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Assessment of periodic homogenisation-based multiscale computational schemes for quasi-brittle structural failure

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Abstract

New methods for the modelling of structural failure by means of multiscale approaches were recently proposed, in which the structural description involves coarse scale discontinuities, the behaviour of which is fed by Representative Volume Element (RVE) computations. Their main asset consists in identifying the material response from fine scale material parameters and computations, including the failure behaviour of the material. One of the distinctions between the available approaches relates to the boundary conditions applied on the RVE. The methods based on classical computational homogenisation usually make use of periodic boundary conditions. This assumption remains a priori debatable for the localised behaviour of quasi-brittle materials. For the particular case of periodic materials (masonry), the level of approximation induced by the periodic assumption is here scrutinised. A new displacement discontinuity-enhanced scale transition is therefore outlined based on energetic consistency requirements. The corresponding multiscale framework results are compared with complete fine scale modelling results used as a reference, showing a good agreement in terms of limit load, and in failure mechanisms at both the fine scale and at the overall structural level.

Key words: Structural analysis, Multiscale discontinuities, Periodic homogenisation, Failure, Fine scale comparison

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1 Introduction

The formulation of macroscopic constitutive laws for the behaviour of damaging quasi-brittle materials is a difficult task. Complex closed-form constitutive laws formats are needed to account for effects such as damage-induced anisotropy. In addition, evolution laws have to be used for the additional parameters entering such equations, which leads to cumbersome and costly experimental identification procedures, especially when initial anisotropy is considered. The masonry material poses all of these challenges simultaneously, due to its strongly heterogeneous microstructure which considerably influences its overall mechanical behaviour.

The focus will here be set on structural computations for masonry structures. In this context, the formulation of closed-form constitutive laws has been pursued in the last decade, see for instance Lourenço et al. (1997a); Berto et al. (2002) for examples of two-dimensional developments. To complement general closed-form constitutive equations, multi-scale techniques have been proposed and applied to non-linear mechanical behaviour with different purposes (material identification vs. structural computations), as well as different range of applicability (periodic or non-periodic materials, quasi-brittle vs. ductile materials). Restricting the overview on textured quasi-brittle materials such as masonry, different approaches were presented recently. A first class of frameworks bears similarities to domain decomposition methods, rather than up-scaling fine scale material behaviour towards coarser scale material response, Brasile et al. (2007a,b); Ibrahimbegovic and Markovic (2003); Markovic and Ibrahimbegovic (2004). In these methods, the structure is decomposed in non-overlapping subdomains. The equilibrium equations are solved on the structure using this domain decomposition, together with compatibility conditions at the interfaces between them. Such an approach allows to incorporate non-linear behaviour features in the computations up to failure. It does not rely on other a priori assumptions, while keeping a significant but distributed computational effort, mainly prescribed by the level of details associated to the chosen microstructural modelling strategy. Another class of frameworks is based on the identification of average (coarse scale) material behaviour features by means of representative volume element (RVE) or unit cell computations. A nested multi-scale computational strategy, known as FE², was proposed in Feyel and Chaboche (2000), Smit et al. (1998), Kouznetsova et al. (2001); and applied to the mechanical behaviour of metallic and polymeric materials, and was later extended to other physical phenomena, Ozdemir et al. (2008a,b). The coarse scale material behaviour of a classical continuum description is then sampled at each quadrature points by using an auxiliary fine scale boundary value problem based on periodic homogenisation averaging principles. This allows to derive numerically the average stress and tangent stiffness for an applied average strain. The applicability of such an approach
is restricted to situations in which the principle of scale separation applies between the fine and coarse descriptions. The computational effort therefore remains important, but substantially decreases with respect to a full fine scale modelling of structures.

A simplified adaptation to cracking in quasi-brittle materials was first proposed in Luciano and Sacco (1997, 1998) with off-line periodic homogenisation, but without structural scale localisation treatment. Two different strategies were proposed recently to tackle damage localisation at the coarse scale by introducing displacement or strain discontinuities in multiscale methods. A first approach consists in feeding the behaviour of coarse scale equivalent displacement discontinuities with information extracted from the aggregation of all fine scale material instabilities present in a unit cell, in the spirit of Belytschko et al. (2008). Another methodology making use of the initially periodic microstructure of masonry is explicitly based on periodic homogenisation of unit cells and based on embedded strain discontinuities, as in Massart et al. (2007). However, periodicity is an assumption which remains strongly debatable in the localised cracking regime, since the principle of scales separation does not apply in that case. Yet, for the initially periodic masonry material, with failure modes clearly dominated by its periodic microstructure, the degree of approximation involved by the local periodicity assumption remains untested, and will be challenged here.

The main objective of this contribution is to analyse the effect of this periodicity assumption. This will be achieved by comparing the results obtained from a homogenisation-based multiscale computation on a confined shear wall test with the results of a full fine scale model based on the same material parameters value, and taken as a reference result. In order to make this comparison possible, an improvement of the framework proposed in Massart et al. (2007) will be presented. The coarse (structural) scale localisation will therefore be described by the introduction of strong discontinuities in the kinematical description in the spirit of Armero (1999). Secondly, a cohesive law-based model will be used at the fine scale in order to improve the efficiency of the computations, and allow a complete fine scale modelling of the confined shearing test.

The paper is structured as follows. A simple scalar damage model with interface elements used for the mortar joints at the fine scale is formulated in Section 2. The essential ingredients of a localisation-enhanced multiscale scheme for failure of periodic quasi-brittle materials are presented in Section 3. The details of the upscaling towards a coarse scale displacement discontinuity are presented in this section with a special emphasis on the aspects differing from Massart et al. (2007), and on the energy consistency argument. The results obtained from this multiscale framework for a confined shearing test are discussed and compared with those of a complete fine scale model in
Finally, the conclusions and prospects are given in Section 5.

