THE KRAJCINOVIC APPROACH TO MODEL SIZE DEPENDENT FRACTURE IN QUASI-BRITTLE SOLIDS

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Abstract

The failure in "quasibrittle" microstructural systems, occurring with no early warning, is a debated problem of great practical importance for the structural engineering community. Available models do not fully account for typical sample-size effects observed in fracture initiation and propagation. The Krajcinovic approach (K-approach) proposed here stems from a posthumous interpretation of Krajcinovic's orginal ideas and offers a new route to tackle such effects by means of an advanced fractal scheme, which consists of the sequential application of the Family-Vicsek scaling laws for the number of damage events $n(\varepsilon;L)$ in the fracture initiation and propagation regimes separately. The procedure is developed and explained in the context of an established lattice models under static tensile testing. Average simulation data for any outer-size L – here ranging from 24 to 192 - is shown to scale nicely by this method, throughout the entire damage process. The proper definition of the damage parameter D allows deploying the deduced scaling laws to deduce the actual stress vs. strain relationship applicable in engineering. The discussion extends with no prejudice to data from real experiments, provided that all necessary information is gathered and all underlying assumptions hold true. The approach shall appeal per se also to the larger scientific community of physicists and mathematicians involved in statistical mechanics and random network failure.

1. INTRODUCTION: QUASI-BRITTLE FAILURE, SIZE EFFECTS AND FRACTALS

Brittle, embrittled, and “quasibrittle” microstructural systems have the tendency to fail catastrophically with little or no early warning as they reach their strength, as shown in Fig.1. Besides the case of a structure containing a critical defect, such failures often develop from diffuse microcracking resulting in fracture initiation and propagation. Modeling and predicting failure of these systems is of utmost importance and has proven to be a formidable task of damage mechanics. In fact, a major complication is represented by the sample-size dependence of both the onset of strain localization and the consequent damage evolution. It is hard to predict the behavior of large structures based on laboratory tests on similarly shaped samples, unless a size-effect model (i.e. a scaling law) can be established to obtain analytical estimates. If a scaling law is available, knowledge of the statistics of a process on one scale allows inferring the statistics of the same process on any other scale. Materials systems of interest involve, for example, concrete, composites, rocks and timber, as demonstrated by a massive experimental evidence reported in literature over the past 40 years

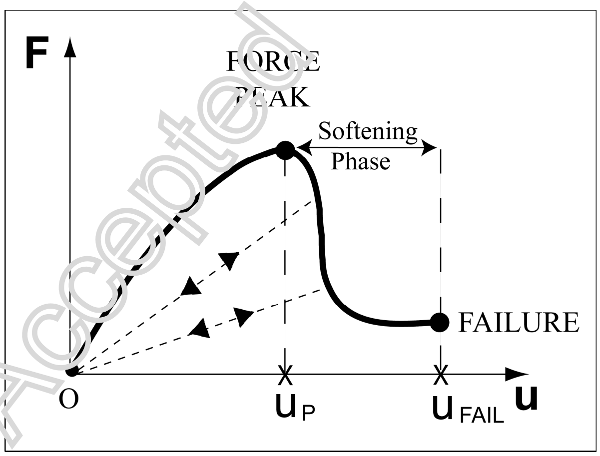

Figure 1. Typical tensile response of a sample made of quasi-brittle material such as concrete, failing from fracture initiation. The softening phase begins with the force peak point and ends with the structural failure. The signature feature of this behavior is the progressive loss of stiffness, as observable from the unloading paths identified solely by the secant slope in each point with no residual strain.

The modeling problem has been under investigation for centuries and many researchers have attempted a number of different strategies. Some modern approaches to fracture and damage have originated from fractal theory and lattice models. For instance, Mishnaevsky Jr (1996) monitored the surface roughness of crack and the specific surface energy needed to form a crack by the mechanism of microcrack coalescence and concluded that the fractal dimension of crack may be monitored during the crack formation process to compute the time-to-fracture in heterogeneous solids. Another group (Cherepanov et al. 1995, Balankin et al. 1996) suggested that the usual LEFM expressions for stress concentration at the crack tip could be replaced by a fractal version based on a roughness-related power law exponent α and a fractal stress intensity factor K_f as

$$\sigma_{ij} \propto K_f \frac{r^{-\alpha}}{l_0} \tag{1}$$

when crack length l falls between a lower cut-off l_0 and a self-affine correlation length ς, $l_0 < l < ς$. Similar continuum-based approaches have followed (Borodich 1997) with some noteworthy contributions that include for example the "Quantized Fracture Mechanics for fractal cracks" (Pugno and Ruoff 2004, Wnuk and Yavari 2008) or the fractional continuum framework of fracture and damage discussed by Tarasov (2013) and Ostoja-Starzewski et al. (2007,2013).
As far as damage initiation in quasi-brittle materials, Carpinteri and coworkers (e.g., 1994, 2012) devoted substantial effort to size effects inherent to fracture in concrete and proposed what they called multi-fractal scaling laws for the strength σ_{PEAK}, which we can rewrite here as:

$$\sigma_{PEAK} \propto \sigma^*_{PEAK} L^{-\beta} \tag{2}$$

where σ^*_{PEAK} is a scale invariant material parameter, β is the fractal exponent ranging from 0 to ½, for the low and high material heterogeneity limits respectively, and L is the sole significant geometrical parameter, provided that only self-similar samples are compared. When applied to experimental data, the authors stated that Eq.(2) provides an empirical method to obtain reasonable values for the fractal dimension damage domain, barring the existence of excessive scatter in the experimental data. They also documented a good agreement with the microcracking process as measured from the acoustic emission (AE) experiments, recovering the power-law and intermittency of avalanches of AE events, as well as the fractal distributions of event locations.

Nonetheless, the multi-scale approach faced also some criticism from exponents of civil engineering community, primarily by Bazant and co-workers. Following an alternative rationale, Bazant (1997a, 1997b) first developed an asymptotic argument and proposed a different model for the fracture initiation problem

$$\sigma_{PEAK} = \sigma^{*}_{PEAK}\left(1+\frac{A}{B+L}\right)^{-1/\beta} \tag{3}$$

where A and B are fitting constants. In subsequent papers (2004,2005), Bazant and co-workers reported a thorough overview of size effects and scaling laws for many different structural systems based on their approach, pointing out the affinity with Weibull statistics and strongly advocating weaknesses of fractal-based models such as (2).

However, a third-party work by Karihaloo and co-workers (Ince et al. 2003) found merits in both approaches when comparing approach (2) vs. (3), one outperforming the other in different size ranges, which ushers in the possibility for such dispute to live on unsettled. At the same time there is the general view in the engineering community that modeling size-effects remains a fertile and urgent research ground for the sake of establishement of reliable models and improvements of current design codes in structural engineering.

In this paper we present a different scaling procedure that we will call “Krajcinovic approach” (K-approach hereafter) as this stems from our posthumous revision of seminal ideas and prior work headed by Dusan Krajcinovic. The original papers by Krajcinovic and Rinaldi (2005a, 2005b) and Rinaldi et al. (2006, 2007) laid the foundation of the work presented here and fostered the usage of fractal theory in connection with lattice model, in a manner very different from Carpinteri’s. Rather than concentrating on the fracture strength, Krajcinovic’s initial exploration focused on establishing the connection between a random heterogeneous microstructured material and the damage parameter D in the constitutive relation throughout the damage process, from the early stage microcracking to the final crack propagation. Noteworthy, D enters the constitutive relations of a material but it is not an intrinsic property, being associated to given boundary conditions and a given loading history. For example, unlike comminution damage in fragmentation problem where the complete loss of stiffness is not achieved at failure (e.g. Mastilovic and Krajcinovic, 1999a, 1999b), the damage parameter for the tensile test is strictly related to loss of stiffness such as $D=\Delta E/E_0$ (Rinaldi, 2009).

Since the damage evolution is a stochastic process that depends on applied load and microstructural disorder of a given sample (i.e. random texture and imperfections), D is a random variable and the problem is better stated in terms of representative average $\langle D \rangle$ (Rinaldi, 2009). More precisely, the macroscale stress-strain response of a damaged heterogeneous quasi-brittle material subject to strain-controlled quasi-static uniaxial test is customarily expressed by the Kachanov's relation[1]

$$\langle \sigma(\varepsilon) \rangle = E_0(1-\langle D(\varepsilon_0; L) \rangle)\varepsilon \quad (4)$$

where $\langle \sigma \rangle$ is the average stress response associated to the imposed strain level ε, E_0 is the initial Young's modulus, and the expected value of the damage parameter $\langle D(\varepsilon_0; L) \rangle$ depends on the loading history ε_0 (i.e., in this case, the maximum strain applied) and on the sample size L. When structural healing is prevented, the damage effect is detected at the macroscale by the (permanent) loss of secant stiffness $\langle E(\varepsilon) \rangle = E_0(1-\langle D(\varepsilon_0; L) \rangle)$ associated with the microcraking process, ranging from $\langle E(\varepsilon) \rangle = E_0$ for $\langle D \rangle = 0$ (i.e. no damage) to $\langle E(\varepsilon) \rangle = 0$ for $\langle D \rangle = 1$ at failure. Krajcinovic's original intention was to scale the average response of a brittle material in Eq. (4) by identifying a suitable scaling law for $\langle D \rangle$

$$\langle D(\varepsilon_0; L) \rangle = f(L) \quad (5)$$

which was sought by means of a fractal-based procedure. However, despite some recognition (e.g. Carpinteri et al., 2012), his ideas were substantially overlooked by the scientific community at large, partly because the fundamental concepts were probably reported in fragmentary and yet incomplete way. The primary objective of this paper is to fill this gap and describe a new scaling procedure in a unitary and finalized form, linking it to prior attempts and explaining in practical terms its usage to practitioners. The method will be illustrated on numerical data from discrete lattice models of different size L. Succinct commentaries of some

