NEED FOR MULTISCALE METHODS**

**Structural Analysis:**
The incorporation of computational tools in structural analysis has allowed improving the complexity of engineering structures.
Materials in structural analysis

Not only the structure has become more complex, but the materials are better known and can be modelled more precisely.

Elastic analysis: $E$, $\nu$

Plastic analysis

Non-linear laminate models

Need for multiscale methods
Materials in structural analysis

However, the complexity of the internal structures of nowadays composites makes necessary to improve the analysis tools, in order to characterize properly the composite performance.

This is specially important when the analysis wants to be conducted in the non-linear range.

In most cases, composite materials are analyzed as an elastic material with orthotropic properties inherited from its constituents (or given by the manufacturer).

Failure is obtained with a comparison criterion such as: maximum strain, maximum stress, Tsai-Hill, Tsai-Wu, etc.

\[ f_1(\sigma_1) + f_2(\sigma_2) + f_{11}(\sigma_1)^2 + f_{22}(\sigma_2)^2 + 2f_{12}(\sigma_1 \sigma_2) + f_3(\tau_{12})^2 = 1 \]

\[ f_1 = \frac{1}{F_{1t}} - \frac{1}{F_{1c}} \quad f_2 = \frac{2}{F_{2t}} - \frac{2}{F_{2c}} \quad f_{12} = \frac{-1}{2F_{1t}} \]

\[ f_{11} = \frac{1}{F_{1t}F_{1c}} \quad f_{22} = \frac{1}{F_{2t}F_{2c}} \quad f_3 = \frac{1}{F_{12}^2} \]

These approaches do not allow knowing the non-linear performance of the composite. Neither the analysis of complex composite micro-structures.
FEM elements for composite analyses

These models can be applied to solid materials, and can be also applied to shell elements using a lamination theory.

In solid elements, different strategies have been developed to characterize some failure modes. In example, for delamination, a quite extended procedure is the using a zero thickness decohesion element:
Required approach to analyze composite materials

There are also specific models to capture some failure modes, such as matrix transversal cracking, fiber buckling, etc.

However, in order to have an accurate prediction of the composite performance, it is necessary to treat it according to what it is: a micro-structure with different components interacting between them.

This can be done with a multiscale procedure.
Multiscale methods – A possible solution

A multiscale method consist on obtaining the material performance of the macro-structure from a micro-model of the material.
With a multiscale approach we are not only coupling "scales", but also disciplines.
The community that works on multiscale analysis can focus in many different aspects:

- Casting
- Forming
- Annealing
- Carburising
- Welding

thermodynamic databases/
discrete models (electronic/atomistic/mesoscopic)

HDF5

Integrated Computational Materials Engineering expert group
Among the different aspects that can be considered in multiscale analyses, this course is focused in one of them.

Our interest, and this course, focuses in the exchange of information between the macro- and the micro- scales.
In the following will be described some multiscale procedures with the aim of providing a better understanding on how these methods work, as well as giving a hint of different existing approaches.

Models based on homogenization procedures:
1. Effective medium approximation
2. Asymptotic homogenization theory
3. Periodic microstructure model
4. Numerical homogenization
5. Homogenization using Lagrange Multipliers
6. Serial/Parallel mixing theory
The effective medium approximation was initially studied by Eshelby, who analyzed the performance of an homogeneous medium with an internal ellipsoidal inclusion.

The solution obtained by Eshelby provided the stresses and strains in the medium.

This solution can be, and is, used to represent different composite materials, such as materials with ellipsoidal or elliptical cracks.
2. Asymptotic homogenization theory

This theory was initially proposed by Sanchez-Palencia in 1987 and can be considered the mathematical basis for most of the multiscale approaches proposed afterwards.

The two scales that are used to solve the problem are related through a parameter $\delta$ that takes into account the difference of magnitude between both scales.

Defining $x$ as macroscopic quantity and $y = x/\delta$, a microscopic quantity, the two-scale process introduced in the partial differential equations of the problem produces equations in $x$, $y$, and in both variables.

Normally, the equations in $y$ are solvable if the microscopic structure is periodic.
3. Periodic microstructure model

This model was developed by Luciano and Barbero in 1995.

The model is written to analyze the following composite:

- Long fiber reinforced matrices
- Fibers with circular cross section
- Rectangular, equally-spaced distribution of fibers in the composite ($a_2$ and $a_3$ are constant in the composite, and $a_2 = a_3$)
- Fibers oriented in x direction
3. Periodic microstructure model

If previous assumptions are fulfilled, the stiffness tensor of the composite can be obtained with the following parameters:

\[
\begin{align*}
C_{11}^* &= \lambda_m + 2 \mu_m - \frac{V_f}{D} \left[ \frac{S_3^2}{\mu_m^2} - \frac{2 S_6 S_3}{\mu_m g} - \frac{a S_4}{\mu_m c} + \frac{S_2^2 - S_3^2}{\mu_m g^2} + \frac{a S_6 + b S_7}{\mu_m g c} + \frac{a^2 - b^2}{4 c^2} \right] \\
C_{12}^* &= \lambda_m + \frac{V_f}{D} b \left[ \frac{S_3}{2 c \mu_m} - \frac{S_6 - S_7}{2 c \mu_m g} - \frac{a + b}{4 c^2} \right] \\
C_{23}^* &= \lambda_m + \frac{V_f}{D} b \left[ \frac{a S_7}{2 c \mu_m g c} - \frac{b a + b^2}{4 c^2} \right] \\
C_{22}^* &= \lambda_m + 2 \mu_m - \frac{V_f}{D} \left[ -\frac{a S_3}{2 \mu_m c} + \frac{a S_6}{2 \mu_m g c} + \frac{a^2 - b^2}{4 c^2} \right] \\
C_{44}^* &= \mu_m - V_f \left[ \frac{2 S_3}{\mu_m} + (\mu_m - \mu_f)^{-1} + \frac{4 S_7}{\mu_m (2 - 2 \nu_m)} \right]^{-1} \\
C_{66}^* &= \mu_m - V_f \left[ -\frac{S_3}{\mu_m} + (\mu_m - \mu_f)^{-1} \right]^{-1}
\end{align*}
\]

Note: The above notation assumes that the stress and strain tensors have the following order: \((x_{11}, x_{22}, x_{33}, x_{23}, x_{13}, x_{12})\)
3. Periodic microstructure model

The parameters that appear in previous equations are:

\[
D = \frac{a S_3^2}{2 \mu_m c} - \frac{a S_6 S_3}{\mu_m g c} + \frac{a (S_6^2 - S_3^2)}{2 \mu_m g^2 c} + \frac{S_3 (b^2 - a^2)}{2 \mu_m c^2} + \frac{S_6 (a^2 - b^2) + S_7 (ab + b^2)}{2 \mu_m g c^2} + \frac{(a^3 - 2b^3 - 3ab^2)}{8 c^3}
\]

\[
a = \mu_f - \mu_m - 2 \mu_f \nu_m + 2 \mu_m \nu_f
\]

\[
b = -\mu_m \nu_m + \mu_f \nu_f + 2 \mu_m \nu_m \nu_f - 2 \mu_f \nu_m \nu_f
\]

\[
c = (\mu_m - \mu_f) (\mu_f - \mu_m + \mu_f \nu_f - \mu_m \nu_m + 2 \mu_m \nu_f - 2 \mu_f \nu_m + 2 \mu_m \nu_m \nu_f - 2 \mu_f \nu_m \nu_f)
\]

\[
g = (2 - 2 \nu_m)
\]

\[
S_3 = 0.49247 - 0.47603 V_f - 0.02748 V_f^2
\]

\[
S_6 = 0.36844 - 0.14944 V_f - 0.27152 V_f^2
\]

\[
S_7 = 0.12346 - 0.32035 V_f + 0.23517 V_f^2
\]

Equations equivalent to those shown can be obtained if \(a_2\) and \(a_3\) distances, defining the distribution of fibers in the composite, are not equal.
3. Periodic microstructure model

The described model is valid under the following assumptions:

- Perfect elastic materials
- Perfect bonding between fiber and matrix
- The material is in a small strain regime
4. Numerical Homogenization

After previous approach, which was solved analytically, Barbero proposed a numerical homogenization in which the composite parameters were obtained from a finite element model of a Representative Volume Element.