2 Simplified fine scale constitutive setting for masonry

Since the aim is to compare multiscale modelling results with a full fine scale representation containing all the heterogeneities of the mesostructure, the same fine scale constitutive laws have to be used in both cases. The choice of a simplified fine scale constitutive setting may be motivated for both modelling approaches. For multiscale computation, the constitutive laws of the constituents are kept simple in order to focus on the extraction of coarse scale averaged behaviour features based on a finer scale description. For full fine scale computations, this allows to get an affordable discretisation in terms of computational cost. Therefore, the failure behaviour of the bricks is not considered in this study and they are assumed elastic. The combined behaviour of the brick-joint interface and of the mortar is modelled by an initially elastic interface element, for which both the normal and tangential stiffnesses ($k_n$, $k_t$) can be related to the elastic behaviour of mortar, Lourenço et al. (1997b). A classical Mohr-Coulomb type strength criterion is used with a tension cut-off and a linear compression cap, as depicted in Figure 1. The parameters $f_t$ and $f_c$ are respectively the tensile mode I strength of the mortar or mortar-brick interfaces, and the compressive strength of masonry as a composite. $c$ is the cohesion, $\varphi$ is the friction angle, and $\vartheta$ is the angle which defines the linear compression cap for the mortar joints.

A scalar damage model with an exponential evolution law is considered. The traction-separation law which links the traction vector $\vec{t}$ across the interface to the relative displacement vector $\vec{\delta}$ is given by

$$\vec{t} = (1 - D) \mathbf{H} \cdot \vec{\delta}$$  \hspace{1cm} (1)

where $D$ is the scalar damage variable growing from zero (virgin material) to one (complete failure) and $\mathbf{H}$ is an elastic stiffness second order tensor which depends on the elastic stiffnesses $k_n$ and $k_t$. Note that (1) implies that no stiffness recovery is taken into account upon crack closure.

The damage evolution law of the mortar joint is given by

$$D(\kappa) = 1 - \frac{f_t}{k_n \kappa} e^{-\frac{G_f(\kappa-k_n)}{f_c}} \text{ for } \kappa \geq \frac{f_t}{k_n}$$  \hspace{1cm} (2)

where $G_f$ is the mode I tensile fracture energy. Since the damage criterion has to take into account the different behaviours in tension and compression, the damage-driving parameter $\kappa$ is taken as the most critical value of an equivalent
relative displacement defined by

$$\delta_{eq} = \max\left\{ \frac{f_t}{c} \tan \varphi \delta_n + \frac{f_t}{c} \frac{k_t}{k_n} |\delta_t| - \frac{f_t}{f_c} \delta_n + \frac{f_t}{f_c} \frac{k_t}{k_n} \frac{1}{\tan \varphi} |\delta_t| \right\}$$

(3)

where $\delta_n$ and $\delta_t$ are the normal and tangential relative displacements, respectively. Note that since only one fracture energy parameter is used, the compressive fracture energy of masonry is implicitly defined by the tensile fracture energy $G_f$ and the relative values of parameters $f_c$ and $f_t$, and cannot be adapted independently. As aforementioned, note that relations (1) to (3) were postulated for the sake of simplicity and to focus on the subject of the paper, i.e. the degree of approximation introduced by the scale transition procedure. More complex mortar formulations including different damage evolutions in mode I and mode II in terms of energy dissipation could be used as well, see Lourenço et al. (1997b). A brick damage model could also be used for instance in order to extend the detection procedure to additional failure modes involving brick failure, see Lourenço et al. (1997b); Massart et al. (2005) for the case of in-plane problems.

3 Homogenisation-based upscaling framework for failure

3.1 Periodic homogenisation of masonry behaviour

To keep this contribution focused, details concerning classical aspects of periodic computational homogenisation will only be sketched, their developments being available in the literature, see Anthoine (1995); Kouznetsova et al. (2001). The essentials of masonry behaviour can be homogenised from the behaviour of its basic constituents, i.e. bricks and mortar joints. Based on its initially periodic microstructure, a unit cell (i.e. a single period RVE) can be used together with averaging relations, see Figure 2. A periodic displacement field of the following form is used, see Anthoine (1995)

$$\tilde{u} = \mathbf{E} \tilde{x} + \tilde{w}$$

(4)

where $\mathbf{E}$ is a coarse scale strain tensor, $\tilde{x}$ is the position vector of an arbitrary point within the cell and $\tilde{w}$ is a periodic mesoscopic fluctuation field, added to the linear displacement field to account for the heterogeneity of the material. Such a displacement field allows to enforce the averaging relation linking fine
and coarse scale strains

\[ E = \frac{1}{V_{\text{cell}}} \int_{V_{\text{cell}}} \varepsilon \left( \mathbf{u} \right) \, dV \]  

(5)

where \( V_{\text{cell}} \) indicates the cell volume. Practically, the periodicity of the fluctuation field is enforced by linear tying relations involving the displacements of opposite boundaries, see Kouznetsova et al. (2001). The work equivalence principle (Hill-Mandel) is used in order to link the mesoscopic and macroscopic virtual work, see Anthoine (1995)

\[ \Sigma : \delta \mathbf{E} = \frac{1}{V_{\text{cell}}} \int_{V_{\text{cell}}} \sigma : \delta \varepsilon \, dV \]  

