Numerical computation of the macroscopic tangent stiffness obtained from a microstructure

1 Introduction

For a microstructure occupying the volume V, the stress tensor $\boldsymbol{\sigma}$ at the scale of the microstructure should satisfy the equilibrium in weak form:

$$\int_V \boldsymbol{\epsilon}(\boldsymbol{v}) : \boldsymbol{\sigma} \, \mathrm{d}V = \int_{\partial V} \boldsymbol{v} \cdot \boldsymbol{t} \, \mathrm{d}S \qquad \forall \boldsymbol{v} \tag{1}$$

where $\boldsymbol{t} = \boldsymbol{\sigma} \cdot \boldsymbol{n}$ is the stress vector at the boundary of V. Eq. (1) is also satisfied for a small variation of the stress which at a given state is linked to the variation of strain through a tangent stiffness tensor $\boldsymbol{C}$, $\delta\boldsymbol{\sigma} = \boldsymbol{C} : \boldsymbol{\epsilon}(\delta\boldsymbol{u})$, resulting in

$$\int_V \boldsymbol{\epsilon}(\boldsymbol{v}) : \delta\boldsymbol{\sigma} \, \mathrm{d}V = \int_{\partial V} \boldsymbol{v} \cdot \delta\boldsymbol{t} \, \mathrm{d}S \qquad \forall \boldsymbol{v} \tag{2}$$

Equation (2) with $\delta\boldsymbol{\sigma} = \boldsymbol{C} : \boldsymbol{\epsilon}(\delta\boldsymbol{u})$ is equivalent to

$$\int_V w(\boldsymbol{\epsilon}(\delta\boldsymbol{u})) \, \mathrm{d}V - \int_{\partial V} \delta\boldsymbol{u} \cdot \delta\boldsymbol{t} \, \mathrm{d}S \leq \int_V w(\boldsymbol{\epsilon}(\boldsymbol{v})) \, \mathrm{d}V - \int_{\partial V} \boldsymbol{v} \cdot \delta\boldsymbol{t} \, \mathrm{d}S \qquad \forall \boldsymbol{v} \tag{3}$$

where $w(\boldsymbol{\epsilon}) = \frac{1}{2}\boldsymbol{\epsilon} : \boldsymbol{C} : \boldsymbol{\epsilon}$.

2 Periodic boundary conditions

For periodic boundary conditions the displacement vector is linked to the macroscopic strain tensor $\boldsymbol{E}$. Any displacement field kinematically admissible with the periodic boundary conditions belongs to the set

$$\kappa(\boldsymbol{E}) = \{\boldsymbol{u} : \boldsymbol{u}(\boldsymbol{x}) = \boldsymbol{E} \cdot \boldsymbol{x} + \tilde{\boldsymbol{u}}(\boldsymbol{x}) \text{ with } \tilde{\boldsymbol{u}} \text{ periodic}\}$$

Since $\delta\boldsymbol{t}$ is anti-periodic we can show that

$$\int_V \boldsymbol{\epsilon}(\boldsymbol{v}) : \delta\boldsymbol{\sigma} \, \mathrm{d}V = \int_{\partial V} \boldsymbol{v} \cdot \delta\boldsymbol{t} \, \mathrm{d}S = \boldsymbol{E} \int_V \delta\boldsymbol{\sigma} \, \mathrm{d}V \qquad \forall \boldsymbol{v} \in \kappa(\boldsymbol{E}) \tag{4}$$

Since $\delta\boldsymbol{u} \in \kappa(\delta\boldsymbol{E})$, we have

$$\int_{\partial V} \delta\boldsymbol{u} \cdot \delta\boldsymbol{t} \, \mathrm{d}S = \int_{\partial V} \boldsymbol{v} \cdot \delta\boldsymbol{t} \, \mathrm{d}S \qquad \forall \boldsymbol{v} \in \kappa(\delta\boldsymbol{E}) \tag{5}$$

and therefore from (3)

$$\int_V w(\boldsymbol{\epsilon}(\delta\boldsymbol{u})) \, \mathrm{d}V \leq \int_V w(\boldsymbol{\epsilon}(\boldsymbol{v})) \, \mathrm{d}V \qquad \forall \boldsymbol{v} \in \kappa(\delta\boldsymbol{E}) \tag{6}$$

