Computational Fracture Mechanics of Concrete Structures: A Retrospective through Multiple Lenses

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ABSTRACT: The history of the application of computational fracture mechanics to concrete structures, now 5 decades old, is interesting from many perspectives. In this paper, a retrospective of computational fracture mechanics in concrete structures (ComFraMCoS) is presented through five lenses. These lenses clarify research trends through an historical overview. We intend to interlace the views through these lenses to sometimes offer admittedly slanted insights, to question the *status quo* and to provoke thought and discussion about future directions of ComFraMCoS.

1 INTRODUCTION

One can easily support the argument that the distinct field of computational fracture mechanics itself arose from concerns about cracking in concrete structures, both plain (e.g. dams, Clough 1962) and reinforced (e.g. beams, Ngo & Scordelis 1967). In past publications there have been many well-written reviews of the work in computational fracture mechanics in concrete structures (ComFraMCoS). Therefore, the goal of this paper is not to serve as a complete summary or technical report, but to extrapolate from the history and suggest future directions for ComFraMCoS research. To do this, we choose a retrospective through 5 lenses: computational resources, software, physics, practice and dimensionality.

The Lens of Computational Resources – George Irwin was doing his best thinking at the same time that electronic computation was being invented. So it was serendipity that the field of fracture mechanics could hop on and ride the still growing wave of computational resources our generation has been lucky to have. But, with teraflops of power, petabytes of storage, and amazing visualization capabilities available for the taking, why has ComFraMCoS appeared mostly to languish on the fringes of this digital revolution? What is inhibiting our field from unleashing all that power on our most fundamental problems?

The Lens of Software – How many distinct ComFraMCoS programs have been written by graduate students worldwide? How many of these programs have broken new ground in numerical methods for solution of boundary value problems, as opposed to revealing new insights into the physical processes they seek to simulate? We see improvements in software as quite different from enhanced understanding of the physics driving fracture processes. The ComFraMCoS community can take pride in contributing significantly to the invention/evolution of smeared cracking, damage mechanics, cohesive constitutive models, meshfree methods, and enriched element methods. But, have we perhaps been a bit too distracted by the novelty of variations in such numerical methods for software implementation rather than finding ways of applying it to answer fundamental questions heretofore intractable?

The Lens of Physics – How much more about incubation, nucleation, microscopically small and large propagation of cracks in reinforced concrete (RC) do we really understand from first principles now compared to 40 years ago? Can the surrogates for physics such as stress intensity factors, damage measures, critical energy release rates, cohesive strengths, whatever your favorite flavor of fracture mechanics, ever capture sufficiently well what is actually happening in a real concrete structure? Our answer is no. What will be required to focus the current generation of graduate students on multidisciplinary approaches, combining computational science and materials science, condensed matter physics and chemistry, and structural mechanics, needed for breakthrough discoveries that will lead to fundamental knowledge in the analysis and design of RC structures?

The Lens of Practice – Is it amazing or embarrassing that after 5 decades, a period during which any

number of other fields of engineering have been born, matured, and completely remade themselves multiple times (e.g., biomedical engineering, MEMS engineering) ComFraMCoS has had so little tangible effect on everyday practice in the analysis and design of concrete structures? It was perhaps naive to think that practice in the field of concrete structures would quickly adopt the more physics-based rules of behavior that have evolved from academic research into the fracture mechanics of concrete. Witness the two-decade struggle to modify the ACI code for size effect in shear. Why haven't full-field, non-linear modeling approaches evolved from ComFraMCoS been adopted?

The Lens of Dimensionality – This lens has two foci: the dimension of the scale of investigation, continuum, meso, micro and atomistic; and the dimension of the space of inquiry, 2D or 3D. More than 20 years ago, truly exciting work began to appear in the ComFraMCoS literature in which the constituents of concrete and small but important details of reinforcement were explicitly represented in both geometry and mesh models. We view these early efforts as precursors to what is now recognized as multiscale modeling. Why, however, in 2007 does the majority of the new ComFraMCoS journal literature have an exclusively continuum focus? Allied fields of composites and even metals have turned their foci downscale towards an integration of condensed matter physics, materials science, and structural mechanics, purposely injecting as much geometrical realism at each length scale as possible into their simulations. Why is the same approach not being taken, for the most part, in ComFraMCoS? And, why, in 2007, with all those teraflops and petabytes lying around, and with uncertainty of planar behavior ever really existing anywhere, is the vast majority of the work in ComFraMCoS still 2D?

It is common to assume at least four distinct length scales comprising concrete: structural, mesoscale, microscale and nanoscale. At the structural length scale, concrete is treated as homogeneous and elastic or elasto-plastic, and linear elastic fracture mechanics is considered applicable for some geometries.

At the mesoscale it is common to include three material phases: aggregate, mortar, and the interfacial transition zone (ITZ) between them. The consensus is that models of this length scale span volumes with edge length $O(10^2 mm)$. The microscale is considered to be the hardened cement paste with characteristic edge length $O(10^{-1} mm)$. The discontinuities at the microstructural length scale are capillary pores. Finally, the nanoscale describes hardened cement gel containing nano-pores (Zaitsev & Wittmann 1981, Cusatis et al. 2006).

We will attempt to show that these lenses are not separate, but rather align, like the multiple lenses in a telescope, each with its own function designed to contribute to a clear and bright image. Carrying this analogy forward, in the last part of the paper we will attempt to rotate this telescope around so that we are peering into the future of ComFraMCoS.

2 LENS OF COMPUTATIONAL RESOURCES

The field of ComFraMCoS has been relatively limited in its scope of investigation due to the perceived computational demands, viewed broadly, of the models developed. Unlike some of our sister disciplines, we seem to have been more self-saddled by an apparent lack of, or lack of will to use, computer power. It is our opinion that this inexplicable malaise can be traced back even to the introduction of smeared cracking to avoid the perceived cumbersome and computational demanding geometrical representation of even a single crack.