[1] Note that a similar (internal variable) constitutive model was applied lately in the context of friction wear by D'Annibale and Luongo.

percolation and finite-size scaling ideas that immediately relate to the lattice models and to the K-approach are presented first.

2. HISTORCAL PERSPECTIVE OF STATICAL METHODS FOR LATTICES

Although fracture models are of primary importance to the structural engineering community, the subject has always appealed significantly to physicists and mathematicians, especially among the statistical mechanics community, which bred a substantial body of results and ideas that are the cornerstone of the methods cited above including ours. Noteworthy, these results flourished over the past 30 years in conjunction with discrete lattice models that provided the possibility to simulate realistically the microstructural disorder of materials and reproduce structural size-effects in a tractable manner. Let us briefly recall the main statistical methods applied to failure of quasi-brittle lattice (ref. Krajcinovic 1996).

2.1 Percolation theory of damage in discrete models

Percolation theory is one of the earliest and simplest approaches to investigate phase transitions in statistical physics (e.g., Stauffer and Aharony, 1994) and has been applied with some success to geometrical and transport properties of mechanical lattices, along with size effects. A damaged lattice can be indeed regarded as a random graph of connected clusters and, as such, it can be studied by means of percolation theory. In that view failure is treated as a phase transition that occurs at percolation condition, that is when the correlation length ξ, associated to the connected/interacting clusters of microcracks, spans the entire finite-size lattice L (or diverges for an infinite lattice as $L \to \infty$). The percolation threshold p_c is defined as the occupation probability p at which an infinite cluster appears in the lattice according to a power-law fractal exponent ν

$$\xi \propto \left| p_c - p \right|^{-\upsilon} \tag{6}$$

For a mechanical network, p roughly corresponds to the density of unbroken springs and p_c is critical point associated to failure. The threshold p_c is defined with respect to an infinite lattice and approached asymptotically in the limit of $L \to \infty$. The application of the results to finite-size systems happens by renormalization group approaches, such as coarse graining techniques (e.g. Christensen, 2002).

Similar scaling laws were sought for many other and diverse parameters (e.g., connectivity, number of microcracks, etc.) and network transport properties (e.g., conductivity, stiffness, etc.) related to the "failure transition" and thereby exhibiting a singularity. As an example, Sen et al. (1985) studied the percolation model for the central-force elastic lattice, finding that bulk modulus (K) and shear modulus (G) scaled as

$$K, G \propto \left(p - p_c\right)^{\beta} \tag{7}$$

with the following numerical estimates $p_c = 0.58, \quad \beta = 2.4 \pm 0.4$ for 2D triangular lattices and $p_c = 0.42, \quad \beta = 4.4 \pm 0.6$ for 3D face centered cubic (FCC) lattices. The same group proposed an effective medium theory of spring-network models, mapping the percolation property of the central-force lattice to a continuum scale, also exploring importance of the coordination number of lattice sites on the scaling (Feng et al. 1985). Many authors (Chelidze 1982, Roux and Guyon 1985, Ostoja-Starzewski 1989, etc.) have reported similar results but, despite the apparent simplicity, the application of percolation ideas to damage has proved to be not straight forward. Krajcinovic (1996) offered a detailed essay on this subject, stressing the importance of percolation theory in damage mechanics and its limitations. Percolation theory ought to be regarded as complementary to mean-field theories of continuum mechanics (e.g. dilute concentration models of damage), granting a way to approach size-scaling issues by means of relations that are universal and supposedly independent of microstructural details. Hansen and Roux (1989), amongst others, investigated the universality problem for central-force lattices. However, one main problem is the estimation of fractal exponents associated to asymptotic behaviors, which require large computations. In time, successive reports have modified earlier accounts and larger simulations have indicated that fracture damage may not comply with basic (uncorrelated) percolation process (Nukala et al. 2006). Another drawback inherent to some percolation studies resides in the preservation of isotropy during the percolation process that proceeds by random either suppression/strengthening of links (e.g. Garcia-Molina et al. 1988), which makes them ill posed to study damage induced anisotropy that immediately arise in quasi-brittle (vectorial) systems (Rinaldi 2009). A critical review by Guyon et al. (1990) represents a relevant and insightful reading on the subject.

