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Can Multiscale-Multiphysics Methods Predict Softening Damage and Structural Failure?

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The multiscale approach was pioneered by Tadmor, Ortiz and Phillips [1] for atomistic-based quasi-continuum analysis of dislocations and hardening plasticity of polycrystalline metals. In that case, the structural failure is due to necking, which is caused by nonlinear geometric effects of finite strain, or to sharp fracture, which is modelled separately (see also [2]). There can be no dispute that the multiscale approach is realistic, delivering to the continuum macroscale an essential information on the physical behavior on the subscale.

However, applying the multiscale approach to failure due to interacting crack systems, or to softening damage such as distributed cracking, is an entirely different matter. To clarify it, let us discuss a few typical multi-scale approaches representative of a flood of recent publications.

Types of Subscale Interactions in Damage or Fracture

The multiscale models are intended to capture two types of interactions on the microscale:

1. Interactions *among orientations* of micro-damage processes, e.g., orientations of tensile or splitting micro-cracks, and frictional micro-slips.
2. Interactions *at distance*, e.g., among different grains or fibers, or among different micro-cracks and micro-slips. These interactions are of two kinds:
   (a) those affecting the *average stress-strain relation*, and
   (b) those *governing localization*, and the material characteristic length *l*0 in particular.

Type 1 interactions are captured not only by the multiscale model but also by the microplane model, although for the latter they are lumped into one continuum point. Type 2(b) interactions are captured by neither, and because 2(b) affects 2(a), type 2(a) interactions are hardly captured by the multiscale model any better than by the microplane model.

So it appears that the current multiscale (and multiscale-multiphysics) approaches only facilitate the computational handling of strong mesh refinement. They fail to capture the physics of localizing distributed softening damage, such as the cracking and frictional slip in the mesostructure of concrete or the propagation of a softening kink band in fiber composites. These approaches offer real advantages over simpler models such as microplane models only if the material is hardening, but not if it exhibits softening damage which can localize into a crack band or shear band and must be described in terms of a material characteristic length, l_0. An archetypical quasibrittle material is concrete. Others include rock, sea ice, consolidated snow, paper, carton and, most importantly, 'high-tech' materials such polymer-fiber composites, tough or toughened ceramics and rigid foams, as well as many bio-materials such as bone, cartilage, dentine and sea shells. All the brittle materials and many ductile materials become quasibrittle on a sufficiently small scale, for instance metallic thin films and nano-composites.

Let us now clarify how the requirement for physical determination of l_0 defeats the usefulness of the multiscale-multiphysics concept.

Types of Multiscale Models and Material Characteristic Length

- Type 1. A discretized subscale material element is embedded into a point of the macroscale continuum, e.g., an integration point of a finite element (slide 1).
- Type 2. A finite region of the macro-continuum coarse mesh is overlapped by a fine mesh or discrete meso-structure model representing the material on the subscale or meso-scale (slide 2).
- Type 3. A finite region of the macro-continuum coarse mesh is replaced with a refined discrete model of the meso-structure (slide 2).
- Type 4. The interactions in a subscale material element among inelastic phenomena of all possible orientations are lumped into one point of the macro-continuum (slide 1). This leads to a microplane model, representing a semi-multiscale model in which the interactions at distance are discarded.

Generally, only types 1 and 2 have been considered as multiscale methods. However, types 3 and 4 are also multiscale models, and they have some significant advantages over types 1 and 2 when the material exhibits softening damage.

For types 1 and 2, one faces various kinds of difficulties with the regularization of the continuum boundary values problem:

1. Inappropriate boundary conditions of the subscale material element that undergoes softening.
2. Ignoring energy release from the whole structure into the front of fracture or strain-localization band.
3. Replacing subscale micro- or mesostructure with an empirically assumed continuum model.
4. Physically unjustified choice of localization limiter for the subscale material element.
5. Lack of any localization limiter to be delivered to the macroscale continuum.

Normally the strain increment at a continuum point (e.g., an integration point of a finite element) is applied on the mesoscale to a material element (an RVE, or larger) with a randomly generated meso-structure (consisting, in the case of concrete, of aggregates and the matrix). The corresponding average strains of the RVE, which can undergo strain-softening, are calculated by a mesoscale program and are then upscaled, i.e., delivered either to an integration point of a finite element of the macro-continuum (Type 1), or transmitted to an overlapping region of a coarse macro-continuum mesh (Type 2).