Indeed, the most detailed, 3D, mesoscale simulations, which include the most elaborate material models with the best available physics, are still intractable in any material system, but at least investigators in many other material systems are trying (McDowell et al. 2003, Attinger & Koumoutsakos 2004)! It is the responsibility of the ComFraMCoS research community to underpin the practice community with ever-increasing understanding of fracture processes and ever-improving means of injecting this understanding into analysis, design, repair, and forensic efforts. "Ever-increasing understanding" means more science and less guessing/simplification/approximation/empiricism. Therefore, we cannot allow our vision to be limited by the PC on one's desk. In the U.S., for example, the National Science Foundation (NSF) has established the TeraGrid (www.teragrid.org), a computing grid with near-petaflop scale computers, high-bandwidth connectivity, petabyte storage, and exotic visualization capabilities, all on a relatively low-traffic 10 Gbps network. *Why are ComFraMCoS researchers not using the TeraGrid?* Possible answers include:

1. We have never built models that need such awesome capability. But at one end of the length scale spectrum, surely we have *concrete structures* with high geometric complexity, dynamic and stochastic boundary conditions, and complex cracking events to demand such capability. At the other end of the spectrum, surely we have *concrete material* which, at the mesoscale and below, has high geometric complexity, stochastic properties, coupled-physics phenomena at work, and exquisitely exciting cracking processes to also demand such simulation capability.

2. A perception that there is overwhelming over-

head in creating and deploying the software components that can use such capability advantageously: the risk is too high compared to the possible reward. But, our community need not be overwhelmed by such fantastic capabilities. There is a huge and ever-widening gap between what's on the desktop and what is on the TeraGrid, and there is plenty of opportunity in between to begin to grow the software and increase model complexity to use cyberinfrastructure more effectively.

3. A perception that our current models are "good enough" for practice. But, this answer begs the question, because it cuts off the principal responsibility of the research community cited above.

It is important to remember that what once was intractable is now commonplace; what once took days on massive supercomputers can now be done in a few seconds on one's laptop. This trend is destined to continue, and the field of computational mechanics will be able to perform elaborate, multiscale, multiphysics simulations previously only imagined. Why not ComFraMCoS?

3 LENS OF SOFTWARE

Our ComFraMCoS community has been a wellspring of innovation in software and algorithms for representation of cracking, and for constitutive models for cracking. In the former category, we have given, or significantly aided the computational fracture community in the development of the following, in roughly chronological order: smeared cracking; discrete cracking with adaptive remeshing; particle and lattice models for cracking; meshfree cracking; and enriched element cracking.

In the latter category of achievements, ComFraMCoS researchers have made vital contributions to: fictitious cracking concept and cohesive zone models; non-local plasticity; and damage mechanics.

However, with all these sterling innovations to our credit, what have they added to our *fundamental understanding* of cracking processes in concrete? For example, what new physical insights at the micro or meso length scales have arisen from application of meshfree or enriched element methods?

Surely, these approaches have made model generation easier, and they should be setting the stage for development of multiscale, multiphysics simulation systems that themselves can perform within TeraGrid-like environments. In our opinion, the principal reason for creating and applying multiscale simulation systems is to expose the sources of variability originating with the material structure at the lower length scale, and to carry this variability upwards to discover its effect on variability of strength at the upper, structure scale. When such a process starts at the micro or meso scale, there will likely be a requirement to represent multiple 3D cracks, to propagate these under as-yet-undiscovered rules of rate and shape change, and to investigate the effects of variability of the geometry and material properties on the resulting evolution of the cracks at such a scale, using, for example, Monte Carlo-like approaches. Feedback to the structure scale would then ensue, and this iterative process would be continued to a desirable termination state. Figure 1 shows the qualitative process for such a multiscale simulation where the major steps are separated into A, B, C, D and E. In Step A, the structural model is analyzed and a critical region identified. In Step B, local boundary conditions are extracted for placement on the model to undergo higher resolution analysis. In Step C, the local model is analyzed to produce the needed fields. In Step D, the cracking criterion is enforced. In Step E, the continuum constitutive model is updated to reflect the response of the local model. The system outlined in this flowchart begs for a TeraGrid-class environment.

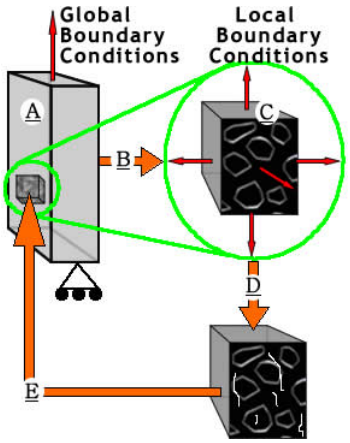

Figure 1. Flowchart describing a multiscale simulation with information flow between length scales

4 LENS OF PHYSICS

In general, the appearance of a crack in a structure and its growth through loading spans multiple time and length scales. A major focus of past research has been to observe the mechanisms of crack growth across *some* length scales and use these observations to develop more accurate models of structural behavior. However, because of difficulties in observing and simulating phenomena at lower length scales, we often resort to simplified *mechanics*, rather than purely *physics*-based models. For example, Figure 2 shows two distinct length scale views of concrete, microscale (top) and mesoscale (bottom). The cracking processes in Figure 2 (bottom) have been simulated using continuum *mechanics*-based models for consti-

tutive behavior and limit states in the hardened cement paste, aggregate and the interface zone. However, this is clearly not a best *physics*-based approach. Figure 2 (top) shows the lower scale at which, even more fundamentally, the cracking process takes place amidst C-S-H rods and other microstructural features. While researchers in other materials systems are analogously creating simulation capability at both of these scales, to the best our knowledge the CoMFraMCoS community is not yet at work at the lower length scale of Figure 2 (top). It is important to consistently seek the most fundamental understanding of the phenomena in a material system in question so that comprehensible, *physics*-based models can eventually be developed.