2.2 Fractal scaling laws of damage in discrete models

Besides percolation models, lattice models represent a fertile playground for the application of many other methods of statistical physics. The fuse lattice by De Arcangelis et al. (1985) illustrated in Fig. 2 is one of the first attempts to depart from percolation ideas and introduce damage by a more realist mechanism of fuse burn-out caused by quenched or annealed disorder as opposed to random link suppression (Krajcinovic 1996).

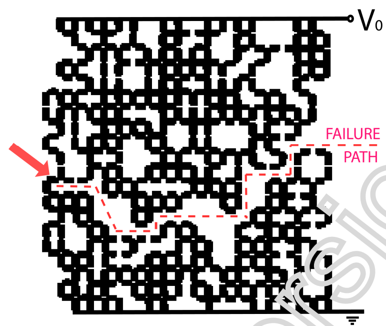

Fig. 2. Example of fuse lattice at the onset of failure, where the suppression of the last fuse pointed by the arrow leads to failure (zero conductance) (redrawn from De Arcangelis et al. 1985).

These fuse models drew immediately a great attention (e.g. Duxbury et al 1986, Alava et al. 2006) as simple scalar models of failure in heterogeneous solids, but were immediately sided by actual "vectorial" mechanical models such as beam and central–force lattices. The latter are indeed significantly more complex and realistic, especially as far as the damage-induced elastic anisotropy and failure patterns are concerned.

The research scope also expanded to consider not just the scaling of one critical point corresponding to the failure threshold, like in percolation, but the entire response of the system during the damage process, particularly after strain localization. The objective was to establish fractal-based transformations that succeed in reconciling the mechanical response of samples of any size by mapping their mechanical response into one scale invariant curve, thus yielding a scaling law for the given damage process.

2.2.1 Family-Vicsek scaling

For our discussion, one specific method called the Family-Vicsek scaling (Family and Vicsek 1991, Barabasi and Stanley 1995) stands prominently above others. It was first used for growth of advancing solidification fronts at the liquid-solid interface. Let us consider the generic function y(x, L) as dependent on a variable x defined over a network domain but also on the size L of the network itself, as depicted in Fig. 3a. The knee-shape typically marks a phase transition at the critical point location (x^*, y^*).

If the Family-Vicsek scaling holds, then the data $y(x, L)$ shall map onto one universal scale-invariant curve such that $f(x/L^\beta, \cancel{L}) = y/L^\alpha$ for any L, as indicated in Fig. 3b, according to the following scaling relation

$$y(x, L) = L^\alpha \; f\left(\frac{x}{L^\beta}\right) \tag{8}$$

Three conditions must be met for this scaling procedure to be feasible:

1. at the transition the y value must be a fractal such that $y(x^*, L) \propto L^\alpha$,
2. the location of the transition must be a fractal such that $x^* \propto L^\beta$,
3. before the transition the data must follow a power law $y(x, L) \propto x^\gamma$.

Consequently only two out of the three exponents {α, β, γ} are independent due to the constraint γ = α / β.

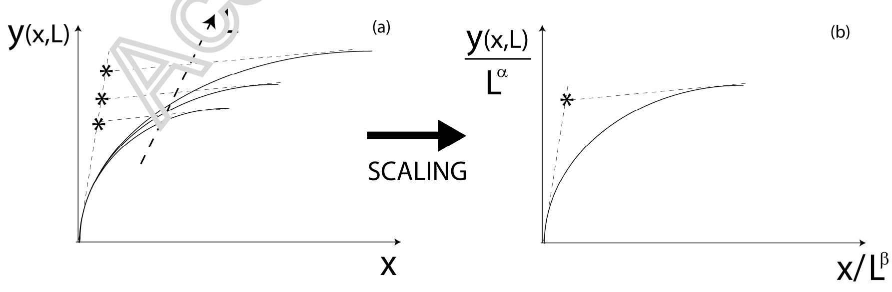

Fig.3. Illustration of the scaling procedure applicable to some non-linear systems that experience a transition governed by a universal law. The response *y* depends on the controlled variable *x* but also on the system size *L*, which controls the occurrence of the transition. A scaling law exists if *y(x,L)* maps into a scale invariant curve upon normalizing *y* and *x* by L^α and L^β respectively.

