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A dissipation-based control method for the multi-scale modelling of quasi-brittle materials

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Abstract

Multi-scale models based on computational homogenisation are nowadays developed for the simulation of complex material behaviour. The use of homogenisation techniques on finite-sized representative volume elements in the presence of quasi-brittle damage may lead to the presence of snap-backs in the macroscopic material response. A methodology to simulate this type of response in the multi-scale technique is proposed, based on the control of the dissipation at the mesoscopic scale. ***To cite this article: T.J. Massart et al., C. R. Mecanique 333 (2005).***

Résumé

Une méthode de contrôle basée sur la dissipation pour la modélisation multi-échelles des matériaux quasi-fragiles. Des schémas multi-échelles basés sur des principes d'homogénéisation numériques sont actuellement développés pour la simulation de comportements matériels complexes. L'utilisation de techniques d'homogénéisation sur des éléments de volume représentatifs de tailles finies en présence d'endommagement quasi-fragile peut causer l'apparition d'effets de snap-back dans la réponse matérielle macroscopique. Une méthode est proposée permettant d'introduire ce type de réponse dans un schéma multi-échelles, basée sur le contrôle de la dissipation à l'échelle mésoscopique. ***Pour citer cet article : T.J. Massart et al., C. R. Mecanique 333 (2005).***

Keywords: Computational solid mechanics; Multi-scale modelling; Localisation; Snap-back; Path following method; Dissipation control

Mots-clés : Mécanique des solides numérique ; Modélisation multi-échelles ; Localisation ; Snap-back ; Méthode de continuation ; Contrôle par dissipation

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Cette Note traite de l'application des schémas multi-échelles numériques dans le calcul de la réponse quasi-statique des matériaux composites quasi-fragiles. Ce type de méthode est basé sur l'extraction de la réponse macroscopique du matériau sur la base du calcul de la réponse d'un élément de volume représentatif (EVR) de taille finie au moyen de relations de transitions d'échelles ([1,2], relations (1)–(3)). Dans les schémas multi-échelles classiques, la réponse de cet EVR est obtenue via un contrôle en déformation macroscopique (Fig. 1). La présence de phases quasi-fragiles dans l'EVR, couplée aux faibles tailles des zones d'endommagement par rapport aux dimensions de l'EVR (fissuration) peut causer l'apparition de points limites de contrôle en déformations (snap-back) dans la réponse matérielle macroscopique. Afin d'introduire une telle réponse dans un schéma multi-échelles, il est nécessaire d'imposer la poursuite de la dissipation dans l'EVR, le contrôle de l'EVR ne pouvant plus se faire uniquement via la déformation macroscopique. Pour ce faire, cet article propose un moyen de compléter les relations de transitions d'échelles afin de contrôler la dissipation au sein de l'EVR, en transférant une variable mésoscopique contrôlant la dissipation vers l'échelle macroscopique (Section 3.1). Cette méthodologie est précisée pour le cas d'un modèle mésoscopique d'endommagement à gradient implicite en détaillant les transitions d'échelles correspondantes (relations (4)–(8)), et est illustrée par le calcul de la réponse d'un EVR de maçonnerie.

1. Multi-scale modelling based on computational homogenisation

To avoid the difficulty of defining reliable constitutive models for complex multi-phase materials, multi-scale computational approaches are nowadays developed, in which two or more scales of representation are coupled in structural (quasi-static) computations [1]. Effects which emerge from the material structure, such as damage-induced anisotropy, are then captured naturally. The first-order multi-scale approach homogenises the lower scale detailed description (here denoted 'mesoscopic') towards a classical stress-strain response using a Representative Volume Element (RVE) of the heterogeneous material [1]. In the framework of an infinitesimal strain description, a macroscopic strain $\mathbf{E}$ is obtained at each iteration of a non-linear macroscopic computation for all macroscopic Gauss points. The solution procedure then requires the macroscopic stress tensor $\boldsymbol{\Sigma}$ associated to the strain $\mathbf{E}$. Instead of using a closed-form constitutive relation for this purpose, $\mathbf{E}$ is applied in an average sense to a RVE. A boundary value problem (BVP) is constructed on the RVE, with boundary conditions defined such that the volume average of the mesoscopic strain on the RVE equals the imposed macroscopic strain. A mesoscopic displacement field of the form

