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Review of "A computational homogenization framework with enhanced localization criterion for macroscopic cohesive failure in heterogeneous materials"

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Reviewer 1 (Vinh Phu Nguyen)

The manuscript presents a two scale computational homogenization (FE^2) model to simulate fracture of composites. Their key contribution remains in the proposal of a geometric scaling parameter (for transition from micro to macro scale) and robust algorithm to determine the crack orientation at the microscale which is suitable for arbitrary crack paths.

This is a well-written manuscript and have suitably highlighted the key contributions of the authors, and suggesting future scope of research in this domain. The findings of the manuscript certainly will be the interest of many readers from computational mechanics, multi-scale modelling, and composites community. Keeping that in mind, the manuscript needs a major revision based on the following points.

Reviewer The authors have proposed an approach to compute the scaling parameter h as the minimum crack spacing in the periodically deformed micro-structure. Then, what will be the value of h if a single crack path is detected in the microstructure by the fracture algorithm? Also, on the same ground, it appears that the proposed calculation is applicable only for discrete fracture model (specifically, cohesive zone model where the fracture algorithm detects multiple possible crack path among which one can propagate in the macroscale). Please clarify.

Authors The authors acknowledge that the name for the proposed geometrical interpretation of scaling factor h may be misleading in the sense that it gives the impression of a distance between multiple active cracks. Actually in the context of a periodic microstructure which is assumed in most research including this manuscript, such a distance means the shortest spacing between the potentially occurring cracks that possess a repeating pattern due to the periodic pattern of the microstructure. For visually interpreting h, a periodic crack pattern is assumed. In fact only one dominant loading crack will eventually propagate through the material on the macroscale. This periodic crack pattern is artificial in the sense that the repeating cracks are not present in reality or in the simulation. Assuming their presence gives a way to show how much unloading material

is present per unit crack length in the RVE simulation, which is ultimately what is needed for the multiscale framework. In order to avoid the confusion, the name 'minimum crack spacing' has been replaced by 'periodic crack spacing' throughout the text. (see page 20 and Fig 21-caption). Besides, the proposed computing method for h is equally applicable for both discrete cracking and continuous damage model. Actually, continuous damage models are essentially equivalent to the discrete cracking model in representing a strong discontinuity as shown in J. Oliver, A.E. Huespe, Comput. Methods Appl. Mech. Engrg. 2004. In both models, failure paths (cracks or damage bands) could be determined. For the continuous damage model, the spacing between two periodic damage bands should then be considered (see page 20).

Reviewer How the scaling parameter h is computed in Section 4.5? Is it using Equation 16 proposed by Svenning et al. (2017)? Is it a case where the proposed definition of h does not work? If yes, then the proposed definition of h has issues related to the arbitrary crack path or to the case of single crack in the microstructure. Please clarify.

Authors Indeed, in Section 4.5 where an arbitrary crack path is tracked, the h for each cohesive micromodel can not be decided beforehand as for simple RVE cases. First, the localization orientation of the crack at the cohesive integration point on macroscale is obtained by the acoustic tensor spectrum analysis. Then with such orientation, h is computed by using Equation (17). For a 2D square RVE the proposed definition is equivalent to the Equation (17).

Reviewer To summarize, $h = d_m$ in Sections 4.1-4.3, $h = d_c$ in Section 4.4, and h is computed based on Equation (16) for Section 4.5. Please mention what is the order of magnitude of h considered in Sections 4.4 and 4.5? Also, can the proposed h (= minimum crack spacing...) be computed on the fly similar to its predecessors, e.g. Eq. (15), Eq. (16)?

Authors The magnitude of h considered in Sections 4.4 and 4.5 is 10^{-3} mm. And yes, it can and should be decided on the fly because it depends on the localization orientation at the bifurcation moment of the bulk material point. For the arbitrary crack path in Section 4.5, the crack orientation can only be determined on the fly, thus h is also computed on the fly by using Equation (17).

Reviewer In Figure 20(a), please make the notch length proportionate to the other geometric dimensions. Also, mark the dimension of the circular inclusion in Figure 20(b).

Authors Both points have been addressed as shown in the new Figure 25 (page 25).

Reviewer Please mark the periodic boundary conditions on Figure 4 for clarity.

