CAN MULTISCALE-MULTIPHYSICS METHODS PREDICT SOFTENING DAMAGE AND STRUCTURAL FAILURE?†

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The possibility of replacing semiempirical constitutive laws with computationally intensive multiscale and multiphysics simulations of complex material behavior on the mesoscale has led to exaggerated expectations. This brief paper shows that this has been the case for the simulation of softening material damage and fracture in quasi-brittle structures. It is argued that the problem of determining the material lengths on the mesoscale and trasmitting them to the macroscale would have to be mastered before realistic predictions of structural damage and failure could be expected.

KEY WORDS: *fracture, damage localization, scaling, scale bridging, material characteristic length, nonlocal models, finite element methods, lattice-particle simulation*

The multiscale approach was pioneered by Tadmor *et al.* (1996) 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 modeled separately [see also Ghoniem *et al.* (2003)]. There can be no dispute that the multiscale approach is realistic, delivering to the continuum macroscale essential information on the physical behavior on the subscale.

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

1. 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 microdamage processes (e.g., orientations of tensile or splitting microcracks, and frictional microslips).
2. Interactions *at distance* (e.g., among different grains or fibers, or among different microcracks and microslips). These interactions are of two kinds:
   a. Those affecting the *average stress-strain relation*
   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.

Thus, it appears that the current multiscale (and multiscale-multiphysics) approaches only facilitate the

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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.

2. 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) (Fig. 1).

Type 2. A finite region of the macrocontinuum coarse mesh is overlapped by a fine mesh or discrete mesostructure model representing the material on the subscale, or mesoscale (Fig. 2).

Type 3. A finite region of the macrocontinuum coarse mesh is replaced with a refined discrete model of the mesostructure (Fig. 2).

Type 4. The interactions in a subscale material element among inelastic phenomena of all possible orientations are lumped into one point of the macrocontinuum (Fig. 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

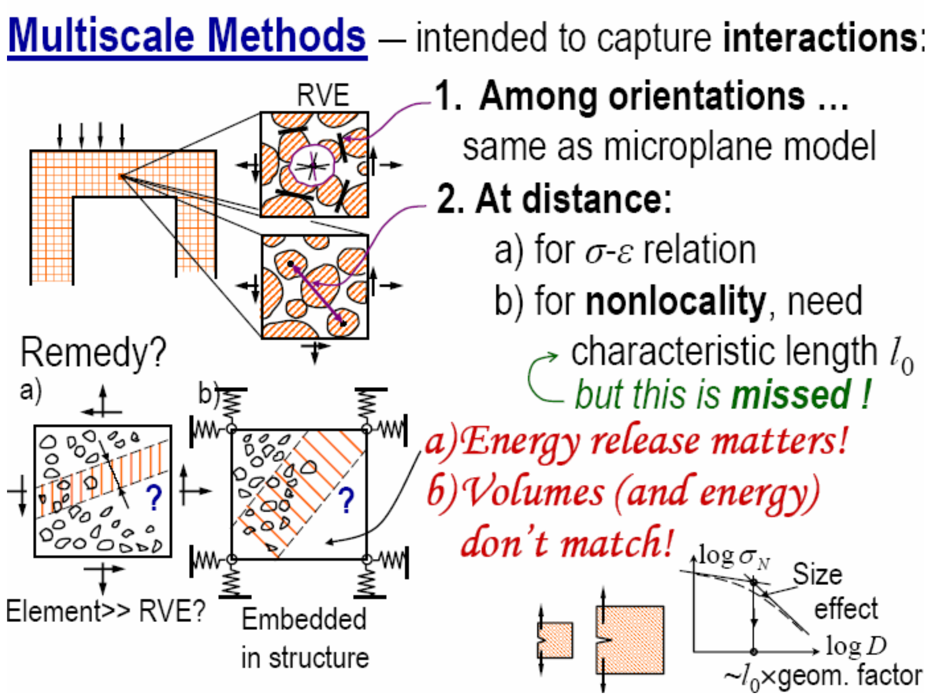

FIG. 1: Top: RCE embedded in a point of macrocontinuum, with interactions among orientations (top right) and at distance (lower right). **Bottom**: Material element larger than RVE, with localization band. Bottom left: Isolated; Bottom right: Interaction with the rest of structure, modeled by springs of tangential stiffness