The stiffness tensor of the composite is obtained by applying different strain tensors on the RVE

\[
\begin{align*}
u_i (a_1, x_2, x_3) - u_i (-a_1, x_2, x_3) &= 2a_1 \varepsilon_{11}^{0} &-a_2 \leq x_2 \leq a_2 \\
& \quad -a_3 \leq x_3 \leq a_3 \\

u_i (x_1, a_2, x_3) - u_i (x_1, -a_2, x_3) &= 2a_2 \varepsilon_{22}^{0} &-a_1 \leq x_1 \leq a_1 \\
& \quad -a_3 \leq x_3 \leq a_3 \\

u_i (x_1, x_2, a_3) - u_i (x_1, x_2, -a_3) &= 2a_3 \varepsilon_{33}^{0} &-a_1 \leq x_1 \leq a_1 \\
& \quad -a_2 \leq x_2 \leq a_2
\end{align*}
\]

\[
C_{\alpha\beta} = \sigma_{\alpha} = \frac{1}{V} \int_V \sigma_{\alpha} (x_1, x_2, x_3) \ dV \quad \text{with} \ \varepsilon_{\beta}^{0} = 1
\]
4. Numerical Homogenization

In example, to obtain the first column of the stiffness tensor:

\[ \epsilon_1^0 = 1 \quad \epsilon_2^0 = \epsilon_3^0 = \gamma_4^0 = \gamma_5^0 = \gamma_6^0 = 0 \]

\[ u_1 (a_1, x_2, x_3) - u_1 (-a_1, x_2, x_3) = 2a_1 \quad -a_2 \leq x_2 \leq a_2 \]
\[ u_2 (a_1, x_2, x_3) - u_2 (-a_1, x_2, x_3) = 0 \quad -a_3 \leq x_3 \leq a_3 \]
\[ u_3 (a_1, x_2, x_3) - u_3 (-a_1, x_2, x_3) = 0 \]

\[ u_i (x_1, a_2, x_3) - u_i (x_1, -a_2, x_3) = 0 \quad -a_1 \leq x_1 \leq a_1 \]
\[ -a_3 \leq x_3 \leq a_3 \]

\[ u_i (x_1, x_2, a_3) - u_i (x_1, x_2, -a_3) = 0 \quad -a_1 \leq x_1 \leq a_1 \]
\[ -a_2 < x_2 \leq a_2 \]

\[ C_{\alpha 1} = \overline{\sigma}_{\alpha} = \frac{1}{V} \int_V \sigma_{\alpha} (x_1, x_2, x_3) \, dV \]

The considerations made on the periodic microstructure model are still valid: elasticity, perfect bonding between materials and small strains.
5. Homogenization using Lagrange Multipliers

This model was initially proposed by Zalamea, Oller in 2001. It consists in obtaining the material performance by solving a finite element model of a representative volume element.
5. Homogenization using Lagrange Multipliers

The representative volume element is defined by cells. These have to be defined respecting the periodicity of the base material. To have the cell perfectly defined, it is necessary to define also the periodicity vectors.
5. Homogenization using Lagrange Multipliers

The periodicity elements will vary depending on the cell defined as Representative Volume Element.
5. Homogenization using Lagrange Multipliers

The deformation obtained in the macro-model is transferred to the micro-model using the average theory.

It is important to remark that the micro-model deformation does not only modify the geometry of the RVE but also the periodicity vectors.
5. Homogenization using Lagrange Multipliers

The use of Lagrange Multipliers to force the periodicity at the RVE increases the computational cost and the complexity of the system. On the other hand, it allows defining periodicity vectors. With these, the same RVE can be used to characterize different composites.
5. Homogenization using Lagrange Multipliers

The results obtained for the simulations previously presented are:

Multiscale procedures. Examples
5. Homogenization using Lagrange Multipliers

Besides the additional complexity provided by the use of Lagrange Multipliers to solve the RVE problem, the major drawback of this homogenization procedure was:

It was proposed in 2001!

Computational capabilities were substantially smaller than today.

The analyses that could be performed were only academic

In example:

Previous case consisted in a macro model with 60 linear 2D elements and a micro model with 108 linear 2D elements.

The problem was solved with a parallel process with 4 processors and required 1h15min to be solved.
6. Serial-parallel mixing theory

This last example differs from the others, as it does not define an specific model to characterize a given composite geometry, but instead provides the mechanical response of the composite by defining specific relations between the constitutive equations of its components.

The serial-parallel mixing theory (SP RoM) can be understood as a phenomenological homogenization or a constitutive equation manager.
In order to understand the performance of the serial/parallel mixing theory we will analyze a basic material:

Parallel behavior
\[ \varepsilon_1 = \varepsilon_2 = \ldots = \varepsilon_n \]

Serial behavior
\[ \sigma_1 = \sigma_2 = \ldots = \sigma_n \]
6. Serial-parallel mixing theory

The serial/parallel mixing theory states that:
1. All components have the same strains in parallel direction
2. All components have the same stress in serial direction
3. All components participate in the composite material proportionally to their volumetric participation

This is:

Parallel direction
\[
\begin{align*}
\varepsilon^c_P &= m \varepsilon^m_P = f \varepsilon^f_P \\
\sigma^c_P &= m k^m \sigma^m_P + f k^f \sigma^f_P
\end{align*}
\]

Serial direction
\[
\begin{align*}
\varepsilon^c_S &= m k^m \varepsilon^m_S + f k^f \varepsilon^f_S \\
\sigma^c_S &= m \sigma^m_S = f \sigma^f_S
\end{align*}
\]
6. Serial-parallel mixing theory

Application of the SP RoM formulation to laminate materials:

Laminates simulated with solid elements:

1) Apply parallel RoM at layer level
2) Apply SP RoM for each layer
3) Obtain stresses with parallel RoM

\[ \varepsilon_i = \varepsilon_1 = \ldots = \varepsilon_n \]
\[ \varepsilon_i \rightarrow \sigma_i \]
\[ \sigma = \sum k \sigma \]

Laminates simulated with shell elements:

1) \[
\begin{pmatrix}
L_i \varepsilon_x \\
L_i \varepsilon_y \\
L_i \gamma_{xy}
\end{pmatrix} =
\begin{pmatrix}
\varepsilon_x^0 \\
\varepsilon_y^0 \\
\gamma_{xy}^0
\end{pmatrix} + Z
\begin{pmatrix}
K_x \\
K_y \\
K_{xy}
\end{pmatrix}
\]
2) SP RoM

\[ L_i \varepsilon \rightarrow L_i \sigma \]
6. Serial-parallel mixing theory

Parallel Load:

Stress-strain graph in the load direction

Stress-strain graph perpendicular to the load direction

ISO-STRAIN Behaviour

ISO-STRESS Behaviour

Multiscale procedures. Examples
6. Serial-parallel mixing theory

Serial Load:

Stress-strain graph in the load direction

Stress-strain graph perpendicular to the load direction

ISO-STRESS Behaviour

ISO-STRAIN Behaviour

Multiscale procedures. Examples
6. Serial-parallel mixing theory

Numerical example. Delamination of composites

One of the most common failure modes of composite laminates is delamination. The SP RoM is capable of predicting this failure mode naturally.

Example: Ply drop-off test
6. Serial-parallel mixing theory

Failure mode of the ply drop-off test:
As materials have increased their complexity, advanced numerical approaches are also required for a correct characterization.

Multiscale procedures are the perfect framework to increase, as much as wanted, the complexity of the model used to define the composite.

Our interest lays in the information exchange between the two scales. The procedure chosen must allow:

• Solve engineering problems
• An accurate material characterization. So all the possibilities of nowadays composites can be taken into account.
2. First Order Computational Homogenization
2. First Order Computational Homogenization (FOCH)
   2.1. Basic Principles
   2.2. Formulation
   2.3. Implementation
   2.4. Numerical examples
A multiscale procedure consists on solving a numerical model, in which the response of some of its components is obtained from a numerical model found in a lower scale.
Multiscale procedures in mechanical problems

If this is applied to the solution of structural mechanical problems, the multiscale procedure consists on:

Transfer the deformation gradient tensor $\varepsilon_M$ to the micro-scale, where is solved a boundary value problem (BVP) over a representative volume element (RVE). The macroscopic stress tensor $\sigma_M$ and tangent stiffness matrix $C_{\text{hom}}$ can be obtained from this scale. (Geers et al. 2010)
Conditions to apply a multiscale procedure

In order to apply a multiscale procedure there are two conditions that must be fulfilled:

1. Periodicity of the RVE
2. Scale separation

$L_m \ll \ll \ll L_e$

There are several studies concerning the most representative size of the RVE, such as:

S.M. Mirkhalaf, F.M. Andrade Pires, Ricardo Simoes: *Determination of the size of the Representative Volume Element (RVE) for the simulation of heterogeneous polymers at finite strains*. Finite Elements in Analysis and Design (119), 2016
The displacement field in the macro scale can be computed as:

Macro scale displacement:

Continuum: \[ d\mathbf{x} = \mathbf{F} \cdot d\mathbf{X} \]

Taylor’s exp.: \[ \Delta \mathbf{x} = \mathbf{F}(\mathbf{X}_0) \cdot \Delta \mathbf{X} + \frac{1}{2} \mathbf{G}(\mathbf{X}_0) : \Delta \mathbf{X} \otimes \Delta \mathbf{X} + \mathcal{O}(\Delta \mathbf{X}^3) \]

with

\( \mathbf{F} = \text{Deformation gradient tensor} \)

\( \mathbf{G} = \text{Gradient of the deformation gradient tensor} \)

\[ \mathbf{F} = \frac{\partial \phi}{\partial \mathbf{X}} \]

\[ \mathbf{G} = \nabla \mathbf{F} = \frac{\partial}{\partial \mathbf{X}} \left( \frac{\partial \phi}{\partial \mathbf{X}} \right) \]
Micro Displacement

The displacement field in the micro scale is a combination of the displacements provided by the macro structure and a micro fluctuation:

\[ \mathbf{x}_\mu (\mathbf{X}_o, \mathbf{X}_\mu) \approx \mathbf{x}_\mu^0 + \mathbf{F}(\mathbf{X}_o) \cdot \Delta \mathbf{X}_\mu + \mathbf{w}(\mathbf{X}_\mu) \]

\[ \Delta \mathbf{X}_\mu = \mathbf{X}_\mu - \mathbf{X}_\mu^0 \]

\[ \Delta \mathbf{x} = \mathbf{F}(\mathbf{X}_o) \cdot \Delta \mathbf{x} + \frac{1}{2} \mathbf{G}(\mathbf{X}_o) : \Delta \mathbf{X} \otimes \Delta \mathbf{X} + \mathcal{O}(\Delta \mathbf{x}^3) \]

This is a FIRST ORDER HOMOGENIZATION because it only considers the first term of the macro displacement field.