This empirical scaling procedure, borrowed from phase transitions and clusters theory, has proved useful to investigate microcracks cooperation and damage localization in multisite cracking and fracture processes, where lattice models had already revealed the existence of several fractals quantities. Hermann, Hansen and Roux sought to apply the scaling to data from numerical experiments on central-force lattice (Hansen et al. 1989) and beam lattice (Hermann et al. 1989), finding satisfactory results only over certain portions of the damage process. Fig. 4 displays raw force-displacement data F(u) for the beam lattice vs. scaled data $F = L^{\alpha} f(uL^{-\beta})$ with scaling exponents $\alpha = \beta = 0.75$. They also sought a scaling relation for other quantities, such as the number of broken links $n = L^{\gamma}\Psi(uL^{-\beta})$. The results of the scaling displayed in Fig. 4 exemplifies that the scaling could be used only up to the force peak.

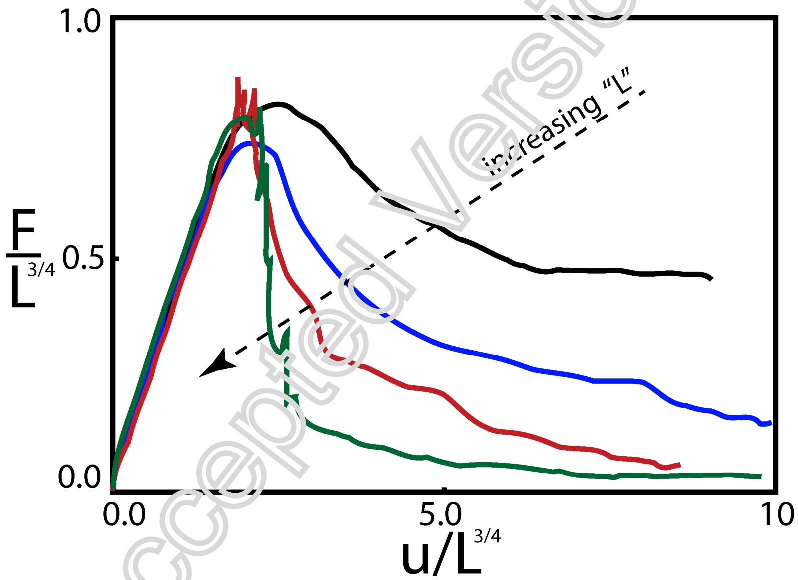

Fig. 4. Results of Family-Vicsek scaling (data from Hermann et al. 1989).

3. The K-approach

The Family-Vicsek scaling is also the cornerstone of the approach featured here, although utilized in a much different manner, along the footsteps of Krajcinovic. As opposed to Fig.4 (and to most other scaling in literature), our strategy does not target the force vs. displacement data directly, but it pursues the nested application of the Family-Vicsek scaling (8) on the curves *n*-*ε* (i.e., number of microcracks vs. strain), which resemble the situation sketched in Fig.3. Note that it is not possible to scale *n*-*ε* with a single application of Eq.(8) because the damage process encompass two stages, each governed by different fractal quantities. Let us first state the principle of our scaling, and then explain the practical application on an example.

Statement #1. The objective of the K-approach is twofold: (i) the formulation of scaling laws for the $n(\varepsilon;L)$, mapping these data into a scale-invariant function valid for any L , and (ii) the linking of such scaling function to the damage parameter D .

Statement #2. The practical procedure consists of applying the Family-Vicsek twice in cascade, according to a two-steps scheme entailing the sequential application of (8) separately to the microcracks prior and after the stress peak, in recognition of the nature of the fracture initiation problem consisting of two distinct phases (ref. Fig.6 later). The two steps are:

Step #1: Application of Eq.(8) to the number of microcracks and, by setting $\alpha=d+\beta$ (d is the applicable Euclidean dimension), the identification of the sole independent fractal exponent β that makes the scaled data "$n(\varepsilon, L)/L^{d+\beta}$ vs. ε/L^{β}" overlap for any L up to the peak strain ε_p, thus yielding the scale-invariant function $g(\varepsilon/L^{\beta})$

$$n(\varepsilon; L) = L^{d+\beta}\, g\left(\frac{\varepsilon}{L^{\beta}}\right) \tag{9}$$

Step #2: Nested application of Eq.(8) to the post-peak increment of microcracks Δn and identification of the exponent β' that delivers a scale invariant function $g'(\Delta\varepsilon/L^{\beta+\beta'})$, making the remaining data of the softening phase overlap for any L up to failure.

$$\Delta n(\varepsilon; L) = L^{d+\beta+\beta'}\, g'\left(\frac{\Delta\varepsilon}{L^{\beta+\beta'}}\right) \tag{10}$$

3.1 Example: application to lattice data

The procedure is illustrated here with respect to the same simulation data used originally by Krajcinovic and Rinaldi (2005a, 2005b) for the random lattice of size L x L depicted in Fig.5, the details of which are recalled in the Appendix. Therein, the average stress responses from the tensile tests for each L represent the primary output from simulations, clearly demonstrating the existence of a strengthening effect with the shrinking L, like in real systems.