(6)

which results in the averaging relation between coarse and fine scale stress tensors

\[ \Sigma = \frac{1}{V_{\text{cell}}} \int_{V_{\text{cell}}} \sigma \, dV \]  

(7)

Based on the periodicity assumption, relations (4)-(7) allow to formulate a boundary value problem on the unit cell, and to control or extract average quantities (strains, stresses, tangent stiffness) from displacements or tying forces at specific controlling points, see Kouznetsova et al. (2001) for details. This methodology was used extensively for material characterisation, i.e. without incorporation within structural computations, initially for elastic behaviour, see Pande et al. (1989); Anthoine (1995). Recent works considered the extension to non-periodic random microstructures using statistically equivalent unit cells, see Zeman and Sejnoha (2007). Their extension to non-linear behaviour showed that physically meaningful results could be obtained in terms of strength and failure patterns, see Pegon and Anthoine (1997); Anthoine (1997); Massart et al. (2004, 2005).

### 3.2 Principles for upscaling the failure behaviour of periodic materials

As presented in Feyel and Chaboche (2000); Smit et al. (1998); Kouznetsova et al. (2001), the upscaling procedure prior to coarse scale localisation consists in applying periodic homogenisation in each coarse scale point of a classical continuum. However, failure at each scale of representation should be carefully treated to obtained meaningful results. At the scale of constituents, classical closed-form constitutive laws can be used, as described in Section 2.

At the coarse scale, and since no a priori postulated constitutive relation is readily available, the detection of localisation has to be based on the average quantities resulting from the upscaling procedure. As a result, the onset of structural localisation is detected from the homogenised tangent stiffness and the associated acoustic tensor. The localisation can be associated to a
condition for the loss of ellipticity of the coarse scale equilibrium problem, based on the non positive-definiteness of the homogenised acoustic tensor for some orientation, see Rice (1976); Rice and Rudnicki (1980). Alternatively, it can be associated to a condition for the loss of uniqueness of the discretised fine scale boundary value problem, i.e. non positive-definite character of the homogenised tangent stiffness, de Borst et al. (1993). As already identified in Massart (2003); Mercatoris et al. (2008), the latter criterion will be used to detect occurrence of localisation and the former to extract the average orientation of the localisation zone. It is emphasised that when periodic homogenisation is used, this coarse scale localisation detection procedure actually introduces a periodicity-related approximation with respect to a fine scale description, since this type of boundary condition may overconstrain the unit cell and overestimate the average tangent stiffness of the material.

An important and debated choice is related to the RVE size. In the present case of quasi-brittle failure, a geometrically linear description is used. The loss of uniqueness can only by associated to material non-linearities, and the localisation detection is not RVE-size dependent, see Massart et al. (2004). As a result, a unit cell will be used here, thereby restricting the model to damage configurations which can be described with such a cell, i.e. single period cracks.

Once structural localisation and its orientation are detected, a discontinuity with this orientation has to be introduced in the coarse scale description to account for the damage localisation, together with elastically unloading surrounding zones, as sketched in Figure 3a. In Massart et al. (2007), a strain discontinuity with a given width (see Figure 3) was used within a relaxed Taylor model to represent the average effect of the localising zone in a coarse scale quadrature point. The presence of this strain discontinuity was not explicitly incorporated in the coarse scale discretisation as such, but was rather embedded in the average behaviour of the considered quadrature point. The behaviour of the localising region was directly obtained from the homogenised behaviour of a further damaging unit cell. Here, the discontinuity will be explicitly introduced in the coarse scale displacement field discretisation in the spirit of Armero (1999), by using a lumped displacement jump. This format requires the extraction of a cohesive response from the average behaviour of a damaging unit cell. This extraction should enforce that the correct amount of dissipated energy is transferred to the coarse scale. Again, it is emphasised that this treatment of structural localisation implicitly carries assumptions if periodic homogenisation is still used to extract this coarse scale cohesive response, since the scale separation assumption is not satisfied anymore upon coarse scale localisation. Furthermore, as an additional choice, the zones surrounding the localising regions are assumed to unload elastically, an assumption which might not be satisfied during the complete loading history of all the concerned points in the structure.
3.3 Incorporation of a strong discontinuity at coarse scale

The structural scale problem is solved using the finite element method and using an embedded strong discontinuity model in which the behaviour of the discontinuity is obtained from fine scale computations. Once structural localisation is detected, the coarse scale displacement field is enriched by a strong discontinuity, as proposed by Armero (1999). A displacement jump $\vec{\xi}$ is introduced along a discontinuity line $\Gamma_d$, the orientation of which is deduced from the acoustic tensor-based criterion. This jump is added to the regular continuous part of the displacement field according to

$$\vec{u}_e = \vec{u} + \Psi \vec{\xi}$$  \hspace{1cm} (8)

where $\Psi$ represents a set of functions exhibiting a unit jump along the discontinuity line. The enhanced strain tensor is obtained by differentiating Equation (8), which leads to

$$E_e = (\nabla \vec{u}_e)_{\text{sym}} = E(\vec{u}) + G(\vec{\xi}) + (\vec{\xi} \cdot \vec{n})_{\text{sym}} \delta_{\Gamma_d}$$  \hspace{1cm} (9)

where $E(\vec{u})$ is the strain tensor based on classical kinematics, $G(\vec{\xi})$ is the regular part of the enhanced strain tensor $E_e$ which depends on the displacement jump and $\delta_{\Gamma_d}$ is the Dirac function centered on the discontinuity line. This Dirac function is integrated along the discontinuity line and therefore does not need regularisation, see de Borst et al. (2001). The details concerning the discretisation of such an enhanced kinematics, among which the construction of the tensor $G$ can be found in Armero (1999), and will be omitted here for brevity.