Although the macro stress-strain relation may get improved by dipping into the subscale, it is still a *local* strain-softening stress-strain relation. Consequently, the macro-scale tangential stiffness matrix is not positive definite, causing the wave speed to be imaginary, the boundary value problem to be ill-posed, and the equilibrium on the continuum level to be unstable. So, the finite element solutions lack objectivity with respect to the mesh choice, exhibiting spurious mesh sensitivity and convergence to material failure that is localized to a zero volume (domain of measure zero) and thus occurs with zero energy dissipation. This blatantly incorrect feature precludes simulating the energetic size effect [3,4,5,6,7], which is the salient aspect of all quasibrittle or softening failures (in fact, the size effect in concrete, laminates, sandwich shells or other quasibrittle materials seems not to have yet been successfully modelled by any multiscale approach).

Therefore, some sort of a localization limiter, associated with a material characteristic length l_0 or material fracture energy G_f (per unit area, not per unit volume), is crucial in order to regularize the boundary value problem (i.e., make it well posed). Realistic estimation of l_0 is inevitable to model strain softening objectively and realistically, and to capture the size effect.

The simulated material element may be taken as the representative volume element (RVE), the size of which, in the case of strain softening, should be taken equal to only about two to three dominant grain or inhomogeneity sizes [8,9] (slide 1). Since no localization can occur within such a small material element, the desired benefit of physical support for the chosen type of regularization is forfeited.

If the simulated material element is taken to be larger than one RVE, say, a cube having the side of 10 grains (and thus a volume 1000 grains), a localized damage band may develop within such an element (slide 1). But regardless of whether the boundary conditions of this element are periodic, or are specified as displacement or force increments, the width and orientation of the localization band will not be realistic, because the band formation depends not only on the stiffness and energy dissipation of the localization band (of unknown size, orientation and location), but also on the rate of *energy release* not just from this element but from the *whole* structure. The energy release, which is what matters, is conveyed to the band in this larger element through the tangential stiffness matrix of the surrounding structure acting on the boundary nodes of the material element (slide 1). This matrix must correspond to proper loading-unloading combinations everywhere in the surrounding structure. Unfortunately, the existing multiscale models do not meet this requirement.

As a related problem, the stresses and strains in an oversize material volume element that contains a localized damage band can be highly non-uniform. This renders their averages unrealistic for transfer to the continuum macroscale.

Another related problem stems from the requirement that the sum of the volumes of the RVEs associated with all the integration points of one macroscale finite element must be equal to the volume of that element. This requirement has typically been ignored. But then the strain energy release delivered to the macroscale integration point as the RVE unloads is incorrect. Hence, the size of the embedded subscale element and the macroscopic finite element size must be uniquely related.

The characteristic length l_0 governing localization essentially represents the minimum spacing of parallel cohesive cracks, or the localization band width, and governs the type 1 size effect [5]. It is different from (though related to) Irwin's characteristic length $l = EG_F/f_t^2$ which controls the length of the fracture process zone and governs the type 2 size effect [5] (E = Young's modulus, f_t = tensile strength). Unambiguous identification of l_0 calls for computational simulation of and matching of scaled size effect tests on the given brittle heterogeneous material. If the small-size and large-size asymptotic power laws are experimentally or computationally identified, their intersection gives a certain characteristic size l_1, and multiplying it by a proper geometry factor yields l_0. Arbitrary imposition of some kind of localization limiter with characteristic length l_1 into a subscale finite element mesh helps, of course, to stabilize strain-softening but certainly does make the model realistic.

Some so-called 'multiscale' models do not try to simulate the actual heterogeneous microstructure on the subscale (meso-scale). Rather, they simply introduce in the subscale material element a refined mesh and adopt arbitrarily some localization limiter (e.g., the micropolar continuum) regardless of its physical justification. There is nothing *physically* multiscale about such computational exercises. They merely serve as a convenient approach to mesh refinement.