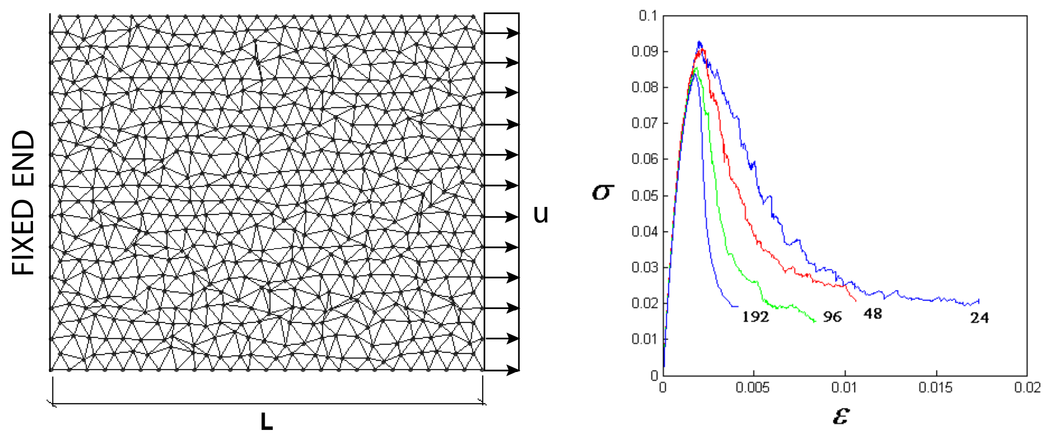

Fig. 5. Irregular triangular lattice of square shape (*L*x*L*) subjected to uniaxial tensile load in a displacement controlled mode. Average stress vs. strain response for L = {24,48,96,192} computed over 10 replicates per size.

However, the K-scaling requires "tracking" the function of broken links (i.e. the microcracks) *n(ε;L)*, which is the object of the scaling. The function *n(ε;L)* is often recognized as the primary source of information about the damage process and is indeed closely related to the damage parameter *D*. In 1-D models, the function n(ε) is actually all that is needed to compute *D*, usually through a closed-form solution (Rinaldi 2011). In higher dimensional problems such as this 2-D lattice lattice, this connection still exists but is more complex, as demonstrated earlier (Rinaldi, 2009). The sample data plotted in Fig.6 allows grasping such a connection between the force response and the microcracks evolution. The micro-stress fields are compared (in absolute value) at four states of the damage process. While the micro-stress distribution "1" is statistically "invariant" for all replicates with same size *L* and corresponds to random damage nucleation, the distributions "2, 3, and 4" all depend on the disorder of the microstructure and reveal damage localization and propagation. The knee in the *n*-*u* curve, overlaid (out of scale) onto the *F*-*u* data, is reminiscent of the scenario in Fig.3 and marks the occurrence of the transition between this two regimes, from homogeneity to heterogeneity (equivalently from nucleation to propagation of damage or from hardening to softening). As discussed elsewhere (Rinaldi, 2007, 2009), damage nucleation is a "diffuse" process with higher rupturing rate whereas damage propagation is a process highly correlated in space and with a (apparently) lower microcracking rate.

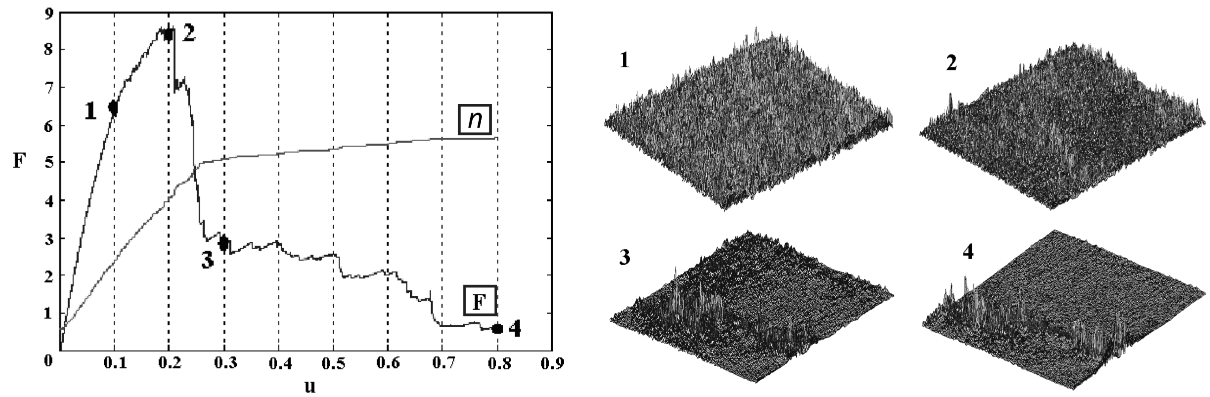

Fig.6. Micro-stress distribution at 4 points of the damage process. Stress (strain) localization is observed at “2” (peak point) from the loss of statistical homogeneity and formation of energy (stress) clusters (i.e. hot-spots).