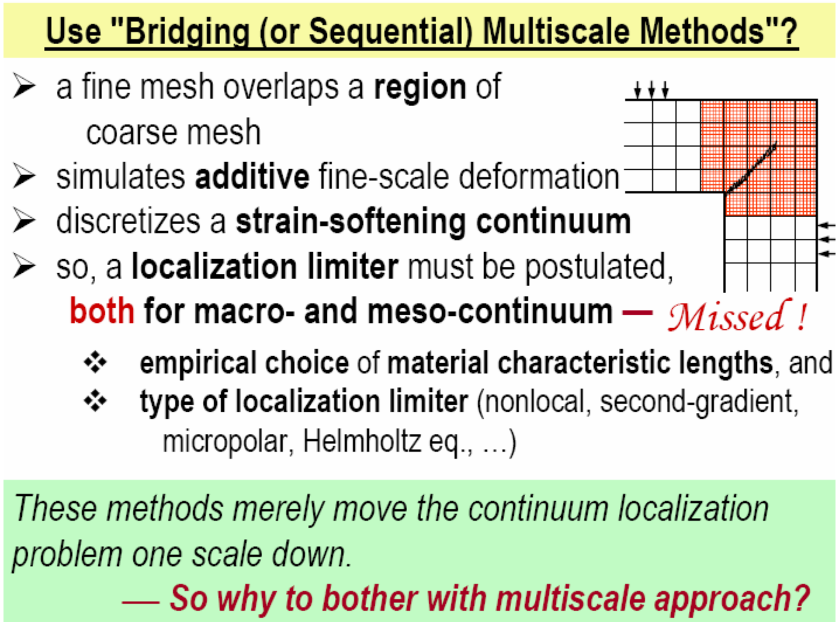

FIG. 2: Region of structure where a fine mesh supposed to represent the mesostructure overlays a coarse mesh that discretizes the macrocontinuum

multiscale models and 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 value problems:

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 [a representative volume element (RVE), or larger] with a randomly generated mesostructure (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 then upscaled [i.e., delivered to either an integration point of a finite element of the macrocontinuum (type 1) or transmitted to an overlapping region of a coarse macrocontinuum 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 macroscale 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. Thus, 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 (Bažant, 1976, 1986, 2002, 2004; Bažant and Planas, 1998), 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 modeled 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 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 (Bažant and Pang, 2006, 2007) (Fig. 1). Because 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), then a localized damage band may develop within such an element (Fig. 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 (Fig. 2). 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 oversized material volume element that contains a localized damage band can be highly nonuniform. 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 (Bažant, 2004). 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 (Bažant, 2004) (E = Young's modulus, f_t = tensile strength). Unambiguous identification of l_0 calls for computational simulation and matching of scaled size effect tests on the given brittle heterogeneous material. If the small- and large-size asymptotic power laws are experimentally or computationally identified, then 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 (mesoscale). 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 mesostructure) model, the choice of a proper type of localization limiter is another major problem. The existing possible choices include the following:

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

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 mesoscale 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.

3. REPLACING A FINITE REGION WITH HETEROGENEOUS MESO-STRUCTURE SIMULATION

An approach that appears to realistically capture the mesoscale behavior is the confinement-shear lattice-particle (CSL) model of the mesostructure (Cusatis and Cedolin, 2007; Cusatis *et al.*, 2006, 2003) (Fig. 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 nonsoftening region. For strain-softening distributed damage, this combination of a continuum with a mesostructural 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 mesoscale but merely serve to reduce the computational burden of strong mesh refinement. They introduce hierarchical, or sequential, overlapping meshes of different refinements (Fig. 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 macrocontinuum displacement and is intended to capture softening damage with its localization (Kadowaki and Liu, 2004; Liu *et al.*, 2006; Fish *et al.*, 1999; Fish and Yu, 2001; Oskay and Fish, 2007).