In order to determine the additional displacement jump field, the weak form of equilibrium is solved together with a weak continuity condition on the stress along the discontinuity line:

$$\int_{\Gamma_d} (\vec{T}_d - \Sigma \cdot \vec{n}) \, d\Gamma_d = 0$$  \hspace{1cm} (10)

where $\vec{T}_d$ is the traction vector across the discontinuity, $\Sigma$ is the stress tensor in the bulk, surrounding the discontinuity, and $\vec{n}$ is the normal to the discontinuity line $\Gamma_d$. A material response which links the traction vector to the displacement jump is required to drive the discontinuity and reads

$$\delta \vec{T}_d = 2 \mathbf{C}_d \cdot \delta \vec{\xi}$$  \hspace{1cm} (11)

where $2 \mathbf{C}_d$ is the discontinuity tangent stiffness tensor. Once the embedded discontinuity is introduced, the bulk of the element is assumed to unload elastically from the state reached at that point.
Note that this strong discontinuity approach is a element-based enrichment of the displacement field. This carries the advantage that the additional displacement jump field may be condensed at the element level. As a corresponding drawback, this implies that the crack path continuity and the displacement jump field continuity across the element boundaries are not ensured, which may have consequences in terms of global energy dissipation. Note also that an extension in this respect could be considered with an XFEM-based implementation at the coarse scale as in Belytschko et al. (2008). However, the extraction of an average discontinuity behaviour from the homogenisation of fine scale computations can lead to the re-orientation of this discontinuity as a result of further fine scale damage evolutions. This fact is particularly important for the case of strongly textured materials as masonry, and should be accounted for to avoid stress locking phenomena at the coarse scale, which is easier to accommodate with an element-based enrichment.

3.4 Upscaling localising behaviour towards the coarse scale discontinuity

In the present contribution, contrary to the approach proposed by Armero (1999) where constitutive laws are given by closed-form laws, both the bulk and discontinuity material behaviours are deduced from fine scale unit cell computations. A material secant stiffness is extracted from the unit cell in which the structural localisation has just been detected. The material behaviour of the discontinuity, described by Equation (11) at the coarse scale, must be extracted from the fine scale description by means of an enhanced upscaling procedure. A further damaging unit cell is used for this purpose, which will be denoted in the sequel as Localising Volume Element (LVE), see Figure 3.

The extraction of the coarse scale discontinuity response requires the definition of an average strain $E_{LVE}$ to be applied on the LVE from the coarse scale displacement jump; as well as the evaluation of $T_d$ and $C_d$ from the results of the LVE computation. An approximate energy consistency argument is used as illustrated in Figure 3 in order to build a relationship between the displacement jump vector $\xi$ across a zero-thickness zone with an orientation $\vec{n}$ used at the coarse scale, and the average strain $E_{LVE}$ applied to a localising region with a finite volume detected at the fine scale. The localisation width $w_n$ defining the volume of the localising region therefore has to enter this relationship to take into account in the coarse scale description the finite fine scale volume on which damage localisation occurs. The introduction of the fine scale localisation width in the scale transition indeed allows to objectively upscale the total energy dissipation independently of the coarse scale discretisation.

Writing the work variation for the idealised band-surrounding representation
(Figure 3b), in which the localising region behaviour is identified from the LVE and the unloading region is associated with an unloading RVE yields

$$\delta W_m = \int_{V_u} \Sigma^{RVE} : \delta \mathbf{E}^{RVE} \, dV_u + \int_{V_l} \Sigma^{LVE} : \delta \mathbf{E}^{LVE} \, dV_l$$  \hspace{1cm} (12)$$

where $V_l$ and $V_u$ represent respectively the volumes of the further loading (damaging) and unloading regions. In the corresponding coarse scale representation (Figure 3c), the localising behaviour is lumped into a zero-thickness cohesive zone and the complete volume of the element is assumed to unload according to the behaviour extracted from the RVE. The corresponding work variation reads

$$\delta W_M = \int_{V_u} \Sigma^{RVE} : \delta \mathbf{E}^{RVE} \, dV_u + \int_{V_l} \Sigma^{RVE} : \delta \mathbf{E}^{RVE} \, dV_l + \int_{\Gamma_d} \mathbf{T}^d \cdot \delta \mathbf{\xi} \, d\Gamma$$  \hspace{1cm} (13)$$

The strain jump variation associated with a strain discontinuity mode vector $\delta \tilde{m}$ along a discontinuity line of normal $\tilde{n}$ is given by

$$\delta \mathbf{E}^{LVE} = \frac{1}{2} \left( \tilde{n} \delta \tilde{m} + \delta \tilde{m} \tilde{n} \right)$$  \hspace{1cm} (14)$$

Assuming that the variations $\delta \mathbf{E}^{LVE}$, $\delta \mathbf{E}^{RVE}$, and $\delta \mathbf{\xi}$ are constant on the domains on which they are integrated, assuming that the traction continuity is enforced along the boundary between the localising and unloading regions, and defining the traction across the coarse scale discontinuity from the LVE average stress, one obtains

$$\tilde{T}^d = \Sigma^{LVE} \cdot \tilde{n} = \Sigma^{RVE} \cdot \tilde{n}$$  \hspace{1cm} (15)$$

Imposing the energy equivalence $\delta W_m = \delta W_M$ then yields

$$w_n (\delta \mathbf{E}^{LVE} - \delta \mathbf{E}^{RVE}) \cdot \tilde{n} = \delta \mathbf{\xi}$$  \hspace{1cm} (16)$$