FOCH – Formulation
Micro Displacement

To simplify the symbolic manipulation and for symmetry purposes, it is convenient to set the origin of the RVE’s coordinate system as:

\[ X_\mu^o = 0 \quad \text{and} \quad x_\mu^o = 0 \]

Therefore,

\[ x_\mu (X_o, X_\mu) \approx F(X_o) \cdot X_\mu + w(X_\mu) \]

And the displacement field of the RVE can be written as:

\[ u_\mu = x_\mu - X_\mu \]

\[ u_\mu (X_o, X_\mu) \approx [F(X_o) - I] \cdot X_\mu + w(X_\mu) \]
Boundary Conditions in the RVE

The first average theorem states that the volume average of the microstructural deformation gradient over the RVE must be equal to the macroscopic deformation gradient:

\[
F \left( X_o \right) = \frac{1}{V_\mu} \int_{\Omega_\mu} F_\mu \left( X_o, X_\mu \right) \, dV
\]

The microstructural deformation gradient can be written as:

\[
F_\mu \left( X_o, X_\mu \right) = \nabla x_\mu \left( X_o, X_\mu \right) \simeq F \left( X_o \right) + \nabla w \left( X_\mu \right)
\]

With some math, it is finally obtained:

\[
\int_{\Omega_\mu} \nabla w \left( X_\mu \right) \, dV = 0
\]
Boundary Conditions in the RVE

Applying the divergence theorem, the last expression becomes:

\[ \int_{\partial \Omega_\mu} \mathbf{w} \left( \mathbf{X}_\mu \right) \otimes \mathbf{N} \, dA = 0 \]

Which can be rewritten as:

\[
\begin{align*}
& \left( \int_{N_X^+} \mathbf{w} \, dA_{yz} - \int_{N_X^-} \mathbf{w} \, dA_{yz} \right) \otimes \mathbf{N}_X^+ \\
+ & \left( \int_{N_Y^+} \mathbf{w} \, dA_{xz} - \int_{N_Y^-} \mathbf{w} \, dA_{xz} \right) \otimes \mathbf{N}_Y^+ \\
+ & \left( \int_{N_Z^+} \mathbf{w} \, dA_{xy} - \int_{N_Z^-} \mathbf{w} \, dA_{xy} \right) \otimes \mathbf{N}_Z^+ = 0
\end{align*}
\]
Boundary Conditions in the RVE

There are several boundary conditions that can be applied to the RVE that fulfil the defined requirement:

• Taylor Model (zero fluctuations):

\[ \mathbf{w}, \text{sufficiently regular} \mid \mathbf{w}(\mathbf{X}_\mu) = 0, \quad \forall \mathbf{X}_\mu \in \Omega_\mu \]

• Linear boundary displacements (zero boundary fluctuations):

\[ \mathbf{w}, \text{sufficiently regular} \mid \mathbf{w}(\mathbf{X}_\mu) = 0, \quad \forall \mathbf{X}_\mu \in \partial \Omega_\mu \]

• Periodic boundary fluctuations:

\[ \mathbf{w}, \text{sufficiently regular} \mid \mathbf{w}(\mathbf{X}_\mu^+) = \mathbf{w}(\mathbf{X}_\mu^-), \quad \forall \text{pairs } \{\mathbf{X}_\mu^+, \mathbf{X}_\mu^-\} \in \partial \Omega_\mu \]

• Minimal constrain:

There is no specific restriction, besides the integral over the fluctuation field.
The macro strain tensor must be equal to the volume average of the micro strain tensor:

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

And the micro strain tensor can be written as:

$$\mathbf{E}_\mu(\mathbf{X}_o, \mathbf{X}_\mu) = \mathbf{E}(\mathbf{X}_o) + \mathbf{E}_\mu^w(\mathbf{X}_\mu)$$

being

$$\mathbf{E}_\mu^w = \frac{1}{2} \left( \nabla \mathbf{w} + (\nabla \mathbf{w})^T \right) = \nabla^s \mathbf{w}$$
The Hill-Mandel energy condition states that the virtual work of the point $X_0$ must be equal to the volume average of the virtual work in the RVE for any kinematically admissible displacement field:

$$ S : \delta E (X_o) = \frac{1}{V_{\mu}} \int_{\Omega_{\mu}} S_{\mu} : \delta E_{\mu} \, dV $$

$$ = \frac{1}{V_{\mu}} \int_{\Omega_{\mu}} S_{\mu} \, dV : \delta E (X_o) + \frac{1}{V_{\mu}} \int_{\Omega_{\mu}} S_{\mu} : \delta E^{w}_{\mu} (X_{\mu}) \, dV $$

Defining the macroscopic stress tensor as the average of the microstructural stress tensor in the RVE domain:

$$ S (X_o, X_{\mu}) \equiv \frac{1}{V_{\mu}} \int_{\Omega_{\mu}} S_{\mu} (X_o, X_{\mu}) \, dV $$
The Hill-Mandel principle will be satisfied if:

\[ \int_{\Omega_\mu} S_\mu : \delta E^w_\mu (X_\mu) \ dV = \int_{\Omega_\mu} S_\mu : \nabla^s \delta w \ dV = 0 \]

RVE variational equilibrium equation
Macroscopic and microscopic stress tensor

The microscopic stress tensor can be obtained as:

\[ S_{\mu} (X_o, X_\mu) = C_{\mu} (X_\mu) : E_{\mu} (X_o, X_\mu) \]

\[ = C_{\mu} (X_\mu) : E (X_o) + C_{\mu} (X_\mu) : E_{\mu}^w (X_\mu) \]

And the macroscopic stress tensor can be calculated as:

\[ S (X_o, X_\mu) = \frac{1}{V_\mu} \int_{\Omega_\mu} S_{\mu} (X_o, X_\mu) \, dV \]

\[ S (X_o, X_\mu) = \bar{C} : E (X_o) + \frac{1}{V_\mu} \int_{\Omega_\mu} C_{\mu} : E_{\mu}^w (X_\mu) \, dV \]

with:

\[ \bar{C} \equiv \frac{1}{V_\mu} \int_{\Omega_\mu} C_{\mu} \, dV \]
Some remarks regarding the macroscopic stress tensor:

1. It does not depend explicitly on $X_\mu$. Therefore, the stresses provided by the RVE are independent of its size. A non-dimensional RVE can be used to characterize the material.

2. The fluctuation strains affect the macro-response of the structure. Depending on the boundary conditions chosen, different macro-stress results will be obtained. The Taylor model returns the classical mixing theory results.
The Finite Element Method for the analysis of structural problems is based on solving the Principle of Virtual Work:

\[ \int_{\Omega} \delta E^T \cdot S \, dV = \int_{\Omega} \delta \bar{u}^T \cdot b \, dV + \int_{\partial\Omega} \delta \bar{u}^T \cdot q \, dV + \sum \delta u_i^T \cdot P_i \]

Which leads to the solution of the linear system of equations:

\[ K \cdot \bar{u} = F \]

being

\[ K = \int_{\Omega} B^T : C : B \, dV \]

And the relation between stresses, strains and displacements:

\[ S = C : E = C : B \cdot \bar{u} \]

IN A LINEAR ANALYSIS!
In a non-linear analysis, the relation between strains and stresses are different to those predicted by the material stiffness matrix. In an implicit approach the displacements are found with an iterative procedure:

\[ F_{(k)} = B \cdot \hat{u}_{(k)} + I, \quad G_{(k)} = H \cdot \hat{u}_{(k)} \]

\[ \hat{u}_{(k+1)} = \hat{u}_{(k)} + K^{-1} \cdot \Delta F \]

\[ \Delta F = |F_{ext} - F_{int}| \leq tol \]

**Flow diagram**

- Initial material and geometric properties + boundary conditions
- Calculate elastic stiffness: \( K = B^T : C : B \)
- \( F_{(n)} = F_{(n-1)} + \Delta F_{(n)} \)
- \( \hat{u}_{(n)} = \hat{u}_{(n-1)} + K^{-1} \cdot \Delta F_{(n)} \)
- \( \hat{u}_{(k+1)} = \hat{u}_{(n)} : F_{ext} = F_{(n)} \)
- \( k = 1, k_{max} \)
- \( F_{(k)} = B \cdot \hat{u}_{(k)} + I, \quad G_{(k)} = H \cdot \hat{u}_{(k)} \)
- \( \hat{u}_{(k+1)} = \hat{u}_{(k)} : K = \hat{T}_{(k)} \)
- \( \Delta F = |F_{ext} - F_{int}| \leq tol \)
- No, \( k = k + 1 \)
- Yes, \( n = n + 1 \)
- END
Solution of the MACROSCALE problem

The material stiffness matrix depends on the RVE microstructure.