$$\vec{u} = \mathbf{E} \cdot \vec{x} + \vec{w} \tag{1}$$

is assumed in each point of the mesostructure, where $\vec{x}$ is the position vector within the RVE, and $\vec{w}$ is a mesoscopic displacement fluctuation field accounting for the heterogeneity of the material. A periodic fluctuation is classically assumed to impose that the average of the mesoscopic strain is the imposed macroscopic strain [2]. Using this periodicity assumption, the macroscopic kinematic quantities are imposed on the RVE through displacements imposed on three control points, as indicated in Fig. 1 for the case of periodic masonry. The response of the RVE is obtained as the solution of this strain-controlled BVP. As a result of periodicity and assuming equivalence of the variations of macroscopic and mesoscopic work for any strain variation, the macroscopic stress $\boldsymbol{\Sigma}$ is obtained as the average of the mesoscopic stress field and is computed from the forces acting on the control points [2]

$$\boldsymbol{\Sigma} = \frac{1}{V_{\mathrm{RVE}}} \int_{V_{\mathrm{RVE}}} \boldsymbol{\sigma} \, \mathrm{d}V_{\mathrm{RVE}} = \frac{1}{V_{\mathrm{RVE}}} \sum_{i=1}^{3} \vec{x}^{(i)} \otimes \vec{f}^{(i)} \tag{2}$$

where $\vec{f}^{(i)}$ is the external force applied to controlling point (i) as obtained by static condensation towards the controlling degrees of freedom, $\vec{x}^{(i)}$ is its position, and $\otimes$ denotes an outer (dyadic) product. The scale transition

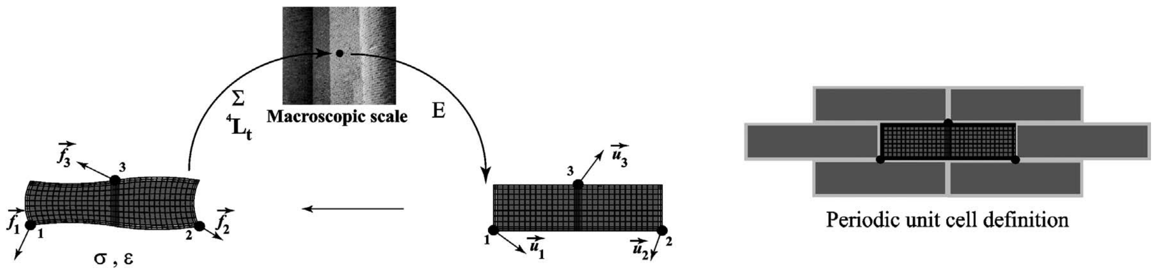

Fig. 1. Principle of first-order multi-scale solution scheme illustrated for a periodic masonry RVE.

Fig. 1. Principe d'un schéma multi-échelles au premier ordre illustré pour un EVR de maçonnerie.

also permits to extract the homogenised constitutive tangent from the condensation of the mesostructural tangent stiffness [2]

$$\delta\boldsymbol{\Sigma} = {}^4\mathbf{L} : \delta\mathbf{E} = \left(\sum_{n=1}^{3} \sum_{p=1}^{3} \vec{x}^{(n)} \otimes \mathbf{K}_M^{(np)} \otimes \vec{x}^{(p)} \right) : \delta\mathbf{E} \tag{3}$$

The scale transition procedure attributes a stress-strain response extracted from a finite mesoscopic volume to a macroscopic material point, which restricts its application to cases in which a sufficient separation exists between the structural and mesoscopic spatial scales. Any type of model can be used for the constituents in the RVE. For masonry, the quasi-brittle nature of the constituents requires some crack modelling strategy such as softening cohesive laws or softening continuum laws with non-locality.