Authors PBCs are now marked in the Figure 4 (page 13) as suggested.

Reviewer Please add some cross-reference for h after Equation 37.

Authors Cross-reference for h is added after Equation (37) (page 11).

Reviewer The manuscript contains a few typos. For example, on page 17, "... has a crack pattern similar to case C from section Section 4.4, ...". On page 3, two references looks same although they are distinct. "This work has been further extended by Toro et al. (2016) and Toro et al. (2016)". On page 10, the union operator $\cup$ should be used instead of the intersection, $\Omega_A^M \cap \Omega_B^M = \Omega^M$.

Authors These typos have been corrected (pages 24, 4, 11).

Reviewer 2 (Thierry Massart)

The paper deals with adaptations of the existing computational multiscale frameworks dealing with failure using an upscaling of the RVE failure process towards cohesive zone models in FE^2 type approaches. The text is well written and structured.

The manuscript contains useful new material related to the implementation of the FE^2 approach with the use of a phantom node approach at the structural upper scale.

Although presented here probably in a more general way with respect to previous contributions, some other aspects in the manuscript are at least partially already present in such previous contributions that may have been overlooked, unless some new ingredients used here escape me. It seems to be the case for the characteristic size d_c (distance between two periodic dissipating

zones of neighbouring RVEs), and more importantly for the use of the acoustic tensor-based localization orientation detection using a discontinuous material bifurcation analysis.
Globally, I think that the manuscript is sound and recaps several ingredients in a neat way (which is useful and nice). However, it gives the feeling to the reader that all these ingredients (including the two mentioned above) were not treated in previous contributions. This impression is reinforced by the title that is too general in my opinion.
Specific comments motivating this global assessment are the following.

Reviewer As duly mentioned by the authors, the upscaling of failure from microstructural models towards some type of localization enhancements at the macroscopic scale have been proposed before, including in references given in the manuscript. The title of the manuscript is in my opinion too general. It sounds as if the purpose of the paper was to propose an original way of upscaling failure that was not proposed before. I think that the title should be revised to avoid such an impression. A suggestion is to somehow pinpoint in the title (as in the abstract) the original aspects of the manuscript (phantom node implementation for cracking at the structural scale, formalization of criterion (31) in the acoustic tensor detection, which is in link with work presented in previous contributions, see next comment).

Authors As commented by the reviewer, the ingredients of the framework in this manuscript are not fully original but an adaptation and improvement of existing contributions. The authors agree that the title should avoid the misconception. Thus, a revised title is given trying to summarize the originality of the manuscript. It is "*A computational homogenization framework with enhanced localization criterion for macroscopic cohesive failure in heterogeneous materials*".

Reviewer The notion of a discontinuous bifurcation analysis for the detection of the (average) cracking orientation was used previously as mentioned in the manuscript. In discontinuous material bifurcation however, the linear comparison solid assumption is not used (i.e. the material outside the localization zone is not assumed to follow the same material tangent as inside it at the bifurcation occurrence). As a consequence, localization may theoretically be possible for the whole fan of orientations for which a negative value of the acoustic tensor is present. This indeed makes it possible for not taking the orientation that matches the global minimum of the acoustic tensor eigenspectrum.

The authors however do not seem to be aware that this fact was already analysed in the context of computational homogenization towards embedded cracks in Massart et al., IJNME, 2007 (cited in the manuscript, but not on this specific aspect). It was further extended in Mercatoris and Massart, EFM, 2009 for out-of plane bending, considering macroscopic cohesive behaviour. As shown in these papers, taking a local extremum (and not the global minimum) could be motivated when matching the acoustic eigenspectrum with microstructural damage patterns (Fig. 8 of the present manuscript is similar to a figure of the 2007 reference and confirms one of the analyses proposed in these two papers for a specific material among other diverse loading cases).

Criterion (31) proposed here makes this procedure even more systematic, which is a useful information worth publishing. However, unless some aspects would have escaped me (in which case the difference with these previous works should be highlighted more clearly), previous contributions on this aspect should be recognized more specifically.

Authors Indeed as the reviewer comments, the previous two journal papers (Massart et al., IJNME, 2007 & Mercatoris and Massart, EFM, 2009) included attention for the very same topic of localization detection in the context of computational homogenization. Unfortunately, we have overlooked this in the first version of manuscript. The references to these papers have been elaborated more specifically in the text (see page 7 and page 10) to recognize their originality and contributions.