There is no constitutive model. The stress tensor corresponding to the applied stresses is obtained from the RVE solution.

IN A LINEAR ANALYSIS, THE RVE HAS TO BE SOLVED ONLY ONCE!
The microscale problem is, by itself, a numerical model that will be solved with the FEM.

The main differences compared to the macroscale problem are:

1. The boundary conditions to be applied to the model are defined by the deformation gradient of the macroscale problem.

2. The result required from the model are the macroscale stresses, which are obtained from the microscale stresses, and the tangent stiffness tensor.
MICRO-STRUCTURE boundary conditions

From the different models that can be applied, the most convenient is the *periodic boundary fluctuations*:

\[ w, \text{ sufficiently regular} \mid w \left( X^+_\mu \right) = w \left( X^-_\mu \right), \forall \text{ pairs } \{ X^+_\mu, X^-_\mu \} \in \partial \Omega_\mu \]

Which can be rewritten as:

\[
\begin{align*}
    u_\mu(X^+_\mu) - u_\mu(X^-_\mu) &= D_1(F - I) \cdot N^+_X, \quad \forall \text{ pairs } \{ X^+_\mu, X^-_\mu \} \in \partial \Omega_\mu|N_X \\
    u_\mu(X^+_\mu) - u_\mu(X^-_\mu) &= D_2(F - I) \cdot N^+_Y, \quad \forall \text{ pairs } \{ X^+_\mu, X^-_\mu \} \in \partial \Omega_\mu|N_Y \\
    u_\mu(X^+_\mu) - u_\mu(X^-_\mu) &= D_3(F - I) \cdot N^+_Z, \quad \forall \text{ pairs } \{ X^+_\mu, X^-_\mu \} \in \partial \Omega_\mu|N_Z
\end{align*}
\]

These boundary conditions are applied by defining master and slave nodes in the RVE model.
MICRO-STRUCTURE boundary conditions

Master and slave nodes in the RVE:

<table>
<thead>
<tr>
<th>Master nodes</th>
<th>a</th>
<th>b</th>
<th>c</th>
<th>d</th>
<th>e</th>
<th>f</th>
</tr>
</thead>
<tbody>
<tr>
<td>Slave nodes</td>
<td>a₁, a₂, a₃</td>
<td>b₁, b₂, b₃</td>
<td>c₁, c₂, c₃</td>
<td>d₁</td>
<td>e₁</td>
<td>f₁</td>
</tr>
</tbody>
</table>
MICRO-STRUCTURE boundary conditions

Position vector of the different nodes:

\[
X_{a_1} - X_a = \begin{bmatrix}
X_{\mu} \\ D_2/2 \\ -D_3/2
\end{bmatrix} - \begin{bmatrix}
X_{\mu} \\ -D_2/2 \\ -D_3/2
\end{bmatrix} = \begin{bmatrix}
0 \\ D_2 \\ 0
\end{bmatrix} = D_2 N_Y^+
\]

\[
X_{a_2} - X_a = \begin{bmatrix}
X_{\mu} \\ D_2/2 \\ D_3/2
\end{bmatrix} - \begin{bmatrix}
X_{\mu} \\ -D_2/2 \\ -D_3/2
\end{bmatrix} = \begin{bmatrix}
0 \\ D_2 \\ D_3
\end{bmatrix} = D_2 N_Y^+ + D_3 N_Z^+
\]

\[
X_{a_3} - X_a = \begin{bmatrix}
X_{\mu} \\ -D_2/2 \\ D_3/2
\end{bmatrix} - \begin{bmatrix}
X_{\mu} \\ -D_2/2 \\ -D_3/2
\end{bmatrix} = \begin{bmatrix}
0 \\ 0 \\ D_3
\end{bmatrix} = D_3 N_Z^+
\]
MICRO-STRUCTURE boundary conditions

Having defined the position vector, the periodic boundary fluctuations condition can be written as:

$$\tilde{u}_{a_1} = \tilde{u}_a + (F - I) \cdot (X_{a_1} - X_a) = \tilde{u}_a + D_2 (F - I) \cdot N_Y^+$$

defining:

$$sm_1 = D_1 (F - I) \cdot N_X^+$$

$$sm_2 = D_2 (F - I) \cdot N_Y^+$$

$$sm_3 = D_3 (F - I) \cdot N_Z^+$$

the displacement of the slave nodes can be obtained as:

$$\tilde{u}_{a_1} = \tilde{u}_a + sm_2, \quad \tilde{u}_{a_2} = \tilde{u}_a + sm_2 + sm_3, \quad \tilde{u}_{a_3} = \tilde{u}_a + sm_3,$$

$$\tilde{u}_{b_1} = \tilde{u}_b + sm_1, \quad \tilde{u}_{b_2} = \tilde{u}_b + sm_1 + sm_3, \quad \tilde{u}_{b_3} = \tilde{u}_b + sm_3,$$

$$\tilde{u}_{c_1} = \tilde{u}_c + sm_1, \quad \tilde{u}_{c_2} = \tilde{u}_c + sm_1 + sm_2, \quad \tilde{u}_{c_3} = \tilde{u}_c + sm_2,$$

$$\tilde{u}_{d_1} = \tilde{u}_d + sm_3, \quad \tilde{u}_{e_1} = \tilde{u}_e + sm_1, \quad \tilde{u}_{f_1} = \tilde{u}_f + sm_2.$$
The micro-structural problem to be solved consists on a RVE in which are known the displacement relations between its parallel faces.

This problem can be solved with two different approaches:

1. Definition of Lagrange Multipliers that relate the displacement relation between master and slave nodes.

\[
\begin{bmatrix}
  K & k_p^T & k_p^T \\
  k_p & I & -I \\
  k_p & -I & I \\
\end{bmatrix}
\begin{bmatrix}
  u \\
  \lambda_1 \\
  \lambda_2 \\
\end{bmatrix}
= \begin{bmatrix}
  F \\
  \Delta D \\
  \Delta D \\
\end{bmatrix}
\]

2. Removing the slave degrees of freedom from the linear system of equations.
Elimination of slave degrees of freedom

The linear system of equations to be solved can be rewritten differentiating internal ($u$), master ($m$) and slave ($s$) nodes:

\[
\begin{bmatrix}
K_{uu} & K_{um} & K_{us} \\
K_{mu} & K_{mm} & K_{ms} \\
K_{su} & K_{sm} & K_{ss}
\end{bmatrix}
\begin{bmatrix}
d_u \\
d_m \\
d_s
\end{bmatrix}
= \begin{bmatrix}
F_u \\
F_m \\
F_s
\end{bmatrix}
\]

\[
\begin{bmatrix}
K_{uu} \\
K_{mu} \\
K_{su}
\end{bmatrix}
\{d_u\} 
+ \begin{bmatrix}
K_{um} \\
K_{mm} \\
K_{sm}
\end{bmatrix}
\{d_m\} 
+ \begin{bmatrix}
K_{us} \\
K_{ms} \\
K_{ss}
\end{bmatrix}
\{d_s\} = \begin{bmatrix}
F_u \\
F_m \\
F_s
\end{bmatrix}
\]

The displacement of the slave nodes can be written as a function of the master nodes:

\[
\{d_s\} = [S_{sm}] \{d_m\} + \{\Delta d\}
The periodic boundary fluctuation condition requires that the sum of forces in the master and slave nodes to be zero:

$$\{ F_m \} + [ S_{ms} ] \{ F_s \} = 0$$
Elimination of slave degrees of freedom

The linear system of equation can be rewritten as:

\[
\begin{bmatrix}
\frac{K_{uu}}{K_{mu} + S_{ms} K_{su}} \\
\frac{K_{us}}{K_{ms} + S_{ms} K_{su}}
\end{bmatrix}
\begin{bmatrix} d_u \\ \triangle d \end{bmatrix} + \begin{bmatrix}
\frac{K_{um} + K_{us} S_{sm}}{K_{mm} + K_{ms} S_{sm} + S_{ms} K_{sm} + S_{ms} K_{ss} S_{sm}}
\end{bmatrix}
\begin{bmatrix} d_m \\ \triangle d \end{bmatrix} +
\]

\[
\begin{bmatrix}
F_u \\
\frac{F_u}{F_m + S_{ms} F_s}
\end{bmatrix}
\]

\[
\begin{bmatrix}
\frac{K_{uu}}{K_{mu} + S_{ms} K_{su}} \\
\frac{K_{um} + K_{us} S_{sm}}{K_{mm} + K_{ms} S_{sm} + S_{ms} K_{sm} + S_{ms} K_{ss} S_{sm}}
\end{bmatrix}
\begin{bmatrix} d_u \\ d_m \end{bmatrix} = \begin{bmatrix}
\frac{F_u - K_{us} \triangle d}{(K_{ms} + S_{ms} K_{ss}) \triangle d} \\
\end{bmatrix}
\]

\[
K_r \cdot d_r = F_r
\]
Solution of the MICROSCALE problem

Input data provided by the macroproblem.
Each gauss point provides a different input data.