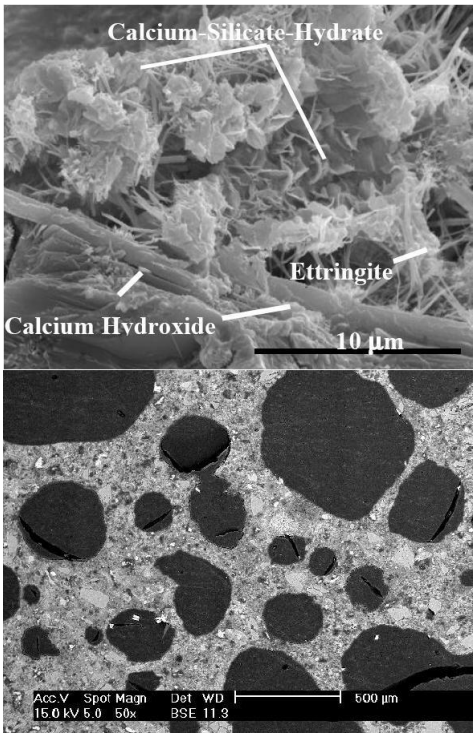

Figure 2. Two distinct length scales of concrete: microscale (top, Stutzman 2001) and mesoscale (bottom, Roels et al. 2002).

As will become clear through the next section, the Lens of Practice, size effect on the nominal tensile strength of concrete is crucially important to concrete structure design. Size effect, like any other observed phenomenon, can be explained through modeling and simulating the fundamental processes of concrete cracking. However, before the discussion of current size effect models, important understanding gained through experimental observation is discussed. This will give a good perspective of how knowledge gained from observation is incorporated within current models and design practice. The following section describes briefly the driving mechanisms of concrete fracture incubation, nucleation, and localization of dominant cracks.

4.1 *Important experimental observations*

As summarized by Slate & Hover (1984), concrete material response is largely dependent on cracks, even under multiaxial compression loading, that incubate, nucleate and propagate during curing and loading. The mesoscale, Figure 2 (bottom), is the focus of the following discussion since most experimental observation and computational modeling have occurred at this scale. As described in our introduction, it has been observed that the ITZ is the main crack initiation site for curing concrete and the "dominant mechanism in concrete fracture" (Vervuurt & van Mier 1995). Each of the constituents in the mesoscale undoubtedly affects the response to loading; but, what exactly are those effects and how are their individual responses coupled? From past observation, it is well-known that crack incubation, nucleation and propagation play a dominant role in concrete response to loading (Kotsovos 1979, Ditomasso 1984, Vervuurt & van Mier 1995, van Mier 1997).

Cracks begin at the lowest length scales and grow through loading, residual or applied. Depending on the material system, these cracks may nucleate in particles, composite constituents, or among many other possibilities along naturally arising interfaces. Often, cracks are introduced before loading takes place; such cracks are termed preloading cracks. One example of a preloading crack location is at the aggregate-matrix interface on the mesoscale. Estimates from numerical techniques suggest that tensile stresses as high as 1800 psi can exist at these interfaces due to shrinkage strains alone (Slate & Hover 1984) and cause crack formation along interfaces before loading. Since these cracks develop on the aggregate length scale, they are termed here as mesoscale cracks.

Such initial mesoscale cracks are the traditionally observed beginning of cracking in concrete. Upon loading, existing interface cracks start to grow and new cracks are incubated and nucleated in the aggregate and cement matrix. A typical stress-strain plot of concrete shows that the response remains relatively linear up to approximately 30% of the ultimate applied load. This linear behavior implies that crack formation and growth during this period is minimal. As inherent cracks propagate and new cracks are incubated and nucleated, the available load paths are reduced; as a result, stress on the intact load paths is increased and the concrete begins nonlinear, inelastic response. Overall, it is evident from experimental observation that cracking during curing and loading dominates the shape of the concrete response curve. Therefore, the many mechanisms by which mesoscale cracks incubate, nucleate and propagate can and should be incorporated in models to simulate the bulk material and structural behavior.

From past observations of the mesostructure, it has

become clear that the nonlinear response of concrete is due to the strain localization caused by microcracking (Bažant et al. 1998). From linear elastic fracture mechanics (LEFM) much of the ability to predict the fracture process comes from the assumption that the fracture process zone (FPZ) is much smaller than a characteristic structural length. The FPZ, in concrete, is characterized by a softened zone near a structural-scale crack tip where tensile stress has exceeded the nominal tensile strength and significant localization of mesoscale cracking has occurred (van Mier 1997, Bažant et al. 1998). The cracks causing softening in the FPZ coalesce with the structural-scale crack as it propagates through the FPZ. If a significant FPZ is present, i.e. the FPZ is not negligible when compared with the structural dimensions, there will exist a size effect on the structural response characteristics that must be considered (Bažant 1992). By size effect, it is meant that structures that are different in size will exhibit different material properties even when the structures are fabricated using the same material and are geometrically similar (Atkins 1999). From experimental observations of fundamental mechanics of concrete, the size effect can be modeled, in full detail, to both increase understanding of these fundamental mechanisms and to improve structural reliability and efficiency. Currently, we resort to empirical methods as outlined in the following section.

5 LENS OF PRACTICE

In general, research in the form of detailed analyses and simulations is directed at improving design codes and overall understanding, which are of utmost importance to structural engineering of concrete structures. Usually, because of a time constraint, completely detailed analyses are not feasible and the general code equations guide the engineer along a quicker, more conservative path to a safe design. Considering the application of fracture mechanics to the design of concrete structures, here are two key questions:

1. Why is detailed analysis/simulation of cracking in concrete necessary? If a concrete structure has developed cracks that are subject to forensics or repair (Ingraffea et al. 1995), then it is unclear how overarching code equations could possibly be developed. In such cases, detailed analysis must be carried out where a code would only be sensible as a guideline for acceptable methods; and

2. Why are simplified, fracture mechanics-based, design equations necessary? For design of concrete structures, a globally accepted size effect theory would provide a more exact means to extrapolate strength characteristics to large scale structures that are too costly or impossible to test. The size effect causes structures to act less ductile as size increases. Currently, a simple linear extrapolation based on the compressive fracture strength of laboratory-sized specimens exists in the ACI code, possibly resulting in unconservative designs (Bažant et al. 2005). Because of this potentially dangerous situation, the inclusion of the size-effect concept in the design of concrete structures would be beneficial.