Without a good subscale (micro- or mesotructure) model, the choice of a proper type of localization limiter is another major problem. The existing possible choices include:

(1) a strongly nonlocal formulation (in the form or an integral over a finite neighborhood, or a coupled Helmholtz equation); or

(2) a weakly nonlocal formulation (in the form of the second strain gradient, or the first strain gradient, as in Cosserat's, Mindlin's or Eringen's micropolar media).

Many more choices exist for orthotropic composites. These arbitrary choices of regularization of the boundary value problem do not yield identical results. For example, the micropolar model, adopted for the meso-scale in some recent studies, is known to be a poor localization limiter; it can control only localization into pure shear bands, but not into tensile cracking bands, compression shear bands or compression splitting bands.

Unfortunately, the requirement for some kind of nonlocal model, with a localization limiter involving a material characteristic length, defeats the main purpose of the multiscale approach—modeling based on the physics of microstructure. Thus, in the case of softening damage, the multiscale approach, while more complex, is actually no more realistic than the simpler microplane approach which, too, delivers no characteristic length of material, and requires this length to be introduced separately.

Replacing a Finite Region with Heterogeneous Meso-Structure Simulation

An approach that appears to capture realistically the meso-scale behavior is the CSL lattice-particle model of the meso-structure [10,11,12] (slide 3). Large three-dimensional structures, of course, cannot be simulated in this manner. But even for large structures, the lattice particle model can be used within a small region of the structure where severe distributed cracking, slipping, fracture, or shear-banding is expected, while the regular finite elements are used for the remaining non-softening region. For strain-softening distributed damage, this combination of a continuum with a meso-structural lattice-particle system appears to be the only viable, fully multiscale, approach at present.

Some recent variants, called "multiscale", e.g. the "bridging multiscale method" are not really aimed at capturing the physics on the meso-scale but merely serve to reduce the computational burden of strong mesh refinement. They introduce hierarchical, or sequential, overlapping meshes of different refinements (slide 2). A region of coarse mesh, in which damage is expected, is overlapped by a fine mesh whose displacement field is considered to be additive to the macro-continuum displacement and is intended to capture softening damage with its localization [13, 14, 15, 16, 17].

However, in some approaches (e.g., the 'bridging multiscale method'), the discretization by a fine mesh does not reflect the actual meso-structure of the material. Rather it consists again of a continuum—a strain-softening continuum. This makes it necessary to introduce a localization limiter in the fine mesh on the sub-scale. This localization limiter must again be some type of a nonlocal or gradient model, which must posses a material characteristic length, l_0. So, again, one cannot avoid a purely empirical choice of both l_0 and the type of localization limiter.

Consequently, despite using the term "multiscale", methods such as the "bridging multiscale method" or "sequential multiscale method" are not really complete multiscale-multiphysics approaches as far as damage and structural failure is concerned. They merely supplant to the damage regularization problem on the macro-scale another damage regularization problem on the subscale.

Some approaches (e.g., the "multi-scale asymptotic expansion method") use a homogenization method for the microstructure on the subscale. The resulting stress-strain relation, however, is good only for hardening behavior because the hypotheses of homogenization procedures exclude damage localization and imply absence of l_0 [17].

So it appears that, thus far, there is no way to eschew, on the subscale, a discrete micro- (or meso-) structure model covering the entire region of potential softening damage localization (slide 2). Only such a lower-scale discrete model can capture both the interactions among orientations and the interactions at distance (including the material characteristic length implied by the dominant spacing of material particles, e.g., the grains of the material).

Damage Modelled as Dispersed Cohesive or Singular Line Cracks

When damage is modeled by dispersed discrete cohesive or singular cracks embedded on the subscale, there is no crack band of a finite width, and so one might think that the problem of characteristic material length cannot arise. But it can. In the case of parallel line cracks, there must exist a certain minimum possible crack spacing [18]. While a softening stress-strain relation (with a fixed post-peak) dissipates finite energy per unit volume and thus gives a zero energy dissipation for a band of elements of vanishing size, a system of parallel cohesive cracks whose spacing tends to zero dissipates infinite energy. So the minimum spacing must be a material property representing a material characteristic length [19], which is physically determined by inhomogeneity sizes or by Irwin's length for mesoscale cracks. Otherwise the computational results may be unobjective when the dispersed line cracks remain dispersed, i.e., when their openings do not localize into the opening of one single crack. Such a nonlocalized crack system will occur, e.g., when parallel cracks grow into a stabilizing compression zone [20] or when they are stabilized by transverse reinforcement; see an example in [19]. If no minimum spacing, based on a physically established characteristic length, is imposed, the results will depend on the element size on the subscale and, for vanishing element size, will exhibit a physically impossible convergence.