Output result are the macro-stress and the material tangent stiffness tensor.
Macro stress and tangent constitutive tensor

The expression that provides the macro-stress tensor as been shown when describing the formulation behind the FOCH:

\[
S(X_o, X_\mu) = \frac{1}{V_\mu} \int_{\Omega_\mu} S_\mu(X_o, X_\mu) \, dV
\]

\[
S(X_o, X_\mu) = \bar{C} : E(X_o) + \frac{1}{V_\mu} \int_{\Omega_\mu} C_\mu : E^w_\mu(X_\mu) \, dV
\]

\[
\bar{C} = \frac{1}{V_\mu} \int_{\Omega_\mu} C_\mu \, dV
\]

The stiffness matrix of the RVE material cannot be obtained from the average of the micro-stiffness matrices, as the effect of the fluctuations would not be considered.
The RVE constitutive tensor (elastic and tangent) is obtained with a numerical derivation by perturbations.

The relation between strains and stresses can be written, in matrix form:

\[
\begin{bmatrix}
\dot{S}_1 \\
\vdots \\
\dot{S}_n
\end{bmatrix} = 
\begin{bmatrix}
C_{11}^{\text{tan}} & \cdots & C_{1n}^{\text{tan}} \\
\vdots & \ddots & \vdots \\
C_{n1}^{\text{tan}} & \cdots & C_{nn}^{\text{tan}}
\end{bmatrix}
\begin{bmatrix}
\dot{E}_1 \\
\vdots \\
\dot{E}_n
\end{bmatrix}
\]

The stress tensor can be also obtained as the sum of \( n \) partial stress tensors, which are defined as:

\[
\dot{S} \equiv \sum_{j=1}^{n} \delta^j S = \sum_{j=1}^{n} C_{j}^{\text{tan}} \cdot \delta E_j
\]

with

\[
C_{j}^{\text{tan}} = 
\begin{bmatrix}
C_{1j}^{\text{tan}} & C_{2j}^{\text{tan}} & \cdots & C_{nj}^{\text{tan}}
\end{bmatrix}^T
\]
The calculation of each one of these columns is obtained by defining a perturbed strain value in the different space directions:

$$\mathbf{C}_{ij}^{tan} = \frac{j \mathbf{S}}{\mathbf{E}_{ij}} \equiv \frac{\delta j \mathbf{S}}{\delta \mathbf{E}_{ij}}$$

***FOCH – Implementation***
In a LINEAR PROBLEM this step is not required. The stresses are obtained with the RVE stiffness matrix.

In a FE² problem, the RVE has to be solved at each load step in order to obtain the updated stresses.

The tangent constitutive tensor has to be recalculated if materials inside the RVE become non-linear.

The boundary conditions applied at the RVE are defined by the deformation gradient tensor.
NUMERICAL EXAMPLES

In the following section three different numerical examples will be described and studied.

1. **Quasi-isotropic material.**
2. **Long fiber composite.**
   These examples will be used to show the basic performance of a multiscale procedure in a linear regime.

3. **Laminated composite.**
   This example will be used to show the performance of the formulation if non-linear effects are considered. It also compares the results obtained with a multiscale procedure and other approaches such as a micro-model and a model using the serial/parallel mixing theory.
Problem description

Simulation of a structure with a heterogeneous material composite. The macrostructure is a rectangle of 20x20 cm section and length 80 cm and the microstructure is a matrix with spherical inclusions.
The macro FE mesh has 256 second order hexahedral element (20 nodes) and 1505 nodes.

It is completely fixed in one end and it has an “x” displacement applied to the other end.
The micromodel is a cube with a length of 10 containing 252 spheres from \( d = 0.7 \) to \( d = 2.2 \). The spheres are randomly distributed. The FE mesh has 87405 first order tetrahedral elements and 15946 nodes. The spheres represent 27% of the total volume.
Two different isotropic materials have been considered in the simulation. Each one is defined with its Young and Poisson Modulus. The shear modulus is obtained from these two.

<table>
<thead>
<tr>
<th>Material ID</th>
<th>E [GPa]</th>
<th>(\nu)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3.5</td>
<td>0.2</td>
</tr>
<tr>
<td>2</td>
<td>210</td>
<td>0.3</td>
</tr>
</tbody>
</table>

These two materials have been combined to create four different RVE models:
Stiffness matrix comparison

The multiscale procedures provides the stiffness matrix of the RVE considered. These are:

<table>
<thead>
<tr>
<th>Model</th>
<th>Matrix</th>
<th>Spheres</th>
</tr>
</thead>
<tbody>
<tr>
<td>RVE 1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>RVE 2</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>RVE 3</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>RVE 4</td>
<td>1</td>
<td>-</td>
</tr>
</tbody>
</table>

**RVE 1**

\[
\begin{bmatrix}
3.89 & 0.97 & 0.97 & 0 & 0 & 0 \\
0.97 & 3.89 & 0.97 & 0 & 0 & 0 \\
0.97 & 0.97 & 3.89 & 0 & 0 & 0 \\
0 & 0 & 0 & 1.46 & 0 & 0 \\
0 & 0 & 0 & 0 & 1.46 & 0 \\
0 & 0 & 0 & 0 & 0 & 1.46 \\
\end{bmatrix}
\]

**RVE 2**

\[
\begin{bmatrix}
8.17 & 1.66 & 1.65 & 0 & -0.03 & 0 \\
1.66 & 8.15 & 1.65 & -0.02 & 0 & 0 \\
1.65 & 1.65 & 8.07 & 0 & -0.02 & 0 \\
0 & -0.02 & 0 & 3.15 & 0 & -0.01 \\
-0.03 & 0 & -0.02 & 0 & 3.10 & -0.01 \\
0 & 0 & 0 & -0.01 & -0.01 & 3.12 \\
\end{bmatrix}
\]

**RVE 3**

\[
\begin{bmatrix}
170.21 & 64.99 & 64.80 & -0.03 & -0.13 & 0.04 \\
64.99 & 170.10 & 64.87 & -0.13 & -0.04 & -0.06 \\
64.80 & 64.87 & 169.48 & -0.01 & -0.06 & 0.05 \\
-0.03 & -0.13 & -0.01 & 52.00 & 0.03 & -0.04 \\
-0.13 & -0.04 & -0.06 & 0.03 & 51.81 & 0 \\
0.04 & -0.06 & 0.05 & -0.04 & 0 & 51.89 \\
\end{bmatrix}
\]

**RVE 4**

\[
\begin{bmatrix}
2.42 & 0.57 & 0.57 & 0 & -0.02 & 0.01 \\
0.57 & 2.42 & 0.57 & -0.02 & 0 & -0.01 \\
0.57 & 0.57 & 2.41 & 0 & -0.01 & 0.01 \\
0 & -0.02 & 0 & 0.91 & 0.01 & -0.01 \\
-0.02 & 0 & -0.01 & 0.01 & 0.91 & 0 \\
0.01 & -0.01 & 0.01 & -0.01 & 0 & 0.91 \\
\end{bmatrix}
\]
Macro structural performance

All macro results are very similar, varying only the stress values due to the different stiffness provided by the RVE model.

**Numerical Example 1**

<table>
<thead>
<tr>
<th>Model</th>
<th>Matrix</th>
<th>Spheres</th>
</tr>
</thead>
<tbody>
<tr>
<td>RVE 1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>RVE 2</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>RVE 3</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>RVE 3</td>
<td>1</td>
<td>-</td>
</tr>
</tbody>
</table>

**STRESS IN RVE 1**
\[ \sigma = 0.35 \text{GPa} \]

**STRESS IN RVE 2**
\[ \sigma = 0.76 \text{GPa} \]

**STRESS IN RVE 3**
\[ \sigma = 13 \text{GPa} \]

**STRESS IN RVE 4**
\[ \sigma = 0.22 \text{GPa} \]
Micro structural performance – RVE 1

Displacements

x strains

x stresses
Micro structural performance – RVE 4

Displacements

x strains

x stresses

FOCH – Numerical Example 1
This example analyzes a clamped beam with a vertical displacement in its free edge. The micro-structure corresponds to a long fibre composite.

<table>
<thead>
<tr>
<th>Material</th>
<th>$E$ [GPa]</th>
<th>$\nu$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Matrix</td>
<td>3.1</td>
<td>0.38</td>
</tr>
<tr>
<td>Fibre</td>
<td>24.1</td>
<td>0.20</td>
</tr>
</tbody>
</table>
LONG FIBER COMPOSITE – Results

Macro and micro results
LAMINATED COMPOSITE – Problem description

In this example the results provided by different theories will be compared in order to assess the improvements provided by the multiscale method, as well as its possible drawbacks and costs.

The problem to study is a double clamped beam made of a laminated structure

The problem will be analyzed reducing the shear stiffness of different layers in the laminate.
Formulations to be tested

The proposed problem will be analyzed with three different approaches:

1. **Micro model.** In which all layers are discretized.
2. **Serial-Parallel mixing theory.**
3. **First Order Computational Homogenization.**

The interest lays on comparing the **accuracy** of the solution provided by the different formulations, as well as the **computational cost** required to conduct the analysis.
Numerical models

**Macro-model:**
Only half of the beam has been simulated using the existing symmetry. The macro FE mesh has 2048 first order hexahedral elements (8 nodes) and 2673 nodes.