For the range of possible applications of fracture mechanics in concrete structure design codes it is postulated that: for cracked structures, usually in the arena of forensics or repair, detailed analysis should be required where the crack(s) are represented so that stress and strain fields can be correctly computed; and for more typical design of large concrete structures, general code equations accounting for the size effect should be utilized. By not accounting for the size effect, crude estimates for the nominal tensile strength of very large concrete structures, by a simple extrapolation of gathered data from smaller concrete specimens, overestimates the nominal tensile strength for concrete by up to 80% (Bažant et al. 2005). The inclusion of a size effect equation to more correctly predict structural strength would effectively introduce some knowledge of fracture mechanics into concrete design, improving structural reliabilty and efficiency (Hillerborg 1989).

The well-known weakest link model, which assumes that failure occurs at the onset of a macroscopic crack in an element, is the classical explanation of the size effect. The model is problematic since, among many other reasons, it does not account for the localization of mesoscale cracking in the FPZ. However, size effect on structures failing at the nucleation of a macroscopic crack, with a negligible FPZ, can be explained well by the weakest link model (Bažant 1992, Bažant 1995). Since the ratio of FPZ size to structural dimension is important to crack growth, there needs to be consideration of this influence on size effect. The following theories account for this ratio through a modified cohesive zone model, which is ignored in the weakest link model.

Currently, there are many theories correlating the size effect with fracture mechanics. In the modeling of size effect, three models are attractive: energetic-statistical; multifractal scaling; and the two-parameter cohesive crack model. These theories, although comparable for structural scales that are at or near the generally tested domain (Planas et al. 1995), differ at very large structural scales, the scales which are subject to representation through a size effect model. Because of their differences at these critical length scales, knowledge of the concepts and assumptions that define the three models is important.

5.1 *Energetic-statistical theory for size effect*

The energetic-statistical theory for the size effect on material characteristics, such as nominal tensile strength, is a combination of both a Weibull (weakest-link) statistical distribution and a deterministic, energetic approach (Bažant et al. 2005). This approach has its origin in the cohesive crack model of Hillerborg (Hillerborg et al. 1976). The combination of the two theories provides the ability to match asymptotic behavior of very large and very small structural scales. For this theory, there are two separate equations modeling the size effect in a SEN(B) beam specimen that represent three major cases: structures having large fatigue cracks or notches with significant FPZ; structures failing immediately after crack and FPZ formation; and structures experiencing stable crack growth with nonzero stresses in the FPZ. The first and third cases are represented by:

$$\sigma_N = B f_t \left[1 + \frac{D}{D_0}\right]^{-\frac{1}{2}} \tag{1}$$

where σ_N is the nominal strength of the beam, B is a constant depending on the cracked structural geometry, f_t is the tensile strength, D is the beam depth and D_0 is dependent on, among other things, beam depth, width and initial crack length (Bažant et al. 2005). It is assumed in the derivation of this equation that the ratio of crack length, a, to beam depth, D, is a constant, which enforces a geometric similarity condition for tested structures and design components that depend on the size effect rule. This means that, in order to make a sensical prediction of the nominal strength of a beam that is too large to test, one must test a geometrically similiar specimen in the lab. To support the assumption that a test specimen is geometrically similar to the large-scale structure, verification using a computational model is suggested (Bažant et al. 2005).

For the case of failure at crack formation, the size effect is represented by:

$$\sigma_N = \sigma_\alpha \left[\left(\frac{D_b}{\eta D_b + D}\right)^{\frac{r n_d}{m}} + \frac{r D_b}{\eta D_b + D}\right]^{\frac{1}{r}} \tag{2}$$

where r, η, n_d, and m are empirical constants, D_b is the thickness of the cracked layer of the tension face of the beam and σ_α is dependent on, among other things, beam depth and width (Bažant et al. 2005). This case is not dependent on a crack size since it is assumed that the structure is failing at the first appearance of a crack.

5.2 *Fractal theory for size effect*

The fractal theory for the size effect of material strength is based on the hypothesis that fractal features of a fractured material can be linked to material characteristics (Carpinteri 1994, Carpinteri & Ferro 1994). Consequently, by using the fractal theory, the material characteristics are scale-invariant and are expressed in noninteger dimensions. The fractal dimension is a nondimensional quantification of the tortuosity of the cracked surface at various resolutions (Carpinteri 1994, Carpinteri & Ferro 1994). It is the contention of supporters of this theory that the constraints imposed by formulating the size effect within Eulerian space, namely that of integer dimensions, must be lifted. By utilizing fractal theory, the integer dimension constraint is lifted and material-dependent constants can be expressed in terms of non-integer spaces (Carpinteri et al. 1999).

The fractal theory also builds on the cohesive crack model proposed by Hillerborg to account for the FPZ and produces a scale invariant, cohesive crack model. Classically, self-similar fractals were the widely utilized fractal sets; however, self similar fractal patterns are not able to capture the size effect at large length scales (Carpinteri et al. 2006). Consequently, theory for self-affine fractal sets has been used to extend the cohesive crack model, which enables the fractal theory to capture the size effect at large length scales.

The three material parameters that are included in the cohesive crack model are nominal tensile strength, fracture energy and critical displacement or strain. In the fractal theory, the size effect on each of these parameters is initially considered separately and then coupled in a final step (Carpinteri et al. 2006). For an intuitive, specific example of the fractal theory for size effect on fracture energy, consider a cracked concrete block loaded in simple tension (Carpinteri et al. 2006). As the crack grows the work of fracture is, based on the cohesive crack model, calculated as $\mathcal{G}_f \times b^2$ where $\mathcal{G}_f$ is fracture energy and b is the block width and depth. This is obviously an idealization for the case of concrete, since the crack surface is not actually flat. The fractal theory represents a crack face tortuosity by employing a fractal pattern, determined from experiment, to obtain the crack surface fractal dimension (sometimes called the crack face roughness). From the observation of fractal features on a fractured surface, the fractal dimension is found and the fractal work of fracture is expressed as $\mathcal{G}_f^* \times b^*$, where $\mathcal{G}_f^*$ is the fractal fracture energy now scale-invariant, unlike $\mathcal{G}_f$, and b^* is the fractal area, which is approximately $b^{2+f_{dim}}$, where f_{dim} is the fractal dimension of the fractal pattern. In the fractal theory, the size effect on nominal tensile strength, fracture energy and critical strain are interdependent; therefore, in order to achieve a model for all three, any two must be computed independently and the third is found through their relationship. (Carpinteri et al. 2006).