2. Mesostructural snap-back caused by mesoscopic damage localisation

Snap-back is a structural phenomenon appearing in quasi-static loading conditions which results from the localisation of dissipation in zones which are thin with respect to the structural size. It occurs whenever an elastic zone releases more elastically stored energy than the energy consumed by the dissipating phase. In quasi-static computations (as performed in the above-mentioned nested scheme), the conventional load control or displacement control procedures fail when applied to a snap-back response. A general class of advanced path following techniques has been proposed in [3] to trace such equilibrium paths computationally. A monotonically increasing quantity is used to control the computation. For problems involving localisation, variables related directly to the damage process zone have been shown to perform better than global variables [4]. Since in the multi-scale scheme the macroscopic material point response is obtained from a mesostructural computation on a finite volume, this behaviour may also show snap-back, particularly if quasi-brittle materials are considered and dissipation tends to localise in the weaker constituents. A typical material exhibiting such effects is masonry, with damage concentrating in the relatively thin mortar joints. Classical non-linear displacement-based finite element procedures used at the macroscopic scale assume that for a given strain a resulting stress can always be determined. The existence of a solution of the mesostructural boundary value problem is thus assumed in the multi-scale scheme. This may not be true for macroscopic strains beyond a snap-back point in the homogenised response, at which the entire multi-scale computation will thus fail.

3. A dissipation control method for mesostructural snap-back handling

3.1. Principle of dissipation control for RVE snap-back

To follow the mesostructural snap-back path in the multi-scale scheme, the macroscopic solution procedure should predict a decreasing macroscopic strain as from the start of the snap-back regime for a solution to the mesostructural problem to exist. The selection of an elastic unloading path should also be prevented. Therefore, along with a decreasing macroscopic strain increment, the scale transition should apply an additional constraint which guarantees dissipation inside the RVE by selecting the corresponding tangent stiffness within the solution procedure at the mesoscopic level. The RVE may be forced to follow a dissipative path if the growth of a properly selected mesoscopic quantity is imposed by the macroscopic solution procedure. The choice of the quantity which allows to enforce dissipation is similar to that used in advanced path following techniques, i.e. a mesoscopic variable related to the damage process zone. This quantity, which is denoted here as α, will be chosen according to the mesoscopic crack modelling strategy. A relative displacement may be chosen if a cohesive zone strategy is used [5], or an independent non-local strain degree of freedom if an implicit gradient framework is used [6]. This mesoscopic quantity α has to be transferred to the macroscopic scale together with a conjugate equation.

The prescription by the macro-scale problem of a value for α gives rise to a conjugate reaction 'force'. In the classical multi-scale framework the prescription of an overall strain increment $\Delta\mathbf{E}$ on the RVE is achieved through six controlling displacement increments $\{\Delta u_M\}$. External reaction forces $\{f_M\}$ conjugate to these displacements are used to compute the macroscopic stress. Similarly, the simultaneous prescription of a mesoscopic quantity $\Delta\alpha$ controlling the mesoscopic dissipation will lead to the appearance of a conjugate 'reaction' or residual f_α, as illustrated in Fig. 2. This residual is the generalised 'reaction' that should be applied externally to the RVE in order to obtain the prescribed value of the increment $\Delta\alpha$, if the associated dissipation is not in equilibrium with the imposed $\{\Delta u_M\}$. This out-of-equilibrium quantity only vanishes if the imposed $\Delta\alpha$ takes the value that corresponds to the dissipating solution in which only the overall strain $\Delta\mathbf{E}$ would be prescribed, hence the term 'residual'. In order to obtain the desired solution, the $\Delta\alpha$ imposed by the macroscopic scale must converge to the value for which $f_\alpha = 0$ along the macroscopic iterations. This equation must be taken from the meso-problem and added to the macroscopic set of equations to obtain the proper correction of $\Delta\alpha$ during the macroscopic iteration process.