As a result, the average strain on the LVE is related to the coarse scale displacement jump according to

$$\delta \mathbf{E}^{LVE} \cdot \tilde{n} = \frac{\delta \mathbf{\xi}}{w_n} + \delta \mathbf{E}^{RVE} \cdot \tilde{n}$$  \hspace{1cm} (17)$$

The first term of this relation expresses that the lumped displacement jump along the discontinuity at the coarse scale should incorporate a measure of the fine scale finite volume on which damage occurs, $w_n$ in this case. Note that this localisation zone width can vary with the failure mode observed at the fine scale. Here it will be taken equal to the size of a unit cell in the direction of the normal to the detected localisation orientation. This carries the implicit assumption that the localisation occurs with single period cracks, which might not hold for given cracking modes, such as for instance vertical brick cracking under horizontal tension. The second term of relation (17) accounts for the fact that the RVE unloading is attributed to the complete volume of the
element at the coarse scale. A part of the material inside the LVE is indeed also unloading upon localisation (namely the brick which behaves elastically), but this effect is already incorporated in the averaging operation on the LVE. This second term allows not to take this contribution twice in the energy consistency argument, under the assumption that the unloading material inside the localising band reacts as the identified surrounding material (i.e. with an secant unloading from the bifurcation point). Since the contribution of this second term is usually small, and for the sake of simplicity, it will be neglected in the sequel. Note that this approximation is theoretically valid for cases in which the localisation width is indeed negligible with respect to the dimensions of the coarse scale elements.

The complete multiscale nested procedure with localisation enhancement is depicted in Figure 4. Note that orientation of the discontinuities after their introduction is not fixed. Subsequent localisation analysis of the tangent stiffness of the LVE may indeed detect rotations in the detected localisation orientation as a result of further (unstable) damage growth. In such case, the coarse scale discontinuity is allowed to rotate in order to avoid stress locking. This rotation is however limited at each step, in order to avoid convergence difficulties linked to sudden and strong rotations.

4 Comparison of multiscale and fine scale results on a structural example

4.1 Problem description and qualitative behaviour

In order to compare fine scale and multiscale approaches, the same structural computation will be performed using both descriptions. The tested geometry is shown in Figure 5. It consists of a planar masonry wall of dimensions $2220 \times 2160 \times 98 \text{ mm}^3$, with bricks of dimensions $120 \times 60 \times 98 \text{ mm}^3$ stacked according to a running bond pattern. Note that the size of the wall remains limited by the computational cost of the full fine scale computation. The aspect ratio of the bricks prescribes a preferential staircase crack pattern orientation of $45^\circ$. A clamping of the top and bottom brick rows in the loading set-up is represented by two bands of elements with elastic behaviour and with a stiffness comparable to concrete. The loading is applied in two phases. In the first phase, the wall is compressed by prescribing a uniform vertical displacement of the top boundary. In the second loading phase, the vertical displacement of the top boundary is kept fixed and a horizontal shearing displacement is prescribed on the top right corner of the wall. For low pre-compression loads, damage is first initiated during the confined shearing phase with the appearance of horizontal tensile cracks at the top left and bottom right corners of
the wall. The extension of these tensile damage zones is lower for higher initial compressions. Their appearance is followed by the formation of a compressive strut between the bottom left and top right corners. Upon further shearing, diagonal cracking appears in the central zone of the specimen in the compressive strut, with a stair-case crack pattern at the fine scale. During this compressive strut cracking phase, a strong interaction occurs between the fine scale preferential cracking orientation, and the coarse scale stress distribution prescribed by the confining boundary conditions. The difference between the respective orientation of the strut and of the fine scale pattern strongly influences the damage-induced energy dissipation. Finally, a structural failure mechanism is formed by the propagation of diagonal cracking towards the compressed corners of the wall. Depending on the compressive strength of the mortar, final failure may occur by compressive crushing at the compressed corners of the wall, associated with brick cracking at the fine scale. Since bricks are assumed elastic, compressive crushing is represented here phenomenologically by the compressive cracking of bed joints, see Lourenço et al. (1997b).

Due to the strong confinement present in this test, the stress distribution in the central part of wall remains rather uniform at the early stages of cracking, and the initial shearing damage zone is therefore quite diffuse. This transition from a distributed damage pattern to a localised cracking is difficult to capture computationally, and requires strong step refinements along the computations even for a full fine scale discretisation. Furthermore, the use of a rather coarse discretisation in multiscale computations needed at the coarse scale to keep the localisation width smaller than the structural scale element size also induces numerical difficulties, linked to the proper evaluation of stress concentrations for the coarse scale discontinuity propagation, especially for uniformly distributed stress states. Therefore, a defect is introduced in the central part of the wall to trigger the damage localisation more easily, both in the fine scale and coarse scale computations, see Figure 5. Finally, since the focus is here set on the assessment of the results obtained with a periodicity-based scale transition, a rather favourable mesh topology is adopted at the coarse scale. A diagonal band of elements with an orientation consistent with the average orientation of the compressive strut is introduced in the coarse discretisation in order to properly capture the stress concentration and to allow the complete separation of two rows of nodes with propagating embedded discontinuities. This allows to avoid numerical crack propagation difficulties. Note that the influence of such a mesh alignment at the coarse scale is the same as if enhanced assumed strain methods were used with closed-form material laws.