Reviewer The use of the phantom node approach is an innovative aspect of the proposed approach. Its combination with the acoustic-tensor based detection brings me the following question. When macroscopic localization is detected, failure at the microstructural scale is well engaged, but not complete yet (i.e. there is not a complete microstructural crack path along which zero stress transfer is achieved, and cracking is not homogeneous along the microstructural damage zones). This means that further dissipation may cause slight rotations of the average macroscopic localization orientation. If I understand well the implementation outlined in the manuscript, in

the phantom node or cutFEM approach used at the structural scale for cracking, the orientation is frozen at the value at the onset of localization. Won't this fixed macroscopic crack orientation induce some stress locking effects in the multiscale procedure? The authors may have not met such problems in most of the reported cases in the manuscript because they deal with cases in which mode I cracking is dominant in the macroscopic sense. A verification that the mixed mode case does not suffer from this (by checking that a continuous decrease of the traction across the macro-interface is obtained) and a comment on how to deal with this would be welcome.

Authors It is true that in the current framework the orientation of a macroscopic cohesive segment is fixed from the moment it is inserted. However, in our view it is not unrealistic to suppose that when a macroscopic crack is growing, the orientation of the microscopic localization band is at some point constrained to remain as it is. Besides, no eminent stress-locking has been encountered in the studied cases with the present framework. As shown in the arbitrary crack path example (Fig. 28) which is a mixed-mode case, tractions with continuous descending branch are obtained (slight fluctuation is caused by the unloading in the macroscale model because of arclength solver). If crack orientation really needs to be updated, the only reasonable point to do it we believe, in phantom node model, is the crack tip element and before the crack propagates to the next element. However, the influence of such adaption to the framework would vanish upon mesh-refinement.

Reviewer The discussion related to the proper upscaling of the energy dissipation is of course useful. The parameter d_c separating the potential cracks at the fine scale (Figure 18) is indeed a useful ingredient, at least in cases in which a periodic microstructure is present. This is in line with the idea of the extraction of a localization zone bandwidth motivated by the same argument in Massart et al., IJNME 2007, in which a periodic material is treated. The idea of correcting the upscaled quantities accounting for the non-dissipating regions of the localizing RVE was also proposed for bending cases in Mercatoris et al., Int. J. Fracture, 2012, by using a (secant) unloading RVE to account for the unloading material inside the localizing RVE. A comment on the difference between this approach and the solution proposed in the manuscript would be a useful complementary information.

Authors The proposed definition of parameter h or d_c is, as commented by the reviewer, in line with the localization zone bandwidth in Massart et al. IJNME 2007. From the geometrical perspective, they both represent the area over which the damage or failure can localize under the assumption of periodic material. This is acknowledged in the revised introduction (page 4) and the results section (page 20) where the definition of h is examined. The difference between the current approach and the previous ones resides in the fact that the contribution from the unloading bulk strain is also included into the enhanced strain tensor term that is used to form the boundary conditions for the softening RVE as shown in Eq. (9). This term is not negligible especially when the crack just opens.

Reviewer 3 (Alfredo Huespe)

The paper aims at modeling fracture in heterogeneous materials using a two scale approach, a macro and a micro scale, respectively. The homogenization is performed at the microscale and some information is scaled upward for the modeling of a propagating crack at the macroscale.

The current interest of this subject in solid mechanics is very high. The authors use a number of techniques taken from previous work in the literature; at the macroscale, they adopt a phantom node methodology for simulating the propagating crack. At the microscale, they adopt an interface with a CZM. Both techniques are well reported in the literature. However, the main contribution of the paper is the full multiscale methodology, considering the BC at the microscale, the technique to compute the width h of regularization at the macroscale crack, etc. The authors present a number of numerical assessments to show the viability of this procedure.

Thus, considering the paper subject, as well as the arguments presented in favor of the methodology, I think that it is potentially acceptable for publication in the journal. However, the authors should consider a number of points, by providing additional explanations, before its final acceptance. The points to be clarified are the following:

Reviewer The assessment of the size h providing microcell size objectivity to the homogenization procedure has not been explained in detail when complex fracture patterns are to be simulated at the microscale. This point should be discussed with greater detail, for example in patterns displayed in Figure 2.