Within this enhanced control approach, a converged solution of the RVE problem is still required at each macroscopic iteration, similarly to the original scheme. The key difference is that the prescription of the increment of the mesoscopic quantity α modifies these intermediate RVE configurations. Hence, at each macroscopic iteration, a particular configuration of the RVE, compatible with this prescribed quantity $\Delta\alpha$, is found. Along the macroscopic iterations, the incorporation of the equation $f_\alpha = 0$ forces the configuration of the RVE towards the one with no external prescription of the mesoscopic quantity α. This strategy allows to pass strain control limit points of the homogenised stress-strain behaviour, and, since it selects the corresponding tangent stiffness, to follow the snap-back dissipative solution.

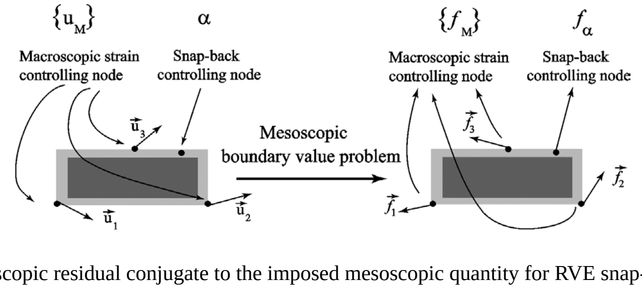

Fig. 2. Mesoscopic residual conjugate to the imposed mesoscopic quantity for RVE snap-back control.

Fig. 2. Apparition d'un résidu conjugué à l'imposition d'une quantité pour le contrôle d'un snap-back de l'EVR par dissipation.

Practically, the residual f_α is obtained directly by condensation of the meso-structural system of equations towards the degrees of freedom used in the macroscopic solution procedure, i.e. $\{u_M\}$ and α. Note that a proper selection procedure must also identify which dissipating quantity α of the RVE to transfer to the macroscopic scale at a given stage of the computation. This selection should evolve as a result of the mesoscopic cracking evolution. At each step, the quantity corresponding to the largest incremental dissipation is selected to control the dissipation in the subsequent increment.

3.2. A dissipation-driven scale transition for a mesoscopic implicit gradient damage model

The dissipation-driven scale transition is now further elaborated for the case of a mesoscopic non-local model [6]. This framework introduces non-locality by use of an averaging field equation, in addition to the equilibrium equation, which requires the discretisation of an independent non-local equivalent strain field $\bar{\varepsilon}$. This field in turn drives damage evolution. The presence of an independent field eases the extraction of the mesoscopic quantity controlling dissipation. The macroscopic tangent operator now consists of four tensors relating variations of the stress $\boldsymbol{\Sigma}$ and the non-local residual $f_{\bar{\varepsilon}}$ to variations of the macroscopic strain $\mathbf{E}$ and of the mesoscopic non-local equivalent strain variable $\bar{\varepsilon}$ controlling dissipation:

$$\delta\boldsymbol{\Sigma} = {}^4\mathbf{C}_M^{uu} : \delta\mathbf{E} + {}^2\mathbf{C}_M^{ue}\delta\bar{\varepsilon}, \qquad \delta f_{\bar{\varepsilon}} = {}^2\mathbf{C}_M^{eu} : \delta\mathbf{E} + \mathrm{C}_M^{ee}\delta\bar{\varepsilon} \tag{4}$$

These tensors ${}^4\mathbf{C}_M^{uu}$, ${}^2\mathbf{C}_M^{ue}$, ${}^2\mathbf{C}_M^{eu}$ and C_M^{ee} can be retrieved from the condensation of the discretized system of equations of the RVE:

$$\left[\mathbf{K}_M^{uu}\right]\{\delta u_M\} + \left\{\mathbf{K}_M^{ue}\right\}\delta\bar{\varepsilon} = \{\delta f_M\}, \qquad \left\langle\mathbf{K}_M^{eu}\right\rangle\{\delta u_M\} + \mathrm{K}_M^{ee}\delta\bar{\varepsilon} = \delta f_{\bar{\varepsilon}} \tag{5}$$