The solution then minimizes w:

$$< w(\boldsymbol{\epsilon}(\delta \boldsymbol{u})) >= \min_{\boldsymbol{v}\in\kappa(\delta \boldsymbol{E})} < w(\boldsymbol{\epsilon}(\boldsymbol{v})) > \tag{7}$$

The minization can also be formulated by a minization with constraint

$$< w(\boldsymbol{\epsilon}(\delta \boldsymbol{u})) >= \min_{\boldsymbol{e},\boldsymbol{v}\text{ periodic}} < w(\boldsymbol{e}) > \quad \text{subject to} \quad \delta\boldsymbol{E} + \boldsymbol{\epsilon}(\boldsymbol{v}) - \boldsymbol{e} = 0 \tag{8}$$

Introduce the lagrangian

$$\mathcal{L}(\boldsymbol{e},\boldsymbol{v},\boldsymbol{\lambda};\delta\boldsymbol{E}) =< w(\boldsymbol{e}) > + < \boldsymbol{\lambda}(\delta\boldsymbol{E} + \boldsymbol{\epsilon}(\boldsymbol{v}) - \boldsymbol{e}) > \tag{9}$$

The solution turns into finding the stationay point of $\mathcal{L}$ on the set of $(\boldsymbol{e},\boldsymbol{v}$ periodic$,\boldsymbol{\lambda})$

$$\mathcal{L}(\boldsymbol{e}^\star,\boldsymbol{v}^\star,\boldsymbol{\lambda}^\star;\delta\boldsymbol{E}) =< w(\boldsymbol{e}^\star) >= \underset{\boldsymbol{e},\boldsymbol{v}\text{ periodic},\boldsymbol{\lambda}}{\text{stationary point of}}\ \mathcal{L}(\boldsymbol{e},\boldsymbol{v},\boldsymbol{\lambda};\delta\boldsymbol{E}) \tag{10}$$

with $\boldsymbol{\epsilon}(\delta\boldsymbol{u}) = \boldsymbol{e}^\star$, $\delta\boldsymbol{u}(\boldsymbol{x}) = \delta\boldsymbol{E}\cdot\boldsymbol{x} + \boldsymbol{v}^\star(\boldsymbol{x})$ and $\delta\boldsymbol{\sigma} = \boldsymbol{\lambda}^\star$. Due to the linearity of the problem $\boldsymbol{\epsilon}(\delta\boldsymbol{u}(\boldsymbol{x})) = \boldsymbol{A}(\boldsymbol{x}) : \delta\boldsymbol{E}$ and thus

$$\mathcal{L}(\boldsymbol{e}^\star,\boldsymbol{v}^\star,\boldsymbol{\lambda}^\star;\delta\boldsymbol{E}) =< w(\boldsymbol{e}^\star) >= \frac{1}{2}\ \delta\boldsymbol{E} :< {}^t\boldsymbol{A} : \boldsymbol{C} : \boldsymbol{A} >: \delta\boldsymbol{E} \tag{11}$$

The tensor $\boldsymbol{C}^{\text{hom}} =< {}^t\boldsymbol{A} : \boldsymbol{C} : \boldsymbol{A} >$ is the homogenized tangent stiffness tensor. It is also given by $\boldsymbol{C}^{\text{hom}} =< \boldsymbol{C} : \boldsymbol{A} >$ through the identity

$$< \boldsymbol{\epsilon}(\boldsymbol{v}) : \delta\boldsymbol{\sigma} >= \boldsymbol{E} :< \delta\boldsymbol{\sigma} > \quad \forall \boldsymbol{v} \in \kappa(\boldsymbol{E}) \tag{12}$$

Therefore it can be shown that

$$\boldsymbol{C}^{\text{hom}} =< \boldsymbol{C} > - < ({}^t\boldsymbol{A} - \mathbf{1}) : \boldsymbol{C} : (\boldsymbol{A} - \mathbf{1}) > \tag{13}$$

3 FE discretization

After a FE discretization (2) turns into:

$$\mathbf{v}\mathbf{K}\delta\mathbf{u} = \mathbf{v}\delta\mathbf{f} \qquad \forall \mathbf{v} \tag{14}$$

where $\delta\mathbf{u}$ and $\mathbf{v}$ are nodal displacement vectors and $\mathbf{K}$ the tangent FE matrix.