Authors In response to this comment, a new case of a microstructure with complex random cracking pattern (case D) has been added in Section 4.4 to discuss the evaluation of h in such scenario.

Reviewer The model objectivity respect of the microcell size (evaluation of the parameter h) has been proved for simplified unrealistic microscale crack patterns. I suggest the authors to include additional discussion about how the evaluation procedure of h behaves in more complex cases of fracture in heterogeneous microstructures.

Authors Indeed, the micromodel size independence has only been shown for a pre-defined vertical micro-crack pattern in Section 4.2 (now Section 4.2.1). Following the suggestion by the reviewer, the study on the case of complex micro-crack patterns is added into the same section to reinforce this aspect of the model (see the new Section 4.2.2). However, the evaluation of h is not extensively discussed here, since it has been elaborated in more detail in Section 4.4 with a new case of complex microscopic crack pattern (case D, see response to previous comment).

Reviewer It is well known in the microscale problem that periodic boundary conditions excessively constraint the formation of general crack patterns. In several parts of the paper, the authors mention that this type of BC is not a fundamental aspect of the methodology. I do not fully agree with this comment because considering less stringent BC is not a simple derivation of the present model.

Authors The authors agree that the strong periodic BCs over-constrain the failure formation inside the RVE if the localization angle is not align with the periodicity. This is well recognized and discussed in the manuscript at several places (pages 10, 24, 27) and related contributions trying to address this issue are also cited. It is not our intention to make this aspect a less fundamental point within the framework.

Regarding the whole procedure of the upscaling framework, however, the choice of the type of BCs is relatively independent as long as it can satisfy the Hill-Mandel condition. The detailed implementation of the BCs stays on the level of micro-BVPs. So the inaccuracy of it does not impair the validity of the two-scale framework. Of course the derivation of the advanced BCs is not simple, but it stays as a detailed point that can be studied separately.

Reviewer In example 4.4 (Figures 15, 16 and 17), it is not physically expected the formation of a stable parallel microcrack pattern. The simultaneous opening of parallel fractures is an unstable process (DNS cannot provide such solution). Considering this observation, the authors should explain with greater detail this aspect of the problem.

Authors The authors totally agree with this comment. Indeed in all three DNS tests, only one crack path is formed as expected physically because it corresponds to the lowest energy level. The misunderstanding is caused by the red lines shown in Fig. 17, 18 ,19 (previous Fig 15, 16 and 17). It looks like they are parallel cracks, but actually they represent the potential crack planes along which zero-thickness cohesive elements are embedded in the mesh. Eventually only one potential crack plane is opening during the simulation, the others just remain closed. This explanation has been added to the text (page 20). The final crack pattern of one case is also added in Figure 22 to further clarify what is happening in the DNS analysis. Additionally, minor changes have been made to the captions of Figures 17, 18 and 19.

Reviewer Furthermore, it is not physically possible that a crack evolves in time (displaying a monotonous opening process) while the surrounding material display hardening (plastic hardening such as shown in example 4.4). The authors should revise this point of the numerical assessments.

Authors Indeed, the bulk material surrounding an actively evolving crack should not follow a hardening behavior. However, in case C in Section 4.4, the plastic region is devised to be in between (not surrounding) the evolving cohesive cracks and therefore is part of the localization band, as

shown in Figure 1 (below). The plastic strain indeed increased eminently from load-step 100 to