To provide qualitative comparison with the other theories, the multifractal scaling law can be written

as:

$$\sigma_N = f_t \left[1 + \frac{l_{ch}}{D}\right]^{\frac{1}{2}} \tag{3}$$

where l_{ch} is a constant, characteristic length of the material and D again is a typical structural dimension (Carpinteri et al. 2006). The characteristic length, l_{ch}, is a representation of the microstructural disorder for the material and defines the transition scale between the fractal scale to the Euclidean scale.

Comparing Equation 3 with 1, it is seen that both of the theories use a power law to express the size effect. In fact, these theories, although fundamentally very different, produce very similar predictions of size effects. This similarity especially holds for structural sizes below the aforementioned l_{ch} transition scale of the fractal theory (Planas et al. 1999).

5.3 *Two-parameter theory for size effect*

The two-parameter theory for size effect is built entirely on the concept of a cohesive crack (Planas et al. 1995, Planas et al. 1999). The cohesive zone concept represents the processes occuring in the FPZ as a fictitious crack surface with a representative stress transfer between crack faces still occurring within the FPZ. Initially proposed by Dugdale and Barrenblatt, Hillerborg extended the concept of a cohesive crack to concrete without the restriction that a structural-scale crack had to exist. Since this model represents the softening due to cracking in the FPZ, the softening regime of the loading response for concrete must be parameterized. It turns out that using two parameters, namely the nominal tensile strength and w_1, both shown in Figure 3, a size effect equation can be deduced by composing two separate laboratory experiments (Bažant et al. 1998).

The two-parameter theory, detailed by Bažant et al. (1998) and Planas et al. (1999), is an iterative, inverse method that can be reduced to the simple procedure given as:

1. The mean splitting tensile strength, $\bar{f}_{st}$, is initially approximated using results of a Brazilian splitting tensile test.

2. The mean flexural strength, $\bar{f}_f$, is measured from SEN(B) specimens with an initial notch length, a_0, and typical structural dimension D.

3. The characteristic material length, l_1, is calculated from a cohesive zone model as:

$$l_1 = \kappa D \left[\frac{13.11}{(x^2-1)^2} + \frac{2.68}{x}\right] \tag{4}$$

where $\kappa = 1 - \alpha_0^{1.45}$, $\alpha_0 = \frac{a_0}{D}$, $x = (\eta_0 \frac{f_t}{f_f})^2$ and $\eta_0 = 3(1-\alpha_0)^2$.

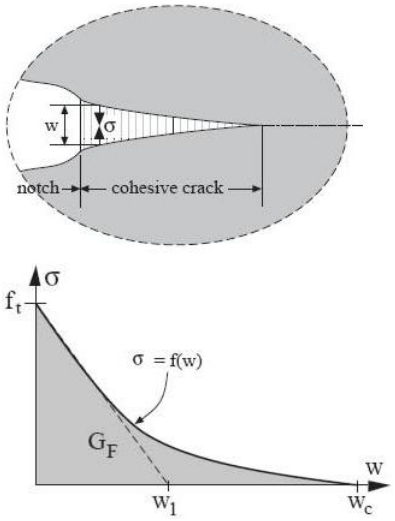

Figure 3. Linear approximation of softening made by two-parameter model (Planas et al. 1999).

4. From the results of the previous step, calculate $\frac{D}{l_1}$ and use the closed-form expression for size effect based on the cohesive zone model:

$$\rho = \frac{f_{st}}{f_t} = \frac{1}{c_1 + c_2 \frac{D}{l_1}} + c_3 \tag{5}$$

which was developed by Rocco et al. (1999). Optimum values for c_1, c_2 and c_3 are given therein for D/l_1 on the interval $[0.4, 10]$ and various ratios of bearing strip width to structural dimension, D. It was found that the width of the bearing strips had a large effect on the splitting tensile strength, $\bar{f}_{st}$ (Rocco et al. 1995, Rocco et al. 1999).

5. The value for nominal tensile strength is now updated by $f_t^{i+1} = f_t^i / \rho$ where i is the current iteration and $f_t^{i=0} = \bar{f}_{st}$.

With an updated value of f_t, a new characteristic material length, l_1 must be recomputed and, consequently, an iteration of steps 3 - 5 is required for increased accuracy. As noted in (Planas et al. 1999), when $f_t^{i+1} - f_t^i \lesssim 2\%$ further iterations are fruitless because of the accuracy of the closed-form solutions utilized in step 3.

6 LENS OF DIMENSIONALITY

The Lens of Dimensionality incorporates both the length scale of the simulation, as well as the spatial dimension of the simulation, 2D or 3D. In this section, we review the contributions of other researchers as they have begun to burrow down scale from the structural scale. It so happens that the spatial dimension of investigation becomes interspersed in the discussion about length scale.

The mesoscale is where the largest body of literature for the Lens of Dimensionality can be found. Consequently, this length scale will be the focus of this section. Discretization in these models contributed to the largest variety in the literature, and, thus, the largest discrepancy of the treatment of fracture, as will be discussed. Typically, if the micro- and nanoscales are included, it is only phenomenologically through effective material models.

6.1 *The mesoscale*

As indicated, the majority of work done in computational fracture mechanics of concrete, at length scales other than the structural, has been focused on the mesoscale. The efforts have only recently turned to three-dimensional representations of the mesoscale. To model the mesoscale, a geometry must be generated, the domain of that geometry must be meshed, the elements of that mesh must be given rules governing their constitutive behavior, and boundary/initial conditions must be assigned.

6.1.1 *Geometry of the mesoscale*

Generation of realistic mesostructural geometry requires considerable discussion. Typically, generating the geometry is a two-step process. First, a representative aggregate geometry is generated independent of location. In the second step, the aggregate is placed in the study volume in a random location. This process is commonly referred to as the take-and-place method.