**Micro-model:**
Different RVE micro-models have been defined to account for different number of layers with reduced shear stiffness (damaged layers).
The material properties defined are those shown in the table.

<table>
<thead>
<tr>
<th>Material</th>
<th>Color</th>
<th>E [GPa]</th>
<th>G [GPa]</th>
<th>$\nu$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lamina 1</td>
<td>Black</td>
<td>210</td>
<td>80.76</td>
<td>0.38</td>
</tr>
<tr>
<td>Lamina 2</td>
<td>Grey</td>
<td>3.5</td>
<td>1.46</td>
<td>0.20</td>
</tr>
<tr>
<td>Lamina 3</td>
<td>White</td>
<td>3.5</td>
<td>0.146</td>
<td>0.20</td>
</tr>
</tbody>
</table>

FOCH – Numerical Example 3
Global damage case – Comparison FOCH vs SP RoM

The first analysis made has been over a laminate in which all layers have the same “damage” value. This comparison has made between the FOCH and the SP RoM approaches.

**Completely undamaged results:**
Different macro-model meshes have been analyzed to study the convergence of the problem.

Micro-model:

SP RoM model:
- Parallel directions: $X$ and $Y$
- Serial directions: $Z$ and shear

---

**Material**

<table>
<thead>
<tr>
<th>Material</th>
<th>Color</th>
<th>E [GPa]</th>
<th>G [GPa]</th>
<th>$\nu$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lamina 1</td>
<td>Black</td>
<td>210</td>
<td>80.76</td>
<td>0.38</td>
</tr>
<tr>
<td>Lamina 2</td>
<td>Grey</td>
<td>3.5</td>
<td>1.46</td>
<td>0.20</td>
</tr>
</tbody>
</table>
Global damage case – Comparison FOCH vs SP RoM

Damage evolution:
The weakest lamina has been analyzed with different values of shear stiffness in order to assess the effect of this value on the results.

<table>
<thead>
<tr>
<th>Material</th>
<th>Color</th>
<th>E [GPa]</th>
<th>G [GPa]</th>
<th>(\nu)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lamina 1</td>
<td>Black</td>
<td>210</td>
<td>80.76</td>
<td>0.38</td>
</tr>
<tr>
<td>Lamina 2</td>
<td>Grey</td>
<td>3.5</td>
<td>varying</td>
<td>0.20</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Model</th>
<th>0%</th>
<th>12.5%</th>
<th>25%</th>
<th>50%</th>
<th>100%</th>
</tr>
</thead>
<tbody>
<tr>
<td>G [GPa]</td>
<td>1.46</td>
<td>1.295</td>
<td>1.131</td>
<td>0.803</td>
<td>0.146</td>
</tr>
</tbody>
</table>

As expected, results are identical for both theories.
Local damage case – All approaches comparison

In this case, the performance of the structure is analyzed when different proportions of layers have a reduced stiffness.

These analyses is made with all three approaches: micro-models, Serial/Parallel RoM and FOCH.

Cases considered:
Five different cases are considered: 0, 12.5, 25, 50 and 100%

---

FOCH – Numerical Example 3
Local damage case – All approaches comparison

Results obtained:

The serial parallel mixing theory, as it assumes a parallel behavior of the different layers of the composite, cannot capture the abrupt variation of stiffness produced by damage in one layer.
Local damage case – All approaches comparison

However, if a global damage is applied to the RVEs of some macro-model elements, the results provided by both theories are very similar.

<table>
<thead>
<tr>
<th>Approach</th>
<th>Reaction</th>
</tr>
</thead>
<tbody>
<tr>
<td>FOCH</td>
<td>357.4 N</td>
</tr>
<tr>
<td>SP RoM</td>
<td>752.8 N</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Approach</th>
<th>Reaction</th>
</tr>
</thead>
<tbody>
<tr>
<td>FOCH</td>
<td>666.4 N</td>
</tr>
<tr>
<td>SP RoM</td>
<td>663.9 N</td>
</tr>
</tbody>
</table>
### Computational cost – Time & Memory

In the following table is shown the computational cost required to perform the analysis of 50% local damage, by the different approaches considered:

<table>
<thead>
<tr>
<th>Item</th>
<th>Micro-model</th>
<th>FE²</th>
<th>Linear FOCH</th>
<th>SP RoM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Real Time (Min:Seg)</td>
<td>6:46</td>
<td>2:27</td>
<td>0:01</td>
<td>0:02</td>
</tr>
<tr>
<td>CPU Time (Min:Seg)</td>
<td>8:44</td>
<td>9:31</td>
<td>0:03</td>
<td>0:17</td>
</tr>
<tr>
<td>Memory (Mbytes)</td>
<td>2690,00</td>
<td>7,45</td>
<td>7,45</td>
<td>15,82</td>
</tr>
<tr>
<td>Reaction Force (N)</td>
<td>236,1</td>
<td>224,7</td>
<td>224,7</td>
<td>576,7</td>
</tr>
</tbody>
</table>

- Micro-model: Excessive CPU time and memory requirements
- FE² model: Excessive time with a substantial reduction of CPU
- Linear FOCH & SP RoM: The most efficient
3. Enhanced First Order Computational Homogenization
3. Enhanced First Order Computational Homogenization (EFOCH)
   3.1. Introduction
   3.2. Formulation
   3.3. Numerical example – Comparison FOCH vs. EFOCH
   3.4. Discussion
Need to account for 2\textsuperscript{nd} order effects

2\textsuperscript{nd} order elements provide a better approximation of the displacement, strain and stress fields:

Shape Functions:

Beam displacements:
Need to account for 2\textsuperscript{nd} order effects

If second order elements are used, the displacement field in the macrostructure uses the gradient of the deformation gradient

\[
\Delta x = F(X_o) \cdot \Delta X + \frac{1}{2} G(X_o) : \Delta X \otimes \Delta X + O(\Delta X_o^3)
\]
The Enhanced First Order Computational Homogenization (EFOCH) uses the first two terms of the macro displacement field

\[ x_\mu (X_o, X_\mu) \cong x^0_\mu + F(X_o) \cdot \Delta X_\mu + \frac{1}{2} G(X_o) : \Delta X_\mu \otimes \Delta X_\mu + w(X_\mu) \]

Defining the origin of coordinates at the center of the RVE, the displacements can be written as:

\[ u_\mu (X_o, X_\mu) \cong [F(X_o) - I] \cdot X_\mu + \frac{1}{2} G(X_o) : X_\mu \otimes X_\mu + w(X_\mu) \]
Boundary Conditions in the RVE

The second order terms are also present in the expression of the microstructural deformation gradient:

$$ F_\mu (X_o, X_\mu) = \nabla x_\mu (X_o, X_\mu) \cong F (X_o) + G (X_o) \cdot X_\mu + \nabla w (X_\mu) $$

And the volume average theorem over the deformation gradient becomes:

$$ \frac{1}{V_\mu} \int_{\Omega_\mu} F_\mu (X_o, X_\mu) \ dV = F (X_o) + G (X_o) \cdot \frac{1}{V_\mu} \int_{\Omega_\mu} X_\mu \ dV + \frac{1}{V_\mu} \int_{\Omega_\mu} \nabla w (X_\mu) \ dV $$

Having defined the origin of the RVE in its center, the first moment of volume is zero:

$$ \int_{\Omega_\mu} X_\mu \ dV = 0 $$

And the BC defined for the FOCH is recovered:

$$ \int_{\partial \Omega_\mu} w (X_\mu) \otimes N \ dA = 0 $$
Boundary Conditions in the RVE

However, in the EFOCH it is necessary to apply the average theorem also to the gradient of the deformation gradient:

\[ G(X_o) = \frac{1}{V_\mu} \int_{\Omega_\mu} G_\mu(X_o, X_\mu) \, dV \]

Defining the gradient of the deformation gradient in the microstructure as:

\[ G_\mu(X_o, X_\mu) = \nabla \left( \nabla x_\mu(X_o, X_\mu) \right) \cong G(X_o) + \nabla \left( \nabla w(X_\mu) \right) \]

The new boundary condition that has to be applied to the RVE becomes:

\[ \int_{\partial \Omega_\mu} \nabla w(X_\mu) \otimes N \, dA = 0 \]
Boundary Conditions in the RVE

Considering an hexahedral RVE, these last conditions can be rewritten as:

\[
\left( \int_{N_X^+} \nabla w \, dA_{yz} - \int_{N_X^-} \nabla w \, dA_{yz} \right) \otimes N_X^+ \\
+ \left( \int_{N_Y^+} \nabla w \, dA_{xz} - \int_{N_Y^-} \nabla w \, dA_{xz} \right) \otimes N_Y^+ \\
+ \left( \int_{N_Z^+} \nabla w \, dA_{xy} - \int_{N_Z^-} \nabla w \, dA_{xy} \right) \otimes N_Z^+ = 0
\]

And, a set of fluctuations that satisfy this last expression is:

\[
\int_{N_X^+} \nabla_X w \, dA_{yz} = \int_{N_X^-} \nabla_X w \, dA_{yz}, \\
\int_{N_Y^+} \nabla_Y w \, dA_{xz} = \int_{N_Y^-} \nabla_Y w \, dA_{xz}, \\
\int_{N_Z^+} \nabla_Z w \, dA_{xy} = \int_{N_Z^-} \nabla_Z w \, dA_{xy}
\]
The expression that defines the microscopic strain tensor is:

$$E_\mu (X_o, X_\mu) = E(X_o) + E^G_\mu (X_o, X_\mu) + E^w_\mu (X_\mu)$$

with,

$$E^w_\mu = \frac{1}{2} \left( \nabla w + (\nabla w)^T \right) = \nabla^s w$$

$$E^G_\mu = \frac{1}{2} \left( G \cdot X_\mu + (G \cdot X_\mu)^T \right)$$

Now, the microscopic strain depends on the size of the RVE!
Hill-Mandel principle and RVE Equilibrium

The Hill-Mandel energy condition states that the virtual work of the point $X_0$ must be equal to the volume average of the virtual work in the RVE for any kinematically admissible displacement field.