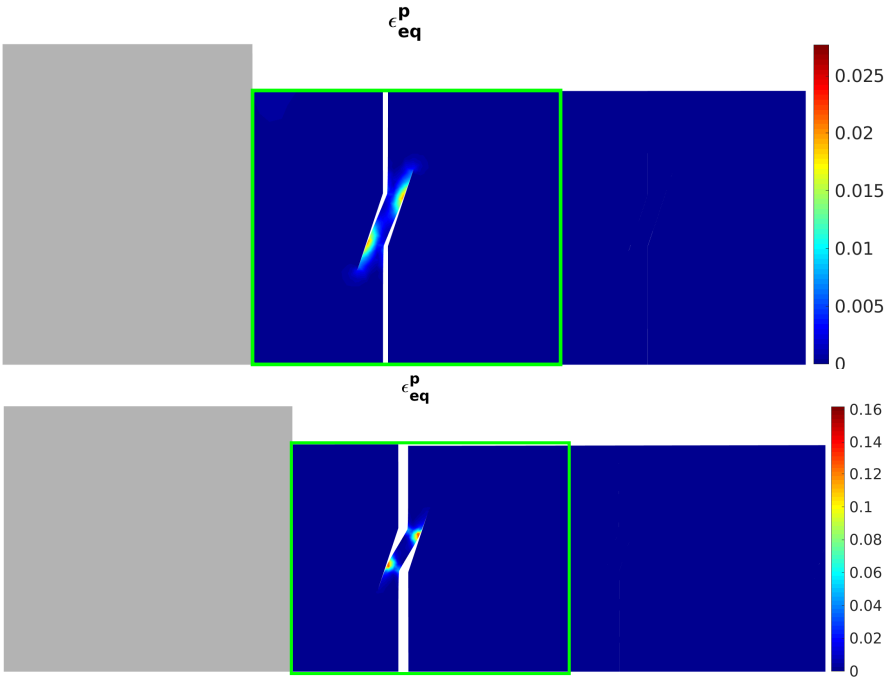

Figure 1 Evolving of equivalent plastic strain of DNS in case C in Section 4.4. Top: Load-step 100; Bottom: Load-step 145.

load-step 145. Even though this is a somewhat artificial case, it is representative of what happens in complex microstructures where global softening with localized deformations takes place while there can still be local mismatch between microcracks in the band.

Reviewer Example 4.5. The experimental test of Galvez et al. displays a macro-crack propagating from the notch root toward the load point. This is not the trend observed in the numerical test presented in the paper. In my opinion, the inaccurate capturing of this crack pattern may be due to the type of BC adopted at the microscale.

Authors The authors agree that strong periodic BCs adopted in this manuscript may give rise to inaccurate development of the crack distribution in the softening RVE. Over-constraining due to the periodicity assumption may cause a delay in the formation of a complete crack path, which overestimates the peak point in the homogenized response curve. And it could also cause deviation of the averaged crack orientation from the correct one to some extent. Another potential cause could be the relatively coarse mesh inside the FE^2 region, which yields poor prediction at the start of the crack. Lastly, the difference of material properties adopted in this manuscript and the experiments also give rise to the fact that an exact same prediction is not expected to obtained. However, as can be seen in Figure 2 (below), the general trend of the obtained crack path is still close to the experimental trajectory. So it is not that bad. As the purpose of this test is to show

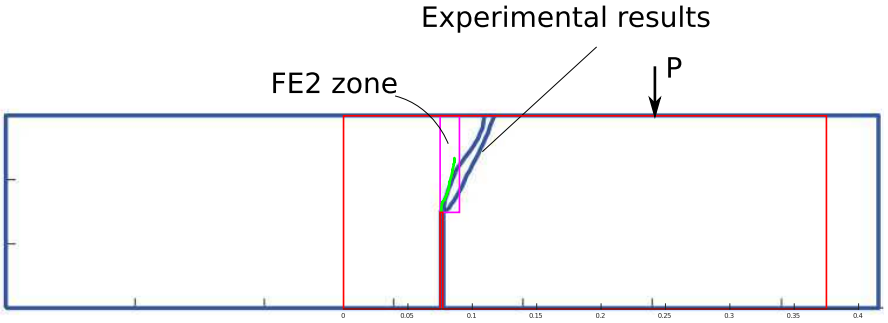

Figure 2 Crack trajectory reference from experiments in Section 4.5

the ability of tracking an arbitrary crack propagation, the results suffice to manifest this point.

Editor's assessment (Laurence Brassart)

The paper proposes a two-scale homogenisation framework to address failure in heterogeneous materials, according to which microscopic failure triggers strain localisation and failure at the macroscopic scale. As noted by the reviewers, the proposed approach builds on a set of existing techniques, which are here combined in a consistent and numerically robust manner. The key novelty is found in the proposal of a geometric scaling parameter dictating the micro-to-macro kinematic transition. All three reviewers acknowledged the scientific quality of the work. Major revisions were however requested to clarify the novelty of the work relative to the state of the art, as well as to clarify several technical points. All three reviewers recommended the paper to be published after the first revision.

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