However, in some approaches (e.g., the "bridging multiscale method"), the discretization by a fine mesh does not reflect the actual mesostructure 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 subscale. This localization limiter must again be some type of a nonlocal or gradient model, which must possess a material characteristic length, l_0. Thus, 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

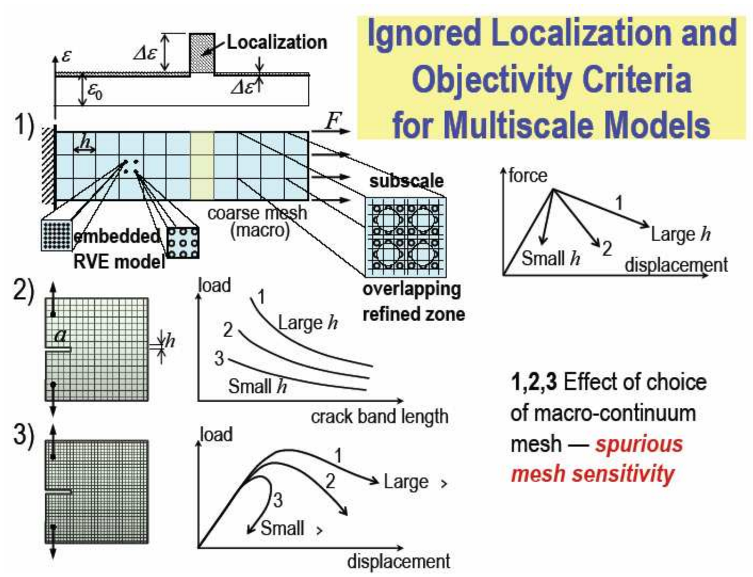

FIG. 3: Objectivity criteria for multiscale models, whose check cannot be ignored

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 macroscale another damage regularization problem on the subscale.

Some approaches (e.g., the "multiscale asymptotic expansion method") uses 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 (Oskay and Fish, 2007).

Thus, 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 (Fig. 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)].

4. DAMAGE MODELED 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 thus 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 (Bažant and Jirásek, 2002). Although a softening stress-strain relation (with a fixed postpeak) 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. Thus, the minimum spacing must be a material property representing a material characteristic length (Bažant, 1985), 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 (Bažant and Wahab, 1979) or when they are stabilized by transverse reinforcement; see an example in Bažant (1985). 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.

5. SPECIAL CASE OF INERTIA DOMINANCE AT HIGH-RATE 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) (Bažant *et al.*, 2000). 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 based 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.

6. 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 (Fig. 3). The simplest is to simulate a homogeneously stressed rectangular specimen (Bažant, 1976). If mesh refinement leads to different postpeak responses, the multiscale model is not suitable for damage and failure analysis (Fig. 3, top). Neither is it if, for a cracked two-dimensional rectangular panel (Fig. 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 (Bažant, 1985, 1986). These simple basic checks should not be ignored.

7. 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 servocontrol 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 the 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.

8. 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 mesostructure of the entire structural region in which softening damage can occur.

REFERENCES

Bažant, Z. P., Instability, ductility, and size effect in strain-softening concrete, *J. Eng. Mech. Div., ASCE.*, vol. **102**(EM2), pp. 331–344, 1976.

Bažant, Z. P. and Wahab, A. B., Instability and spacing of cooling or shrinkage cracks, *J. Eng. Mech. Div., ASCE*, vol. **105**, pp. 873–889, 1979.

Bažant, Z. P., Mechanics of fracture and progressive cracking in concrete structures, *Fracture Mechanics of Concrete: Structural Application and Numerical Calculation*, G. C. Sih and A. DiTommaso, Eds., Dordrecht:Martinus Nijhoff, pp. 1–94, 1985.