The aggregate size is described by a cumulative distribution known as the Fuller curve, and given by

$$F(d) = \left(\frac{d}{d_{max}}\right)^{\alpha} \tag{6}$$

where d is a characteristic dimension (eg. diameter for a sphere), d_{max} is the largest value of d (eg. sieve size), and α is an exponent that controls the degree of fineness (for concrete $\alpha \approx \frac{1}{2}$). There are a number of schemes in the literature that use the Fuller curve to guide the gradation of the set of aggregates (e.g. Zaitsev & Wittmann 1981, Cusatis et al. 2006). In particular, Häfner et al. (2006) give the number of spherical aggregate within the size range $[d_1, d_2]$ in a 3D model as

$$N[d_1, d_2] = \left(\frac{\alpha}{\alpha - 3}\right)\left(\frac{6(d_1^{\alpha-3} - d_2^{\alpha-3})}{\pi\left(d_{max}\right)^{\alpha}}\right) V_{agg} \tag{7}$$

where d_1 and d_2 are bounds on the characteristic dimension, and V_{agg} is the total volume of aggregate in the specimen. Furthermore, the characteristic dimension in the range $[d_1, d_2]$ is randomly generated by

$$d = \left(X_1\left(d_2^{\alpha-3} - d_1^{\alpha-3}\right) + d_1^{\alpha-3}\right)^{\frac{1}{(\alpha-3)}} \tag{8}$$

where X_1 is a uniformly distributed random number on the interval $[0, 1]$. For two-dimensional studies, special care must be taken to adjust the Fuller curve to give aggregate diameter (Wittmann et al. 1985).

An algorithm to generate the mesostructure using Equations 7 and 8 would first determine V_{agg} based on the percentage of aggregate content in the mix design. Then the a minimum aggregate size, d_{min}, would be chosen based on the fidelity of the model desired, and a maximum aggregate size, d_{max}, would be determined based on the sieve size. Next, a suitable number of discrete intervals on $[d_{min}, d_{max}]$ would be chosen and for each interval the following operations performed:

1. use Equation 7 to determine the number of aggregates in this interval, N
2. *take* a random characteristic aggregate using Equation 8
3. *place* the aggregate at a randomly generated position and check for overlapping
4. repeat steps 2 and 3, N times

Up to this point in the discussion, the morphology of the individual aggregate has been assumed spherical. Gravel aggregates are characterized by smooth surfaces, and can be closely approximated with spherical or ellipsoidal geometries. Crushed gravel aggregates, on the other hand, have more complex geometry with sharp corners that, when embedded in a heterogeneous structure, create stress concentrations. There is no hope of reproducing accurate fields with a computational model that does not realistically represent the geometry. Hence, an attempt to account for aggregate morphology is important in the model.

An analytical expression to modify the morphology of the sphere is given by

$$\left|\frac{x}{r_1}\right|^n + \left|\frac{y}{r_2}\right|^n + \left|\frac{z}{r_3}\right|^n = 1 \tag{9}$$

where, if $n = 2$, the r_i are the semiaxes of an ellipsoid (Häfner et al. 2003). Figure 4 shows the consequence of different values of n, and shows that Equation 9 could work well to represent the geometry of gravel aggregate. However, additional methods must be considered to obtain the sharper corners present in crushed-stone.

In two-dimensions, a Fourier series can be used to represent the surface of roughened aggregates (Wittmann et al. 1985). In this approach, the boundary of the aggregate is represented by a set of vertices given in polar coordinates originating at the center of mass of the aggregate. The polar coordinates of each vertex are then described based on measurements of actual aggregate used in the mix. A three-dimensional analog to this is proposed in which spherical harmonics are used to extend the Fourier series

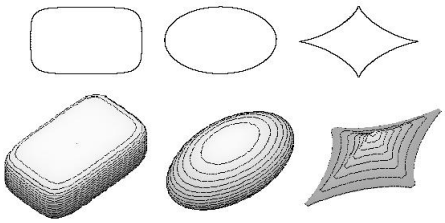

Figure 4. Variations on ellipsoids using Equation 9 with $n = 5, 2$ and 0.7 (Häfner et al. 2003).

idea (Garboczi 2002). In this reference, x-ray computed tomography is used to obtain voxelated descriptions of aggregates from an actual cured specimen. Then, the voxels are used to obtain spherical coordinates of a set of surface vertices. Figure 5 shows the voxelated description of one aggregate (top) and the representation based on its spherical expansion (bottom).

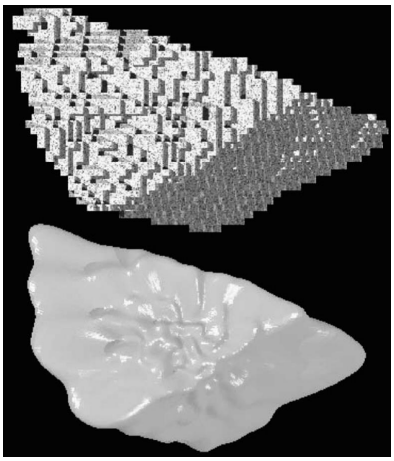

Figure 5. A digital image obtained through x-ray tomography of an aggregate (top). The spherical harmonic expansion of the aggregate (bottom) (Garboczi 2002).

It should be noted that the digital image in the top of Figure 5 could easily have been taken at higher resolution. Also, we would like to point out that x-ray tomography is unnecessary if a statistical analysis of the aggregates were performed prior to pouring. Other, less costly, digital imagery could be used, and a database of aggregate sources from different geological regions could be maintained.

6.1.2 *Discretization of the mesoscale*

The vast majority of computational modeling of concrete at the mesoscale has been done using the finite element method to solve the boundary value problem. Thus, a discretization of the domain is necessary. There are two general approaches used to discretize the domain: a digitized discretization, and a domain conforming discretization. In the digitized discretization the mesh is created independently of the mesostructural geometry and then superposed onto the mesostructure. Thus, elements could overlap the domain of multiple phases. In the domain conforming discretization, the mesh is chosen so that the geometry of the mesostructure is preserved. For this discretization, the geometry of the mesostructure necessarily has to be generated before meshing, and individual elements belong to the domain of only one material phase.