where the matrices $[\mathbf{K}_M^{uu}]$ and $\{\mathbf{K}_M^{ue}\}$ couple external force variations to the displacement variations at the three control points and to the variation of the selected non-local degree of freedom. The line matrix $\langle\mathbf{K}_M^{eu}\rangle$ and the scalar K_M^{ee} link the non-local residual variation to the control displacements variations and to the mesoscopic non-local degree of freedom variation. Relations (5) may be re-written in a tensor-vector format by separating the contribution of each control point:

$$\delta\vec{f}^{(n)} = \sum_{p=1}^{3}\mathbf{K}_M^{uu(np)}\cdot\delta\vec{u}_M^{(p)} + \vec{\mathbf{K}}_M^{ue(n)}\delta\bar{\varepsilon}, \quad n=1,2,3, \qquad \delta f_{\bar{\varepsilon}} = \sum_{p=1}^{3}\vec{\mathbf{K}}_M^{eu(p)}\cdot\delta\vec{u}_M^{(p)} + \mathrm{K}_M^{ee}\delta\bar{\varepsilon} \tag{6}$$

where $\mathbf{K}_M^{uu(np)}$ is a second-order tensor extracted from matrix $[\mathbf{K}_M^{uu}]$ relating the variation of the displacement of control point (p) to the external force variation at control point (n). The vector $\vec{\mathbf{K}}_M^{ue(n)}$ which relates the external force variation at control point (n) to the variation of the selected non-local degree of freedom is extracted from the column matrix $\{\mathbf{K}_M^{ue}\}$. Using (2), the variation of stress is related to the variation of the external forces applied to the control points. By accounting for (6), noting that $\delta\vec{u}^{(p)} = \vec{x}^{(p)}\cdot\vec{\nabla}_M\delta\vec{u}$ and accounting for the symmetry of the infinitesimal strain tensor, we have

$$\delta\boldsymbol{\Sigma} = \underbrace{\frac{1}{V_{\mathrm{RVE}}}\left(\sum_{n=1}^{3}\sum_{p=1}^{3}\vec{x}^{(n)}\otimes\mathbf{K}_M^{uu(np)}\otimes\vec{x}^{(p)}\right)}_{{}^4\mathbf{C}_M^{uu}} : \delta\mathbf{E} + \underbrace{\frac{1}{V_{\mathrm{RVE}}}\left(\sum_{n=1}^{3}\vec{x}^{(n)}\otimes\vec{\mathbf{K}}_M^{ue(n)}\right)}_{{}^2\mathbf{C}_M^{ue}}\delta\bar{\varepsilon} \tag{7}$$

A similar development may be performed for the variation of the non-local residual conjugate to the mesoscopic non-local strain degree of freedom, yielding

$$\delta f_{\bar{\varepsilon}} = \underbrace{\frac{1}{V_{\mathrm{RVE}}}\left(\sum_{p=1}^{3}\vec{\mathbf{K}}_M^{eu(p)}\otimes\vec{x}^{(p)}\right)}_{{}^2\mathbf{C}_M^{eu}} : \delta\mathbf{E} + \underbrace{(\vec{\mathrm{K}}_M^{ee})}_{\mathrm{C}_M^{ee}}\delta\bar{\varepsilon} \tag{8}$$