For the multiscale computation, the masonry wall is discretised at the structural scale by using 3-noded plane stress finite elements with one Gauss integration point. The clamped top and bottom brick rows are discretised with 4-noded linear elements with $2 \times 2$ Gauss integration points. The coarse scale mesh consists of 388 elements and of 536 displacement degrees of freedom.
(excluding the displacement jumps condensed at the element level). The unit cell computations use a rather coarse discretisation with quadratic 2D and interface elements. For the complete fine scale computation, the bricks are discretised using 8-noded quadratic plane stress finite element with $3 \times 3$ Gauss integration points. The mortar joints are represented by 3-noded quadratic interface finite elements with 3 Lobatto quadrature points. Each brick was discretised using 6 by 5 elements, resulting in a model consisting of 160000 dofs. All meshes used for the different levels of descriptions are sketched in the Figures in the next subsections.

Note that the choice of this test calls for several comments regarding the use of periodic homogenisation. Homogenisation with such boundary conditions is known to overestimate the average stiffness of the material, an approximation which is particularly debatable near free boundaries for instance. In the presented test setup, the strong initial confinement in the central zone of the wall allows to decrease the importance of this issue. As a result, the periodic assumption is not expected to be a too penalising assumptions for the detection of localisation in the diagonal strut. Conversely, this assumption may prove quite crude for localisation in the bed joints in the first cracking stages. In the same line, it is recognised that the use of periodically homogenised properties for localised behaviour itself remains untested since the scale separation principle does not apply anymore in this case. This is particularly the case here given the dimensions of the tested wall (which are prescribed by the cost of the full fine scale computation), as the size of the fine scale localisation volume is not much smaller than the coarse scale material points volume. The use of the periodicity assumption for the localised regime will thus be challenged here by using the most critical conditions for its application.

Note that the compressive and shearing loading phases of the wall in both simulations and the cell computations in the multiscale approach are controlled by displacement. In particular, no path following technique is used at the coarse scale in the multiscale computation. Therefore, the multiscale and full fine scale computations results are quantitatively compared until the limit load of the structural response is reached.

The material parameters used for the computations are defined at the fine scale for both approaches, see Section 2, and their values are reported in Table 1. The tensile fracture energy of mortar joints is however increased with respect to realistic values (at least for tensile mode I fracture) in order to avoid any snap-back effect in the unit cell average response, see Massart et al. (2005).

Note that the computation cost is not challenged in this contribution. The size of the structure has been chosen such that a full fine scale model is feasible. The computation costs of the both multiscale and full fine scale approaches are therefore comparable. Practically, a multiscale method would definitely be
used to deal with larger structures. In this case, a multiscale approach would of course be much more effective in terms of computation cost than a full fine scale computation.

Finally, due to the nested incremental iterative scheme, the presented multiscale procedure has a rather high computational cost even with coarse discretisations at both fine and coarse scales. Since all cell responses may be computed independently, the proposed multiscale method is well suited for parallel computations. The multiscale computation reported here was performed with such an implementation.

4.2 Comparison of results

The results of both approaches are compared in this Section, based both on the overall response of the wall (load-displacement response in the second phase and identification of the failure mechanisms), and on the obtained damage patterns at critical spots.

The load-displacement response of the second loading phase is depicted in Figure 6. As can be seen, the multiscale simulation overestimates the initial stiffness by more than 22% with respect to the full fine scale modelling. The load bearing capacity of the wall given by the multiscale computation is however underestimated by only 1.1% with respect to the full fine scale solution. The multiscale peak load appears for a shearing displacement smaller by 7% with respect to the full fine scale solution. This may be associated to the fact that the overestimation of the initial global stiffness leads to stronger stress concentrations and therefore earlier cracking appearance in terms of the imposed shearing displacement.

For each of the three points of the load-displacement curve denoted by a capital letter, a detailed view of the structural state is given in the next Figures. The damage distribution is illustrated on the undeformed structural configuration for the complete fine scale solution. For the same value of the shearing displacement (point A and B) and for the response peak (point C), the coarse scale discontinuities are depicted on the undeformed shape of the coarse scale discretisation of the multiscale computation. The damage distributions of the unit cells corresponding to typical positions in the structure are also given.

As can be seen in Figure 7 representing the damage state at point A in the load-displacement curve, the initial stage of horizontal mode I cracking in bed joints is qualitatively reproduced by the multiscale computation. The overestimation of the initial stiffness of the wall and the rather coarse meshes used in the multiscale approach may explain the difference in the extension of these cracks. In the complete fine scale solution, the horizontal mode I cracking is
localised in the upper left and lower right tensile bed joints. The multiscale computation shows a less localised horizontal cracking due to the fact that the stress concentrations are partly smoothened by the rather coarse discretisation in this zone. The fine scale damage patterns is nevertheless well reproduced, see unit cell (1) in Figure 7. A rather localised damage state promoted by the defect appears in the central zone in the complete fine scale simulation, represented as well in the multiscale framework by embedded discontinuities. Note that their orientation is consistent with the unit cell staircase damage patterns and the full fine scale simulation, see unit cell (2) in Figure 7. In the multiscale solution, the extension of the embedded discontinuities corresponding to the diagonal cracking is larger, probably due to the overestimation of the initial global stiffness. Note that around the staircase cracking fronts in the full fine scale solution, the damage distribution is rather diffused and only the head-joints are partially damaged. This damage pattern is also well reproduced by the multiscale computation in non-localised states (no coarse scale discontinuity in this zone), see unit cell (3) in Figure 7. In the compressed corners, the full fine scale solution shows a slight initiation of damage in the head-joints while bed joints are partially damaged in the multiscale solution, see unit cell (4) in Figure 7.