There are also two general classes of elements used to connect the spacial discretization: one-dimensional elements, and continuum elements. When one-dimensional elements are used, the nodes in the mesh are connected with spring, truss or beam elements. The continuum elements are 2D or 3D elements chosen to match the dimension of the space of their domain. For example, in a two-dimensional mesostructure model, triangular or quadrilateral elements are used to discretize aggregate or mortar, while 1D interface elements are used at the ITZ.

To completely describe the connectivity of the finite element model, a discretization method must be coupled with a choice of elements. There are mesostructural models in the literature that use all four of the possible combinations: a digitized domain with one-dimensional elements (DD1D); a domain conforming discretization with one-dimensional elements (DC1D); a domain conforming discretization with continuum elements (DCnD); and a digitized domain with continuum elements (DDnD). Discussion of the combination of choices is left to the following section where the results of some of the models are also discussed.

6.1.3 *Mesoscale results from the literature*

Much work has been done in two-dimensions with the DD1D approach. The most popular choice of element, in this case, is the Euler-Bernoulli beam element (Schlangen 1993). In these models, known as lattice models, the domain is arbitrarily discretized into a grid of beams. Subsequently, the mesostructural geometry is projected onto the grid and element properties are assigned depending on the mesostructural feature that projects onto them. Figure 6 shows the projection of the mesostructure onto the grid of elements.

Studies were performed to determine the optimum characteristic beam length (mesh size) and orientation. A pseudo-fracture criterion was used, whereby an element in the lattice was removed when the axial stress exceeded a specified tensile strength. Beams were linear elastic until fracture. The use of beam elements versus, say, truss elements assisted in the stability of the structure upon element removal, and gave more realistic predicted crack shapes. Finally, the impact of including the rotational degrees of freedom of the beams, i.e. bending, was studied. It was concluded

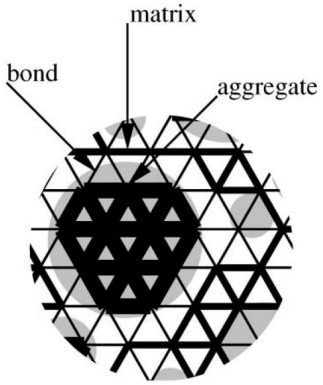

Figure 6. Mesostructure projected onto a lattice of beams (Lilliu & van Mier 2003).

that the bending degrees of freedom were required for the best results (Chang et al. 2002).

With the simple axial stress fracture criterion, the uniform grid was shown to bias the fracture pattern (Schlangen & Garboczi 1996). An attempt to eliminate the mesh bias using a randomly generated lattice showed improvement, but was not totally successful. Consequently, an effective nodal stress was determined based on the sum of the axial and shear forces at a node (Schlangen & Garboczi 1997). With the sum of forces, a plane which maximized its normal force was determined and the area of the connecting beams projected onto that plane. The effective nodal stress was then determined as this normal force divided by this projected area and used in the fracture criteria for each beam. The same study used a scanning electron micrograph and image processing to model an actual specimen. The results showed good qualitative agreement with observed crack patterns; however, the mesostructural models reacted in a more brittle manner than the experiments.

In one interesting DD1D study, the lattice model was used to answer some important modeling questions about the inherent stochasticity of the mesostructure. The consequence of explicitly modeling the mesostructure versus using a uniform lattice with randomly distributed strength was investigated. Two random distributions were investigated, Gaussian and Weibull. The result showed that the correct cracking response could not be reproduced with Gaussian distribution of strength; the Weibull distribution did better; but, neither was as accurate as explicitly representing the mesostructure (van Mier et al. 2002).

Finally, lattice models have been recently extended to 3D mesostructures in uni-axial tension (Lilliu & van Mier 2003). In general, the 2D methods were easily extended; however, the effective nodal stress was not used. Rather, for 3D they returned to the comparison of beam axial stress to strength. A parallel processing algorithm was used to accommodate the size of the problem. Here again, qualitative agreement was found for crack paths and peak load. However, the load-displacement curve shows an unrealistically large, unstable energy release immediately following the peak load.

There is also a body of work which uses the DD1C approach. The original effort, for two-dimensional mesostructures, linked the center of the aggregates with truss elements and used tributary areas and a springs-in-series model for the stiffness (Bažant et al. 1990). In this work, known as a particle model, a bilinear stress/strain law was used to model fracture in a similar fashion to the well-known fictitious crack model. The fracture energy $\mathcal{G}_f$ and element length were used to tune the softening branch of the curve. The model worked quite well. For a set of virtual uniaxial tension specimens, the results conformed to Bažant's size effect model (refer to Eqn. 1). Similar agreement was found for a set of virtual SEN(B) specimens. This agreement is to be expected since both the numerical model and the size effect model are based on the fictitious crack model. Consequently, although the numerical data closely reflected the predictions of the size effect model, they did not closely reproduce experimental results. This discrepancy could be a result of idealizing the mesostructure as two-dimensional, or perhaps more care was necessary in generating the mesostructure and assigning material properties to the truss elements.

The DC1D particle model has evolved into a three-dimensional model of spring members which include shear, major axis bending, and mid-length translational degrees of freedom (Cusatis et al. 2003a, Cusatis et al. 2003b). In this model, the stiffness properties are assigned based on the tributary volume of a lattice member. A recent improvement uses a Voronoi-type tessellation to assign stiffness properties that more closely reflect the mesostructure (Cusatis et al. 2006). Additionally, fracture, friction and decohesion are now included in the constitutive relations. With these improvements, the validation of the particle model reveals close agreement with observed experiments.

A two-dimensional digitized domain with two-dimensional elements (DDnD) has been investigated. In this investigation, the multigrid method is used to allow a fine grid that could represent the mesostructure (Häfner et al. 2006).