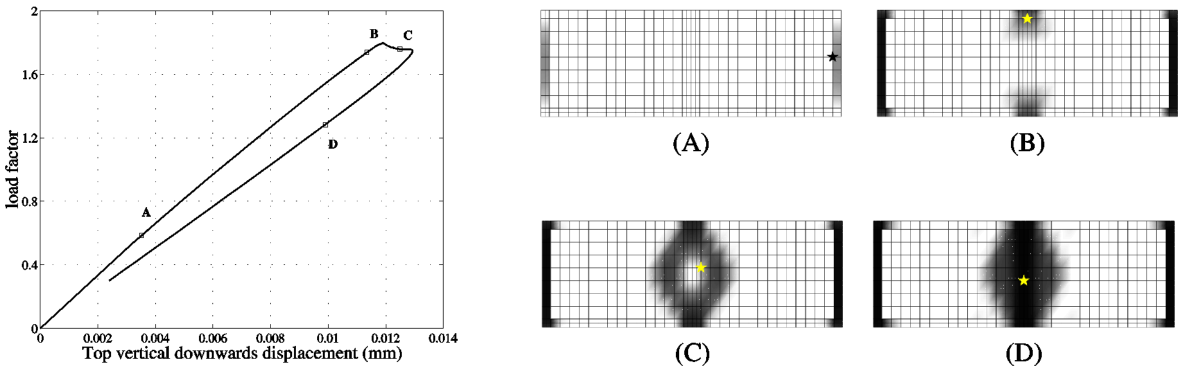

Fig. 3. Load-displacement curve with snap-back obtained by the multi-scale modelling for homogeneous macroscopic tension–compression loading with related damage distributions.

Fig. 3. Réponse avec snap-back obtenue par traitement multi-échelles pour un chargement homogène biaxial de tension–compression.

4. A numerical example

The use of the dissipation-driven multi-scale framework is illustrated here for a mesostructural RVE snap-back for the case of running bond masonry. The macroscopic 'structure' consists of a single finite element under homogeneous macroscopic loading. Horizontal tension is combined with vertical compression along the proportional stress path $(\Sigma_{xx}, \Sigma_{yy}, \Sigma_{xy}) = (0.2, -1, 0)$. The macroscopic response is assumed to remain homogeneous and as masonry is initially periodic, a single period RVE (unit cell) is considered [7]. Damage criteria and material properties used for the brick and mortar joints may be found in [7]. Since the macroscopic response is homogeneous, the RVE response is the only possible cause of snap-back in the homogenised material response. It is dealt with by using the proposed dissipation control strategy. The load factor evolution is represented in Fig. 3 as a function of the top vertical displacement of the structure, which is a direct measure of the macroscopic vertical strain. The damage distribution in the RVE is depicted at different stages of the computation identified by capital letters. The evolving mesoscopic non-local quantity selected for the snap-back control is identified by a star in the damage distributions. These selected quantities are related to the highest incremental damage growth. This figure shows that the enhanced scheme allows to pass the strain control limit point in the homogenised stress-strain response.

5. Closure

The methodology presented in this paper enhances the scale transition used in the classical multi-scale scheme based on computational homogenisation. It allows to account for the finite size of RVE in computations involving quasi-brittle failure, potentially resulting in snap-back effects in the RVE response and in the homogenised stress-strain response. The principle of the method implemented here for an implicit gradient description at the mesoscopic scale may be extended to other types of mesoscopic failure laws, e.g. cohesive laws. Subsequent developments are needed in order to deal with macroscopic localisation.

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References

[1] R.J.M. Smit, Toughness of heterogeneous polymeric systems. A modeling approach, PhD thesis, Eindhoven University of Technology, 1998.
[2] V.G. Kouznetsova, W.A.M. Brekelmans, F.T.P. Baaijens, An approach to micro-macro modeling of heterogeneous materials, Comput. Mech. 27 (2001) 37–48.
[3] M.G.D. Geers, Enhanced solution control for physically and geometrically non-linear problems. Part I – The subplane control approach, Int. J. Numer. Methods Engrg. 46 (1999) 177–204.
[4] R. de Borst, Computation of post-bifurcation and post-failure behavior of strain-softening solids, Comput. & Structures 25 (2) (1987) 211–224.
[5] P.B. Lourenço, Computational strategies for masonry structures, PhD thesis, Delft University of Technology, 1996.
[6] R.H.J. Peerlings, R. de Borst, W.A.M. Brekelmans, J.H.P. de Vree, Gradient-enhanced damage for quasi-brittle materials, Int. J. Numer. Methods Engrg. 39 (1996) 3391–3403.
[7] T.J. Massart, Multi-scale modeling of damage in masonry structures, PhD thesis, Eindhoven University of Technology & Université Libre de Bruxelles, 2003.