In our case, the average *n*-*ε* curves associated to the stress curves in Fig.5 are plotted per each *L* in Fig.7a. Remarkably, the proposed scaling procedure can be illustrated on such lattice data with no loss of generality since it applies seamlessly to real systems, being the needed *σ*-*ε* and *n*-*ε* data in Figs. 5 and 7 obtainable also experimentally, e.g. through AE techniques (e.g. Carpinteri et al. 2012).

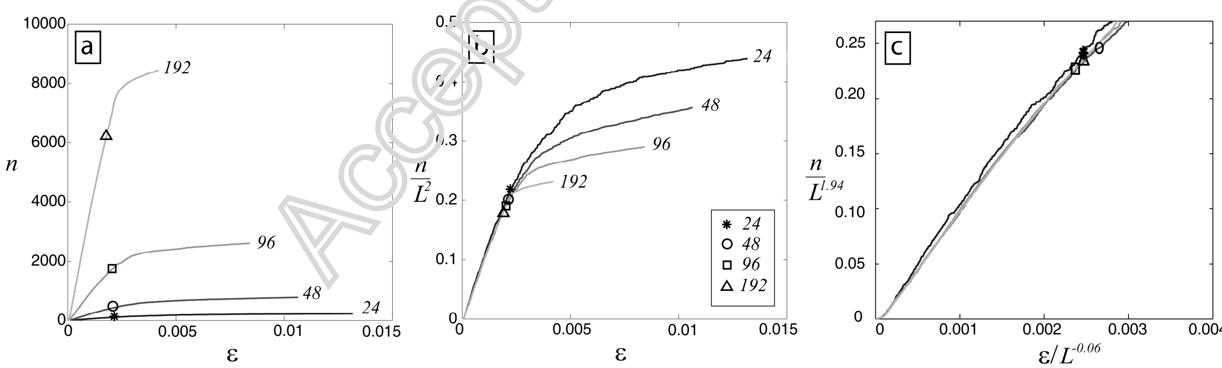

Fig. 7. Plots of (a) $n-\varepsilon$, (b) $\rho-\varepsilon$, (c) $g-\varepsilon$**.** (b) Normalizing n by L^2 yields a microcracks density ρ and produces a first substantial data overlap regardless of *L*; yet, the marked peak points depend on *L*. (c) Scaling data from (b) to (c) causes data collapse up to the peak and renders the complete Family-Vicsek in Eq.(9) for *n(ε;L)*.

3.1.1. Step#1: pre-peak region

With regard to the Step#1 of the procedure, the best results shown in Fig.7c are obtained for the exponent β=-0.06 in the scaling Eq.(9), which specializes as

$$n(\varepsilon, L) = L^{1.94}\, g\left(\frac{\varepsilon}{L^{-0.06}}\right) \tag{11}$$

A substantial overlap is achieved from (11) among all transformed datasets, with near-clustering of all peak points. Accuracy of this deduction is always limited in reality by the finiteness of the simulation/experimental sample, which is used to infer an asymptotic property, i.e. the scale invariant transformation $g(\varepsilon/L^{\beta})$.

Apart from practical usage, a few observations help gaining a better insight of Eq.(9) and about the rationale underlying step#1. Let us note first that the intermediate normalization of n by $L^{d=2}$ in Fig.7b renders an "average microcracks density" $\rho = n / L^2$ and produces a substantial data collapse and causes all transformed curves to exhibit equal slope. This intermediate result had been observed phenomenologically (e.g. Hansen et al., 1989) and has been demonstrated to be necessary on a theoretical ground by Rinaldi (2007). However, this does not suffice to deliver a scale invariant, because the peak strains are still different. Then, a subsequent Family-Vicsek transformation bring us from Fig.7b to Fig.7c by using the constraint $\alpha=\beta=-0.06$ in Eq.(8) to map the peak points into one while preserving the slope agreement. Such a logical construction is evidently reflected in Eq.(9).