The next stage in the cracking process is still located in the rising part of the load-displacement curve (point B). It matches the transition from a diffuse damage pattern in the central zone of the compressive strut towards localisation. Figure 8 depicts this state of the wall for both approaches. Note that the orientation of the slanted embedded discontinuities in the diagonal band of elements is independent of the coarse scale mesh but consistent with the full fine scale modelling and the unit cell staircase damage patterns, see unit cell (1) in Figure 8. The orientation of these embedded discontinuities in fact evolves towards the average staircase orientation given by the brick stacking geometry. Note that the discrepancy between the fine scale preferential orientation (45°) and the compressive strut average direction (about 50°, as illustrated from the fine scale solution of Figures 9 and 10), is the cause for the presence of several diagonal cracks and therefore influences the global energy dissipation. These parallel staircase cracks with respect to the main one are accounted for in the multiscale approach by non-localised damage zones as illustrated by cell (2) in Figure 8. In the top right and bottom left zones, compressive and shearing failure in bed joints appeared in the multiscale framework, see unit cell (3) in Figure 8, which matches rather well with the full fine scale solution. The multiscale solution also shows quasi fully damaged head-joints near the compressed corners, see unit cell (4) in Figure 8, which matches the damage patterns of the full fine scale solution.

Upon completion of the propagation in the compressive strut, the compressed corners fail under compressive crushing at the peak load of the wall response (point C). This compressive crushing failure (represented here phenomenolog-
ically by joints compressive failure) is correctly captured by both the complete fine scale and the multiscale descriptions, see unit cells (1) and (2) in Figure 9. In each description, this damage pattern occurrence matches the peak load of the curve. As expected, the stress redistribution stops the horizontal cracks propagation in the upper and lower bed joints. For the sake of completeness, Figure 9 shows that the multiscale framework properly detects the appearance of bed joint failure along free edges of the wall as in the full fine scale solution, see unit cell (3) in Figure 9. Finally, unit cell (4) in Figure 9 shows that certain joints of the wall remain safe during the loading phase in accordance with the full fine scale simulation results.

To further illustrate the global failure mechanisms, the deformed configurations at the peak load (point C) are depicted in Figure 10 for the both full fine scale and multiscale computations. The tensile and compressive failure of the bed joints in the corners are well reproduced by the multiscale computation, see unit cells (1) and (2) in Figure 10. The staircase opening in the central zone of the compressive strut of the multiscale solution matches as well the failure mechanism of the full fine scale solution. In this zone, the head-joints fail with a tensile mode whereas the damaged part of bed joints present a rather shearing failure mode, see unit cell (3) in Figure 10. Finally, note that the orientation of embedded discontinuities matches the average orientation of the staircase opening in the full fine scale solution, see Figure 10. The full fine scale solution also shows the effect of a different orientation of the fine scale preferential damage orientation and of the global compressive strut. Three staircase cracks are indeed recognizable in this simulation, resulting in an average orientation of the damaged compressive strut of $50^\circ$.

4.3 Discussion

The first observation is related to the presence of an overestimation of the stiffness in the initial stage of the second phase loading. This overestimation can be attributed to the use of periodic homogenisation, as well as to the use of a rather coarse discretisation in the multiscale approach, both at the coarse scale and in the unit cell computations. The use of a coarse discretisation at the structural scale was needed here to keep the localisation width smaller than the structural scale element size. Note that in practical applications of the multiscale framework, larger structures would be considered. A mesh refinement at the structural scale would restrict the stiffness overestimation such that the sole contribution brought by the periodicity assumption would remain.

It is emphasised that the periodicity assumption of the computational homogenisation procedure gets increasingly challenged along the shearing load-
ing phase; even though it may be argued that this assumption keeps its validity before any localisation detection, due to the confined character of the stress distribution. Upon localisation in the bed joints under mode I loading, periodicity is clearly lost as shown in Figure 7 (fine scale). Nevertheless, the presence of these cracks is detected in the multiscale procedure at the correct shearing displacement. This suggest that the overestimation of the initial stiffness does not affect strongly the initiation of the cracking process. Upon localised behaviour, the local periodicity assumption is strongly challenged, especially because the localised bandwidth is comparable to the coarse mesh size. The stress distribution in the centre of the wall remains rather diffuse when the tensile cracks of bed joints are initiated. As a consequence, the periodicity assumption remains a good approximation for non-localised states in the compressive strut. Further in the shearing loading phase, the crack propagates in the compressive strut until the complete development of the failure mechanism when the compressed corners fail (corresponding to the overall response peak). The cohesive behaviour of the coarse scale discontinuities is obtained on a periodic unit cell. As a result, the coarse scale dissipation is directly controlled by the periodicity assumption, even though the cracking in the compressive strut does not consist in many parallel active cracks, as depicted in Figure 10. However, the good agreement between the simulations both in the global response and in the obtained damage patterns shows that the periodicity assumption does not prevent from reaching quantitative results for the treated wall. The load bearing capacity seems to be controlled mainly by the global failure mechanism since the peaks of both approaches match, in spite of the difference in the initial global stiffnesses.

This consideration gives a motivation for the limit analysis assumptions where the load bearing capacity is related to the considered failure mode, as for instance in Milani et al. (2006). The limit analysis approaches focus on the identification of the limit load of structures without considering stable crack situations. The proposed multiscale framework is therefore considered as a complementary approach, since it allows to capture the crack patterns along the loading path and therefore allows to model cracking for loading levels well below the limit loads.

It is also emphasised that the proposed multiscale framework is tested here using the most challenging conditions for its application in terms of the scale separation issue. In particular, its use in much larger structures would result in larger scale jump. As a result, the localised behaviour would be modelled with a better estimation of the energy dissipation.