Bažant, Z. P., Mechanics of distributed cracking, *Appl. Mech. Rev.*, vol. **39**, pp. 675–705, 1986.

Bažant, Z. P. and Planas, J., *Fracture and Size Effect in Concrete and Other Quasibrittle Materials*, Boca Raton: CRC Press, 1998.

Bažant, Z. P., Adley, M. D., Carol, I., Jirásek, M., Akers, S. A., Rohani, B., Cargile, J. D., and Caner, F. C., Large-strain generalization of microplane model for concrete and application, *J. Eng. Mech. ASCE*, vol. **126**(9), pp. 971–980, 2000.

Bažant, Z. P., *Scaling of Structural Strength*, 2nd updated ed., London: Hermes Penton Science, New York: Elsevier (2005), French translation, Paris: Hermès Science Publ. (2004), 2002.

Bažant, Z. P. and Jirásek, M., Nonlocal integral formulations of plasticity and damage: Survey of progress, *ASCE J. Eng. Mech.*, vol. **128**(11), pp. 1119–1149, 2002.

Bažant, Z. P., Scaling theory for quasibrittle structural failure, *Proc., Nat. Acad. Sci.*, vol. **101**(37), pp. 14000–14007, 2004.

Bažant, Z. P. and Pang, S.-D., Mechanics based statistics of failure risk of quasibrittle structures and size effect on safety factors, *Proc. of Nat. Acad. Sci.*, vol. **103**(25), pp. 9434–9439, 2006.

Bažant, Z. P. and Pang, S.-D., Activation energy based extreme value statistics and size effect in brittle and quasibrittle fracture, *J. Mech. Phys. Solids.*, vol. **55**, pp. 91–134, 2007.

Cusatis, G., Bažant, Z. P., and Cedolin, L., Confinement-shear lattice model for concrete damage in tension and compression: I. theory, *J. Eng. Mech. ASCE*, vol. **129**(12), pp. 1439–1448, 2003.

Cusatis, G., Bažant, Z. P., and Cedolin, L., Confinement-shear lattice CSL model for fracture propagation in concrete, *Comput. Methods Appl. Mech. Eng.*, vol. **195**, pp. 7154–7171, 2006.

Cusatis, G. and Cedolin, L., Two-scale study of concrete fracturing behavior, *Eng. Fract. Mech.*, vol. **74**, pp. 3–17, 2007.

Fish, J., Yu, Q., and Shek, K., Computational damage mechanics for composite materials based on mathematical homogenization, *Int. J. Numer. Methods Eng.*, vol. **45**, pp. 1657–1679, 1999.

Fish, J. and Yu, Q., Multiscale damage modeling for composite materials: theory and computational framework, *Int. J. Numer. Methods Eng.*, vol. **52**, pp. 161–191, 2001.

Ghoniem, N. M., Busso, E. P., Kioussis, N., and Huang, H., Multiscale modeling of nanomechanics and micromechanics: An overview, *Philos. Mag.*, vol. **83**(31–34), pp. 3475–3528, 2003.

Kadowaki, H. and Liu, W.-K., Bridging multi-scale method for localization problems, *Comput. Methods Appl. Mech. Eng.*, vol. **193**, pp. 3267–3302, 2004.

Liu, W.-K., Karpov, E. G., and Park, H. S., *Nano Mechanics and Materials: Theory, Multiscale Methods and Applications*, Wiley, Chichester, UK (Sec. 6.8), 2006.

Oskay, C. and Fish, J., Eigendeformation-based reduced order homogenization, *Comput. Methods Appl. Mech. Eng.*, vol. **196**, pp. 1216–1243, 2007.

Tadmor, E. B., Ortiz, M., and Phillips, R., Quasicontinuum analysis of defects in solids, *Philos. Mag. A.*, vol. **73**(6), pp. 1529–1563, 1996.