When using a second order theory to describe the displacement field in the macro model, it is assumed that there is a virtual work of the point corresponds to an average of a macro-volume $\Omega_M$ around the point. Therefore,

\[
\frac{1}{V_M} \int_{\Omega_M} S : \delta E \ dV = \frac{1}{V_\mu} \int_{\Omega_\mu} S_\mu : \delta E_\mu \ dV
\]
Hill-Mandel principle and RVE Equilibrium

Operating over the last expression and defining the homogenized stress tensor as:

\[ \hat{S} \equiv \frac{1}{V_M} \int_{\Omega_M} S \, dV \equiv \frac{1}{V_\mu} \int_{\Omega_\mu} S_\mu \, dV \]

And the homogenized second order stress tensor as:

\[ \hat{Q} \equiv \frac{1}{V_M} \int_{\Omega_M} S \otimes \Delta X \, dV \equiv \frac{1}{V_\mu} \int_{\Omega_\mu} S_\mu \otimes X_\mu \, dV \]

The final variational equilibrium equation becomes:

\[ \int_{\Omega_\mu} S_\mu : \nabla^s \delta w \, dV = 0 \]

Which is the same that was obtained for the FOCH
Macroscopic and microscopic stress tensor

Microscopic Stress Tensor:

The microscopic stress tensor is calculated as:

\[ S_\mu = C_\mu : E(X_o) + C_\mu : E^G_\mu (X_o, X_\mu) + C_\mu : E^w_\mu (X_\mu), \]

It has to be noted that now, the stresses on the different elements of the RVE depends on the position of these elements in the RVE!

Macroscopic Stress Tensor:

The macroscopic stress tensor is obtained using the expression:

\[ \hat{S} = \frac{1}{V_M} \int_{\Omega_M} S \, dV \equiv \frac{1}{V_\mu} \int_{\Omega_\mu} S_\mu \, dV \]
Macroscopic and microscopic stress tensor

Which leads to:

\[ \hat{\mathbf{S}} = \mathbf{C} : \mathbf{E}(X_o) + \mathbf{B} : \mathbf{G}(X_o) + \frac{1}{V_\mu} \int_{\Omega_\mu} \mathbf{C}_\mu : \mathbf{E}_\mu^w(X_\mu) \ dV \]

\[ \mathbf{B} \equiv \frac{1}{V_\mu} \int_{\Omega_\mu} \mathbf{C}_\mu \otimes X_\mu \ dV \]

\( \mathbf{B} \) 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, \( \mathbf{B} = \mathbf{0} \), and therefore:

\[ \mathbf{S}(X_o, X_\mu) = \mathbf{C} : \mathbf{E}(X_o) + \frac{1}{V_\mu} \int_{\Omega_\mu} \mathbf{C}_\mu : \mathbf{E}_\mu^w(X_\mu) \ dV \]
Numerical Example – Cantilever Beam

3. Numerical example

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

Properties

<table>
<thead>
<tr>
<th></th>
<th>E (GPa)</th>
<th>v</th>
</tr>
</thead>
<tbody>
<tr>
<td>Homogeneous mat.</td>
<td>26.56</td>
<td></td>
</tr>
<tr>
<td>Matrix</td>
<td>4.52</td>
<td>0.36</td>
</tr>
<tr>
<td>Long. Fiber (40%)</td>
<td>235</td>
<td>0.21</td>
</tr>
</tbody>
</table>

Mesh Elements L (mm)

<table>
<thead>
<tr>
<th>Mesh</th>
<th>Elements</th>
<th>L (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Macro1</td>
<td>8x1x2</td>
<td>1.3525</td>
</tr>
<tr>
<td>Macro2</td>
<td>16x2x4</td>
<td>0.6762</td>
</tr>
<tr>
<td>Macro3</td>
<td>32x4x8</td>
<td>0.3381</td>
</tr>
<tr>
<td>Macro4</td>
<td>64x8x16</td>
<td>0.1691</td>
</tr>
</tbody>
</table>
Cantilever beam – Homogeneous material

Microstructure Results

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

Analytical Sol. 
Sxx = 100 MPa

3. Numerical example
3. Numerical example

Cantilever beam – Homogeneous material

Macrostructure Results

<table>
<thead>
<tr>
<th>Rz (N)</th>
<th>LE&amp;FO</th>
<th>%</th>
<th>QE&amp;FO</th>
<th>%</th>
<th>QE&amp;EFO</th>
<th>%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Macro1</td>
<td>679,09</td>
<td>13,18</td>
<td>600,43</td>
<td>0,07</td>
<td>600,43</td>
<td>0,07</td>
</tr>
<tr>
<td>Macro2</td>
<td>620,03</td>
<td>3,34</td>
<td>600,12</td>
<td>0,02</td>
<td>600,12</td>
<td>0,02</td>
</tr>
<tr>
<td>Macro3</td>
<td>605,09</td>
<td>0,85</td>
<td>600,09</td>
<td>0,01</td>
<td>600,09</td>
<td>0,01</td>
</tr>
<tr>
<td>Macro4</td>
<td>601,34</td>
<td>0,22</td>
<td>600,08</td>
<td>0,01</td>
<td>600,08</td>
<td>0,01</td>
</tr>
</tbody>
</table>

Analytical Sol.

R_z = 600 N

![Reaction force vs. number of elements](chart.png)
# Cantilever mean – Composite material

## Microstructure Results

<table>
<thead>
<tr>
<th>Sxx (MPa)</th>
<th>Fiber</th>
<th>Matrix</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>LE&amp;FO</td>
<td>QE&amp;FO</td>
</tr>
<tr>
<td>Macro1</td>
<td>454,56</td>
<td>543,31</td>
</tr>
<tr>
<td>Macro2</td>
<td>534,71</td>
<td>584,90</td>
</tr>
<tr>
<td>Macro3</td>
<td>578,97</td>
<td>606,60</td>
</tr>
<tr>
<td>Macro4</td>
<td>603,02</td>
<td>617,54</td>
</tr>
</tbody>
</table>
DISCUSSION. Are second order terms 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?

**YES**

2\textsuperscript{nd} order terms are NOT NEEDED

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

**NO**
Are second order terms really needed?

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

Including 2\textsuperscript{nd} 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.
4. Discussion

Are second order terms really needed?

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

Taking into account 2\textsuperscript{nd} 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 2\textsuperscript{nd} 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.
4. Non-Linear Analyses Using Multiscale Methods
4. Non-Linear Analyses Using Multiscale Methods
   4.1. Different approaches to conduct non-linear analyses
   4.2. Proposal of a Non-Linear Strategy (NLS + SFS)
   4.3. Numerical Examples
As engineers, when analyzing a structure, we want to know its mechanical response and its safety factor.

\[
\text{Stress} \leq \text{Maximum material strength}
\]

If a multiscale method wants to be useful, it must provide the same information.
A linear procedure is capable of providing the structural performance. This is, the forces and displacements on the macro-structure. But it does not provide the safety factor.

This loop is not done and the component stresses are unknown.

Different approaches
A FE2 consists on using the RVE as a constitutive equation, therefore it is solved at each load step, for each gauss point.

**Different Approaches:**

1. **FE²**

   - **Advantage:** It is the most accurate method
   - **Drawback:** Humongous computational cost
2. Failure Characterization

A failure characterization procedure consist on analyzing, after completing the macro-analysis, the most critical RVEs with the exact strain values obtained from the macro-analysis, increasing them until failure.

Advantage: With an affordable computational cost it is possible to know the SF in the macro-structure and the material failure of the RVE.

Drawback: Difficult to know with certainty which is the most critical RVE.
3. Micro-constitutive equation

The RVE can be used as an experimental sample and it can be tested to obtain the parameters required by a given constitutive equation.

The constitutive equation can be either an existing one (i.e. damage with a Von-Mises yield surface) or can be defined explicitly.
3. Micro-constitutive equation

An explicit constitute equation is obtained by loading the RVE in different characteristic directions and recording its damage evolution and stress-strain in that direction.

The macro-model will use the stress-strain curve recorded in the direction given and, if it does not exist, it will interpolate it from the closest ones.