The use here of coarse scale embedded localisation zones as proposed in Armero (1999) is a major difference with the approach proposed in Belytschko et al. (2008), which makes use of XFEM techniques. The lack of crack path continuity in the approach here could lead to strong approximations in terms
of energy dissipation if coarse meshes are used at the structural scale. This is particularly the case for mode I loading, a case in which an XFEM implementation would yield better results, as illustrated in Belytschko et al. (2008) for a three point bending configuration. As a result, it could be expected that the early bed joint cracking in the wall would be modelled more accurately in an XFEM-enhanced multiscale framework. Conversely, the compressive strut cracking is obtained with a fine scale damage evolution which leads to reorientations of the averaged cracking zone, a feature which can be more easily incorporated in an embedded discontinuity formulation, than in an XFEM-based description. Furthermore, for compression dominated average failure modes, more distributed damage states are obtained as illustrated in the case of the wall, in which case, several embedded zones can appear to account for this fact. Finally, it should be noted that the representation of the compressive failure of the corners by means of a cohesive zone is questionable, since it consists in a volume-driven dissipation. Here, a proper representation of this failure mechanism and of the associated energy dissipation is obtained because the size of the unit cell is comparable to the coarse scale element size. If larger structures have to be modelled with compressive failure zones, a proper volume energy dissipation should be accounted for by adapting specifically the localisation size $w_n$ for the compressive stress states.

5 Conclusions

A periodic homogenisation-based multiscale method was proposed for the modelling of quasi-brittle structural failure. In order to upscale failure information, a new displacement discontinuity-enhanced scale transition was developed based on approximate energetic consistency requirements. This framework was assessed by a comparison with a complete fine scale model on a confined shearing wall test, in order to estimate the impacts of the periodicity and scale separation assumptions.

In the case of the confined shearing wall test, it was shown that the multiscale modelling yields results in good agreement with respect to complete fine scale computations results provided stress distributions are confined. In spite of an overestimation of the initial stiffness by the multiscale modelling, the cracking patterns are correctly reproduced, with a good estimation of the failure mechanisms at the both structural and fine scale. Furthermore, the multiscale approach also allows to obtain quantitative information on the limit load, which is obtained with less than 2% error with respect to the full fine scale simulation.

The results obtained here suggests that further studies could be useful in order to extend their scope. First, a parametric study should be performed in order
to analyse the results obtained for different mesh refinements at the coarse scale, different fine scale geometrical features (size of the unit cell, aspect ratio of the unit cell), and different material features (fracture energies). Secondly, additional features could be introduced in the fine scale laws. This would include brick cracking (leading to more localised patterns in the compressive strut), as well as more refined mortar joints laws (independent fracture energies for mode I, mode II and compressive fractures). Finally, the extension of the framework to out-of-plane failure should be performed, based on the results of Mercatoris et al. (2008), and is under way (Mercatoris and Massart (2009)).

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References

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Table 1
Brick (a) and mortar/mortar-brick interface (b) material parameters, see Lourenço (1996).

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\[ E \quad \nu \quad k_n \quad k_l \quad f_l \quad G_f \quad c \quad \varphi \quad f_c \quad \vartheta \]

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Fig. 1. Mohr-Coulomb criterion for the mortar joint/mortar-brick interface with tensile cut-off and linear compressive cap.
Fig. 2. In-plane periodicity of running bond masonry, see Anthoine (1995).
Fig. 3. Identification of a coarse scale discontinuity from a fine scale damage pattern. (a) fine scale damage pattern, (b) identification of a further damaging and localising band of volume $V_l$ and of an unloading surrounding regions of volume $V_u$, (c) aggregation towards a strong discontinuity at coarse scale. Comparison of (a) and (b) defines the localising volume, while the energetic consistency originates from the equivalence between (b) and (c).
Fig. 4. Complete localisation-enhanced nested scheme
Fig. 5. Confined shearing wall test description. The loading is applied in two successive phases: (a) compressive load applied on the top boundary layer, (b) horizontal shearing. The dark grey area depicts the staircase crack defect introduced in the central zone of the wall to initiate localisation of damage in the diagonal compressive strut (decrease of the tensile strength and the cohesion of 50%).
Fig. 6. Confined shearing wall test. Comparison of the load-displacement responses for full fine scale modelling (dashed line) and multiscale simulation (solid line). The capital letters match states for which detailed damage maps are compared in the following Figures.
Fig. 7. Damage maps at point A of the confined shearing load-displacement response of the wall: (left) damage maps of the complete fine scale computation (black lines indicate fully damaged joints and gray lines indicate partially damaged joints), (right) coarse scale discontinuities for the multiscale computation and (bottom) related damage state of unit cells.
Fig. 8. Damage maps at point B of the confined shearing load-displacement response of the wall: (left) damage maps of the complete fine scale computation (black lines indicate fully damaged joints and gray lines indicate partially damaged joints), (right) coarse scale discontinuities for the multiscale computation and (bottom) related damage state of unit cells.
Fig. 9. Damage maps at point C of the confined shearing load-displacement response of the wall: (left) damage maps of the complete fine scale computation (black lines indicate fully damaged joints and gray lines indicate partially damaged joints), (right) coarse scale discontinuities for the multiscale computation and (bottom) related damage state of unit cells.
Fig. 10. Deformed configuration at point C of the confined shearing load-displacement response of the wall (the displacements of the wall are magnified by a factor of 200): (left) deformed configuration of the complete fine scale computation, (right) deformed configuration of the multiscale computation and (bottom) related deformed unit cells (the displacements of the cells are magnified by a factor of 50).