Finally, some of the original computational investigations into the mesostructure of concrete used domain conforming, two-dimensional elements (DCnD) to compute the effective elastic modulus and the effective diffusion coefficient (Wittmann et al. 1985). The same approach was extended later to predict fracture in direct tension specimens (Sadouki & Wittmann 1988). In these investigations, the fictitious

crack model was used in the mortar phase and interface elements, with a softening rule and friction implemented on the interface between phases. The load-displacement response was reasonably predicted with this model, and cracking patterns qualitatively matched experimental data. More recently, this investigation was carried further with the implementation of an advancing front meshing algorithm and an additional fracture criterion (Wang et al. 1999, Kwan et al. 1999). This is interesting work, but needs to be further developed and validated.

The implementation of DCnD models to study physical behavior of the mesoscale has fallen into disfavor. This is largely because of the perceived difficulty in meshing and threat of exorbitant computational expense. However, the successful 20-year-old works cited above seem to suggest that mesoscale modeling of concrete with domain conforming discretization and continuum finite elements is quite feasible. In fact, Figure 7 shows the computational model of a polycrystalline microstructure.

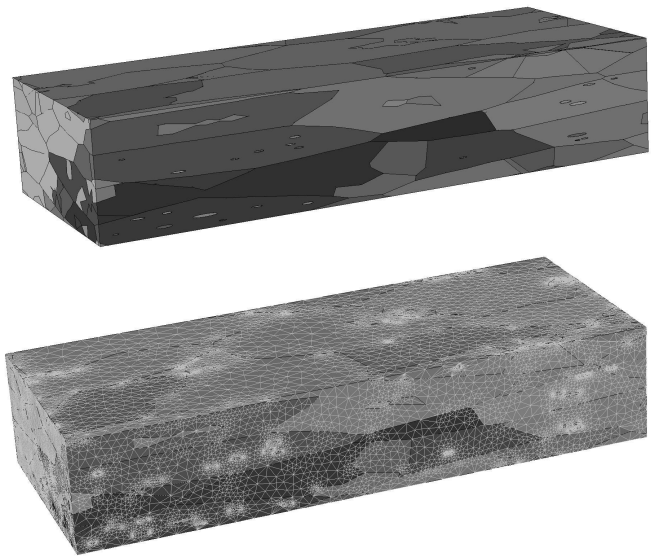

Figure 7. A geometry model of a two-phase polycrystal including 134 grains and 28 second-phase particles (top). The meshed model (bottom).

The dimensions of the model in Figure 7 are $76\mu m$ x $152\mu m$ x $380\mu m$ and it has 134 separate grains with 28 second-phase particles. The finite element model contains 3.6 million quadratic tetrahedra. The meshing was performed *automatically* in serial in a little over an hour. One can compute the stress and strain fields within this polycrystal using a polycrystalline plasticity constitutive rule (Matous & Maniatty 2004) in parallel with 240 Intel Xeon 3.6 GHz processors in about 64 hours up to 1.0% strain.

6.2 *Multiscale simulation*

Multiscale simulation can mean many things to many people. At a bare minimum, it means incorporating the physical phenomena of lower length scales into a higher length scale model (Lackner et al. 2004). A most robust multiscale procedure would allow information to flow from the continuum scale down to the lower scales, and the evolving material response would percolate back up. Currently, there does not appear to be any work being done using such an approach in concrete materials. We hope we are wrong on this observation. However, one of the original investigations into lower length scale analysis of fracture in concrete considered it to be "a multi-level hierarchy-system" (Zaitsev & Wittmann 1981). In this model, analytical stress intensity factors were used with the geometrical features of multiple length scales to determine realistic cracking patterns in concrete compression specimens.

This novel concept should inspire us today. Where could we go if a hierarchical multiscale scheme could determine, with a fast, first-order tool, where strain localization would most likely occur? What if, then, in those locations, a computational tool could burrow down scale and simulate the mechanics and physics of the meso-, micro- and even nano-length scales to determine the patterns of microcracking and predict the consequence? What if this system could be automated to allow engineers with solid practical skills to use such tools?

7 CONCLUSION

Fundamentally, fracture is the development of new surface area. Clearly, in the limit, this means the separation of the bonds between previously attracted atoms. To accurately simulate crack incubation, nucleation and growth, then, it is reasonable to assume the best place to start would be at the atomistic length scale. Obviously, this would lead to a great deal of practical difficulty; we cannot, at present, model every atom in an entire reinforced concrete structure. However, we can begin to reduce the length scale of investigation, as many researchers have done in other material systems.

The Lens of Physics observed the physical phenomena responsible for size effect by focusing on substructural length scales, down to the microscale. This cracking is a direct result of the stochastic nature of the meso- and microstructure; this cracking is diffuse and is virtually guaranteed, often occurring as a result of curing even before mechanical loading.

The Lens of Practice described several empirical approaches to capturing size effect. The approaches require the use of computational models as guidance. Specifically, the computational models should be used to validate the assumption of geometric similarity be-

tween the design structure and the test specimens supporting the equations. Also, size effect models idealize all structures as beams or columns and assume structural analysis is the result of Euler-Bernoulli beam theory; stresses are the result of shears and moments. Currently, the size effect is restricted to bending stress and does not include arbitrary stress in arbitrary geometry. Furthermore, there is some disagreement in the literature as to which of these is the most *fundamentally* justifiable. However, it is clear that no *empirically*-based approach can ever capture the *fundamental* physical behavior.

Through the Lens of Dimensionality, it seems promising that the true nature of the physical phenomena known as size effect can be captured and simulated using a multiscale approach. Size effect is, after all, a result of strain localization due to distributed microcracking. A multiscale framework that explicitly reproduces the stochasticity of the sub-continuum length scales, which includes the best known physical models of damage at those length scales, and which allows information to flow freely between those length scales would necessarily capture the microcracking process. The skeptic says, "It cannot be done". The brave scientist says, "Watch me try".

This is not to suggest that well developed, understood and meaningful empirical formulae that provide reliable estimates for design are obsolete. To be sure, they are indispensable. However, 40 years ago when the crew of the Star Ship Voyager used their handheld, portable communicators to talk to anyone in the galaxy, who would have believed that today every student roaming a college campus would be carrying a wireless telephone? Will we be able to model every atom in a concrete structure 40 years from now? Definitely not, if we don't try.

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