For the matrix column $\tilde{\mathbf{u}}$ associated to the periodic displacement field $\tilde{\boldsymbol{u}}(\boldsymbol{x})$, there is a $n \times m$ matrix $\mathbf{P}$ (n = nb of dof, m = nb of relationships between displacement components) so that

$$\mathbf{P}\tilde{\mathbf{u}} = 0 \tag{15}$$

The traction field $\delta\boldsymbol{t}(\boldsymbol{x})$ being anti-periodic, we have

$$\tilde{\mathbf{v}}\mathbf{K}\delta\mathbf{u} = 0 \qquad \forall\tilde{\mathbf{v}} : \mathbf{P}\tilde{\mathbf{v}} = 0 \tag{16}$$

Hence there are m Lagrange multipliers or a m-components vector λ

$$\mathbf{K}\delta\mathbf{u} = {}^t\mathbf{P}\lambda \tag{17}$$
$$\mathbf{P}\delta\mathbf{u} = \mathbf{P}(\delta\boldsymbol{E}\cdot\mathbf{x}) \tag{18}$$

where $\delta\boldsymbol{E}\cdot\mathbf{x}$ is the matrix column formed with the displacement field obtained from the homogeneous deformation gradient $\delta\boldsymbol{E}\cdot\boldsymbol{x}$ so that $\delta\mathbf{u} = \delta\boldsymbol{E}\cdot\mathbf{x} + \tilde{\mathbf{u}}$.

The number of the reduced unknowns is $n-m$. We note $\tilde{\mathbf{u}}_r$ the reduced unknown vector and there is a $(n-m)\times n$ matrix $\mathbf{B}$:

$$\tilde{\mathbf{u}} = \mathbf{B}\tilde{\mathbf{u}}_r \tag{19}$$

resulting in

$$\mathbf{P}\mathbf{B} = 0 \tag{20}$$

From the above equations

$$\mathbf{K}_r\tilde{\mathbf{u}}_r = \mathbf{f}_r = -{}^t\mathbf{B}\mathbf{K}(\delta\boldsymbol{E}\cdot\mathbf{x}) \tag{21}$$

with $\mathbf{K}_r = {}^t\mathbf{B}\mathbf{K}\mathbf{B}$. The homogenized tangent stiffness tensor $\boldsymbol{C}^{\text{hom}}$ can be identified through the equivalence of the work forms

$$V\delta\boldsymbol{E} : \boldsymbol{C}^{\text{hom}} : \delta\boldsymbol{E}' = \delta\mathbf{u}\mathbf{K}\delta\mathbf{u}' \tag{22}$$

where $\delta\mathbf{u}$ (resp. $\delta\mathbf{u}'$) is the solution asssociated with $\delta\boldsymbol{E}$ (resp. $\delta\boldsymbol{E}'$), so

$$V\delta\boldsymbol{E} : \boldsymbol{C}^{\text{hom}} : \delta\boldsymbol{E}' = (\delta\boldsymbol{E}\cdot\mathbf{x})\mathbf{K}(\delta\boldsymbol{E}'\cdot\mathbf{x}) - \tilde{\mathbf{u}}_r\mathbf{f}'_r \tag{23}$$

which is the discretized form of (13). If $\mathbf{K}$ is symmetric we can ensure the symmetry of $\boldsymbol{C}^{\text{hom}}$ as follows:

$$V\delta\boldsymbol{E} : \boldsymbol{C}^{\text{hom}} : \delta\boldsymbol{E}' = (\delta\boldsymbol{E}\cdot\mathbf{x})\mathbf{K}(\delta\boldsymbol{E}'\cdot\mathbf{x}) - \frac{1}{2}\left(\tilde{\mathbf{u}}_r\mathbf{f}'_r + \tilde{\mathbf{u}}'_r\mathbf{f}_r\right) \tag{24}$$

The computation of $\boldsymbol{C}^{\text{hom}}$ can be performed by the successive use of Eqs (21) and (23 or 24). Indeed during the iterative process of the FE method, at each iteration the matrices $\mathbf{K}_r$ and $\mathbf{K}$ are built and linear sets of equations with left hand sides similar to that of (21) are solved. Then Eq (21) can be solved for $\tilde{\mathbf{u}}_r$ six times with right hand side obtained by setting $\delta\boldsymbol{E} = 1/2(\boldsymbol{e}_k\otimes\boldsymbol{e}_l + \boldsymbol{e}_l\otimes\boldsymbol{e}_k)$. So six resolutions should be performed. Eq (23 or 24) is then used to calculate the corresponding components of $\boldsymbol{C}^{\text{hom}}$.