Special Case of Inertia Dominance at High Impulsive Loads

In the case of dynamics of impact and groundshock, the mass inertia, coupled with the viscous strain rate effect or other damping, may delay any pronounced damage localization beyond the duration of impact event. In that case, the aforementioned regularization of softening damage can be ignored, though only as an approximation (which becomes progressively worse with the passage of time because localization begins to develop already during the impact event) [21]. For this reason, it is appropriate that the finite elements have roughly the size of the material characteristic length (or the width of the localization band). Such an approach corresponds to what is called the crack band model.

Even for high-rate loading problems, it is usually necessary to relate the tensorial constitutive equation base on material properties obtained in standard material tests, uniaxial as well as multiaxial, which are necessarily static. This relationship cannot be realistic if the material characteristic length is not properly captured.

Objectivity Checks for Multiscale Models

The lack of objectivity is best detected by simulating mesh refinement or, equivalently, the size effect in geometrically similar structures (slide 3). The simplest is to simulate a homogeneously stressed rectangular specimen [3]. If mesh refinement leads to different post-peak responses, the multiscale model is not suitable for damage and failure analysis (slide 3, top). Neither it is if, for a cracked two-dimensional rectangular panel (slide 3, middle and bottom), the curves of load versus crack band length, or load versus deflection, change significantly with mesh refinement, or with the scaling of panel size at constant mesh size [19,4]. These simple basic checks should not be ignored.

Analogous Problem in Seismic Structural Tests with Real-Time Simulation of Damaging Zone

In recent experimental studies of seismic resistance of structures, it has become fashionable to use computer-driven servo-control to simulate a cracking zone of a reinforced concrete structure. One technique is to measure a small displacement increment of the surrounding structure, then compute according to a previously calibrated model of the cracking zone the corresponding displacement increments, and then impart these increments, in real time, by fast computer-controlled hydraulic jacks, onto the rest of the structure. Unfortunately, seismic loading is not fast enough to shield this technique from all the aforementioned problems. The simulated cracking zone behaves just like the embedded subscale material element already discussed. As long as this zone is hardening, there is, of course, no problem. But as soon as softening begins, which is what is of main interest, the localization of cracking damage within this zone will differ from reality. The reality is not imposed displacement increments but a two-way interaction (with energy release and proper tangent stiffness constants) of the damage zone with the rest of the structure. To expect a real seismic behavior of concrete structures to be reproduced by such a technique is wishful thinking.

Conclusion

As long as the simulation of subscale mesostructure does not yield the material characteristic length and the type of localization limiter, the multiscale modeling is not a valid approach to softening damage. At present, the only valid approach is a discrete (lattice-particle) simulation of the meso-structure of the entire structural region in which softening damage can occur.