Advantage: It is possible to create a material library and, with it, the solution of the macro-structure is very cheap.

Drawback: It is not a proven method and it is possible to lose some failure modes.
4. Non-Linear Strategy

A non-linear strategy has been developed to analyze, only the RVEs that are close to failure.

Advantage: It reduces enormously the computational cost compared to a FE\(^2\) method.

Drawback: It is still expensive, specially when failure occurs.
The NLS defined aims reducing the computational cost of analyzing a large structure, with a double scale homogenization method, taking into account material non-linearities.

This is achieved with two different procedures:

1. Definition of a **Non-Linear Activation Function (NLAF)**
2. Definition of a **Smart First Step (SFS)** algorithm

It is important to remark that NLS does not try to reduce the computational cost by extrapolating some non-linear results (as reduction models do). Instead, it is designed to solve the minimum number of RVEs (those that have a non-linear performance)
The objective of the NLAF is to have a threshold in the macro-model that tells when the micro-model will become non-linear. And, therefore, if it is necessary to calculate it.

NLAF must be calculated in the macro-model and must depend on damage activation of the micro-model.
The NLAF is defined using the elastic energy density of the material:

For each integration point, we can calculate:

\[ \Psi_e = \frac{1}{2} \sigma : \varepsilon \]

Each integration point is represented by an RVE, which has a maximum elastic energy density of: \( \Psi_e^{\text{Lim}} \)

The threshold function is defined as:

\[ \Psi_e - \Psi_e^{\text{Lim}} \leq 0 \]

In order to calculate the limit elastic energy density in the macro model, \( \Psi_e^{\text{Lim}} \), the following assumption is made:
The material becomes no-linear when the first material point of the RVE becomes non-linear.

For a given strain-stress state we can calculate, in the RVE, for each integration point \( (k) \):

\[
\Psi_{ek} = \frac{1}{2} \sigma_k : \varepsilon_k \\
\Psi_{eLim} = \frac{1}{2} \sigma_{Lim,k} : \varepsilon_{Lim,k}
\]

We can define a function \( f \) that relates how close is any integration point of the RVE to its elastic energy threshold:

\[
f_k = \frac{\Psi_{ek}}{\Psi_{eLim,k}} \quad \text{Extrapolation to macro-model} \quad f = \max\{f_k\}
\]

Therefore:

\[
\Psi_{eLim} = \frac{\Psi_e}{f}
\]

Non-Linear Strategy
The elastic energy density limit calculated defines the amount of energy in the material before its failure, for a given strain state.

If the strain state changes, the elastic energy density limit will also change.

It makes necessary to verify, at each load step, $\varepsilon_n \sim \varepsilon_0$, and recalculate $\psi^{Lim}_e$ if the proportionality is not verified.

**Result if proportionality is not verified**

**Result verifying proportionality**
The final flow diagram of the Non-Linear Activation Function is:

\[ \sigma_{ep} = \bar{C} : \bar{\varepsilon}_i \]
\[ \Psi^e_i = \frac{1}{2} \sigma_{ep} : \bar{\varepsilon}_i \]
\[ \bar{\varepsilon}_i \]
\[ mp = \text{mat. properties} \]
\[ iv = \text{internal variables} \]
\[ ep = \text{elastic predictor} \]
\[ i = \text{umpteenth step} \]

\[ \Psi^e_i - \Psi^e_{\text{Limit}} \leq 0 \]
\[ \Psi^e_{\text{Limit}} = \Psi^e_i \]

\[ \bar{\varepsilon}_{ref} : \bar{\varepsilon}_i \approx 1 \]
\[ \bar{\varepsilon}_i \]

\[ \bar{\varepsilon}_i \]
\[ \sigma_i : \bar{C}^T \]
\[ iv_i \]

Solve Micro

Exit

Solve Micro

Non-Linear Strategy
The proposed procedure requires analyzing the RVE of each integration point in the first load step, in order to calculate $\psi_{e Lim}$.

However, in many simulations, there are many strain-stress states that are proportional from the very beginning:

It is possible to define a *Smart First Step* that minimizes the number of RVEs that must be analyzed to obtain the elastic energy limit of all integration points.
The flow diagram of the Smart First Step is:

The flow diagram involves variables such as $\bar{e}_i$ and $\bar{\psi}_i$, with conditions and loops for $k=1$ to $k=tk$. The flowchart includes steps for solving, updating, and exiting the process. The variables and conditions are crucial for the Non-Linear Strategy.
1. Once an integration point becomes non-linear, it will remain non-linear. The RVE has to be solved at each load step from then on.

2. A material non-linear analysis requires a good approximation of the tangent stiffness tensor. In an homogenization procedure, this is calculated by numerical derivation. This requires analyzing the RVE 6 more times after convergence, with the consequent increase of computational cost.

Concluding: A non-linear analysis is expensive, independently of the strategy used.
Both materials are characterized with an explicit scalar damage model.

### Numerical examples

<table>
<thead>
<tr>
<th>Property</th>
<th>Grey mat.</th>
<th>Blue mat.</th>
</tr>
</thead>
<tbody>
<tr>
<td>E [GPa]</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>ν</td>
<td>0.15</td>
<td>0.15</td>
</tr>
<tr>
<td>σ\text{lim} [MPa]</td>
<td>102</td>
<td>100</td>
</tr>
<tr>
<td>Gf [kJ/m²]</td>
<td>10</td>
<td>10</td>
</tr>
</tbody>
</table>
Results obtained. Damage parameter
Force-Displacement graphs for the different models analyzed.

**Computational cost:**

If this simulation stops at $\text{Displ} = 0.08\text{mm}$, the speed ratio is 7.0

<table>
<thead>
<tr>
<th>Model</th>
<th>FE$^2$</th>
<th>NLS</th>
<th>Speed ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mesh1-Micro1</td>
<td>1h 21’ 53”</td>
<td>28’ 19”</td>
<td>2.89</td>
</tr>
<tr>
<td>Mesh1-Micro2</td>
<td>8h 41’ 19”</td>
<td>3h 10’ 44”</td>
<td>2.73</td>
</tr>
<tr>
<td>Mesh2-Micro1</td>
<td>11h 19’ 49”</td>
<td>2h 29’ 28”</td>
<td>4.55</td>
</tr>
<tr>
<td>Mesh2-Micro2</td>
<td>76h 40’ 33”</td>
<td>18h 39’ 33”</td>
<td>4.11</td>
</tr>
</tbody>
</table>
### NUMERICAL EXAMPLE – PLATE WITH A HOLE

Improvement of the computational cost thanks to the Smart First Step strategy

<table>
<thead>
<tr>
<th>Model</th>
<th>Without SFS</th>
<th>With SFS</th>
<th>Speed ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Time</td>
<td>RVE solved</td>
<td>Time</td>
</tr>
<tr>
<td>Mesh1-Micro1</td>
<td>18’’</td>
<td>2,880</td>
<td>1’’</td>
</tr>
<tr>
<td>Mesh1-Micro2</td>
<td>1’ 48’’</td>
<td>2,880</td>
<td>6’’</td>
</tr>
<tr>
<td>Mesh2-Micro1</td>
<td>2’ 12’’</td>
<td>23,040</td>
<td>3’’</td>
</tr>
<tr>
<td>Mesh2-Micro2</td>
<td>14’ 06’’</td>
<td>23,040</td>
<td>12’’</td>
</tr>
<tr>
<td>Material</td>
<td>Model</td>
<td>E [GPa]</td>
<td>v</td>
</tr>
<tr>
<td>------------------</td>
<td>---------</td>
<td>---------</td>
<td>-----</td>
</tr>
<tr>
<td>Fibre (Carbon)</td>
<td>Elastic</td>
<td>235</td>
<td>0.21</td>
</tr>
<tr>
<td>Matrix (Epoxy)</td>
<td>Damage</td>
<td>4.52</td>
<td>0.36</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>TenCate core</td>
<td>Elastic</td>
<td>56.1</td>
<td>55.6</td>
<td>4.5</td>
</tr>
</tbody>
</table>
NUMERICAL EXAMPLE – Industrial component

Results obtained. Damage parameter

Note: Damage parameter in the macro-model is calculated based on the lost of stiffness of the whole RVE, and not as the integral of the damage over the RVE volume.
Expected failure regions:
Higher value means lower elastic energy available.
Value equal to 1.0 means that all elastic energy has been consumed.

Computational cost:

<table>
<thead>
<tr>
<th>Model</th>
<th>FE²</th>
<th>NLS</th>
<th>Speed ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mesh1-Micro1</td>
<td>32d 14h 46’</td>
<td>11h 36’</td>
<td>67.4</td>
</tr>
</tbody>
</table>

98.5 % reduction of the computational cost!
This work presents a Non-Linear Strategy procedure that makes possible the analysis of structures using homogenization procedures.

The NLS is based on reducing the number of times in which the RVE has to be solved. In other words, in solving the RVE only when it is strictly necessary.

Validation examples have shown the excellent performance provided by the NLS, which in large problems can reduce the computational cost in a 98.5%.

These sort of strategies are a must in order to use homogenization procedures in non-linear analysis of structures.

**Conclusions**
Acknowledgements

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