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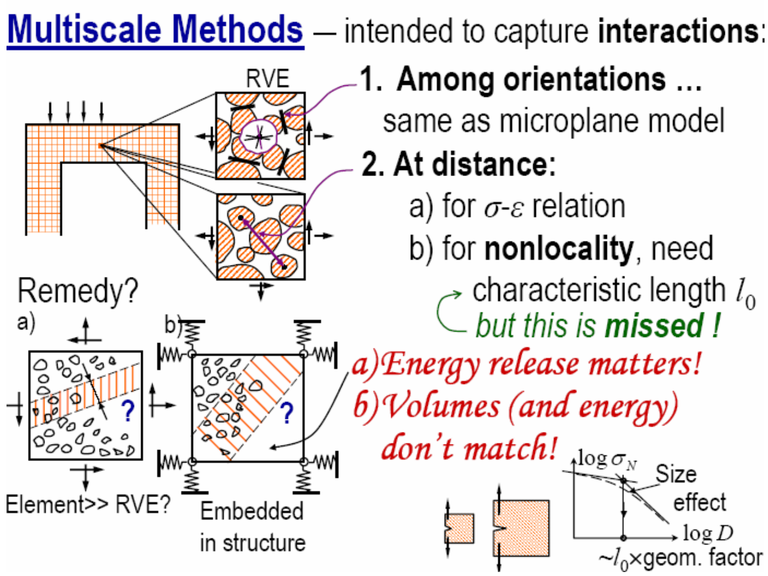
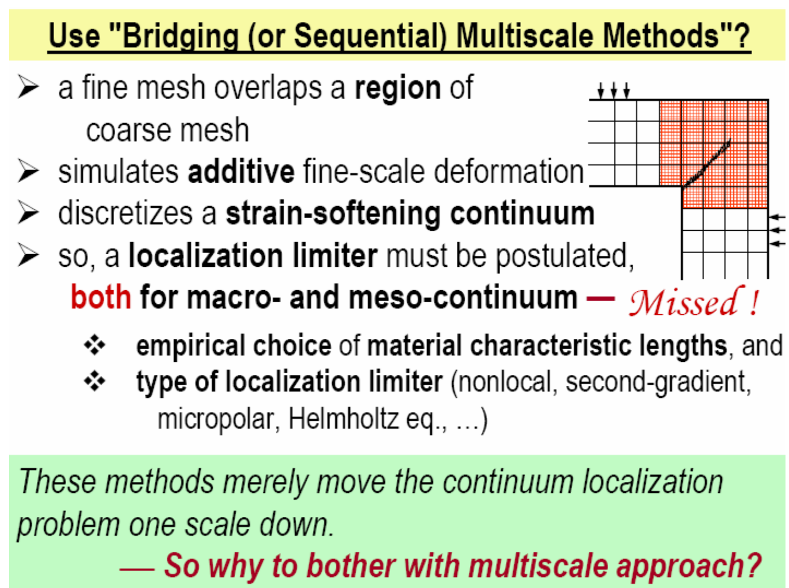
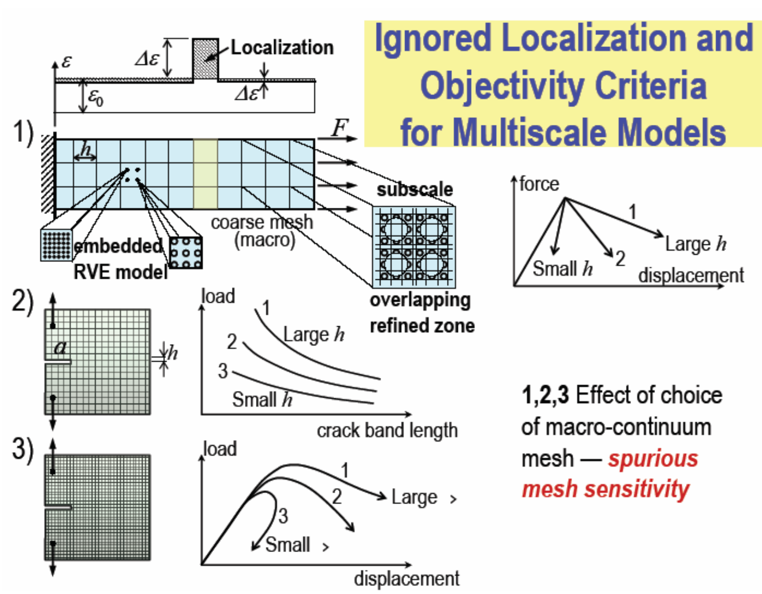


Slide 1: Representative volume element (RCE) embedded in a point of macro-continuum, with interactions among orientations (top right) and at distance (lower right).

Bottom: Material element larger than RVE, with localization band. Bottom Left: Isolated; Bottom Right: Interaction with the rest of structure, modeled by springs of tangential stiffness.



Slide 2 Region of structure where a fine mesh supposed to represent the meso-structure overlays a coarse mesh that discretizes the macro-continuum.



Slide 3 Objectivity criteria for multiscale models, whose check cannot be ignored.