In agreement with the fundamental hypotheses of the Family-Vicsek scaling enlisted in Section 2.2.1, the successful scaling in Fig.7c implies that that the number of microcracks at the peak N_p and peak strain are both fractal quantities that scale as $N_p \propto L^{d-\beta}$ and $\varepsilon_p \propto L^{\beta}$ respectively. In support of this view, in Fig.8 we can check that the microcracks scale as $n(\varepsilon;L) \propto L^2$ before the peak and as $n(\varepsilon_p;L) = N_p \propto L^{1.94}$ at the peak, in agreement with Fig.7c.

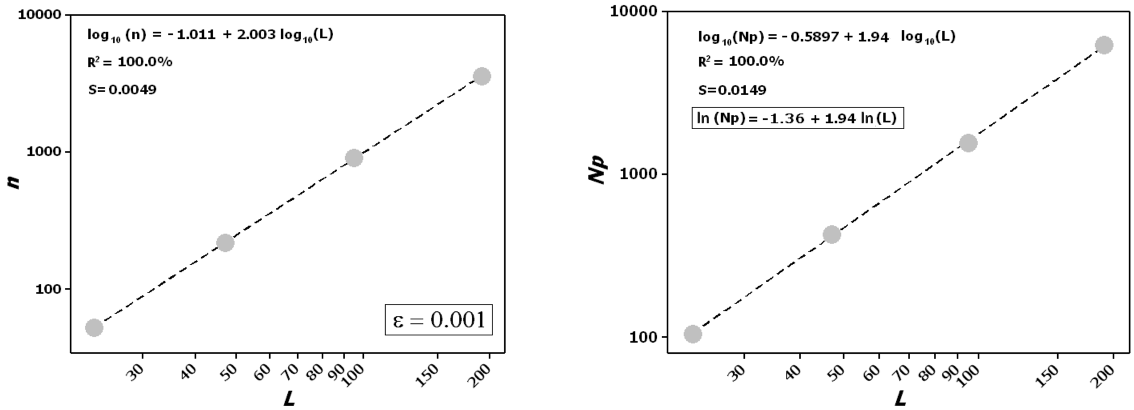

Fig.8. Comparison of fractal behavior of $n(\varepsilon;L)$ at $\varepsilon = 0.001$ vs. peak strain (Np), demonstrated by the linearity of log(n) vs. log(L). In the former case the exponent is ~2 and lowers to ~1.94 at the peak, matching Fig.7c. For convenience-sake, the power law of Np is expressed also in base e such that $N_p = e^{-1.36}L^{1.94}$.

Next, we need to determine the damage parameter D valid up the strain peak for the system under consideration. Based on the results from Krajcinovic and Rinaldi (2005a), our lattice is known to behave in a manner identical to the corresponding "fiber bundle model" (see Appendix) and we can adopt the following definition,

$$D(\varepsilon;L) = \frac{n(\varepsilon;L)}{2N_p} \tag{12}$$

To conclude our task, by virtue of Eq.(11) and because $N_p = e^{-1.36}L^{1.94}$ from Fig.8, we can rewrite it in scale-invariant form as

$$D(\varepsilon) = \frac{g(\varepsilon / L^{-0.06})}{2e^{-1.36}} \tag{13}$$

An analytical form can be obtained by replacing g with an approximating function fitted to the data in Fig.7c in different ways, e.g. via regression methods. In this case, we can for example assume the linearity $n / L^{1.94} \propto \varepsilon / L^{-0.06}$ throughout the range and perform a first order Taylor expansion around ε=0 such that $'' n / L^{1.94} = \partial(n / L^{1.94}) / \partial(\varepsilon / L^{-0.06})\big|_{\varepsilon=0} \cdot \varepsilon / L^{-0.06} ''$, which leads to

$$g(\varepsilon / L^{-0.06}) = \partial\rho / \partial\varepsilon\big|_{\varepsilon=0} \frac{\varepsilon}{L^{-0.06}} \tag{14}$$

with $\partial\rho/\partial\varepsilon\big|_{\varepsilon=0}$ being evaluated numerically as the initial slope either in Fig.7b or Fig.7c. The damage parameter is estimated as

$$D(\varepsilon) = \frac{\partial\rho/\partial\varepsilon\big|_{\varepsilon=0}}{2e^{-1.36}} \frac{\varepsilon}{L^{-0.06}} \tag{15}$$

For this specific example the value of the damage parameter at the peak is invariably $D_p=0.5$. The corresponding peak strain, marking the range of validity of Eq.(13), is

$$\varepsilon_p = \frac{e^{-1.36}}{\partial\rho/\partial\varepsilon\big|_{\varepsilon=0}} L^{-0.06} \tag{16}$$

and Eq.(12) can be back-computed in terms of strain as

$$D(\varepsilon;L) = \frac{\varepsilon}{2\varepsilon_p} \tag{17}$$

The results of the Eq.(18) vs. simulation data provide the validation of the formulated model.

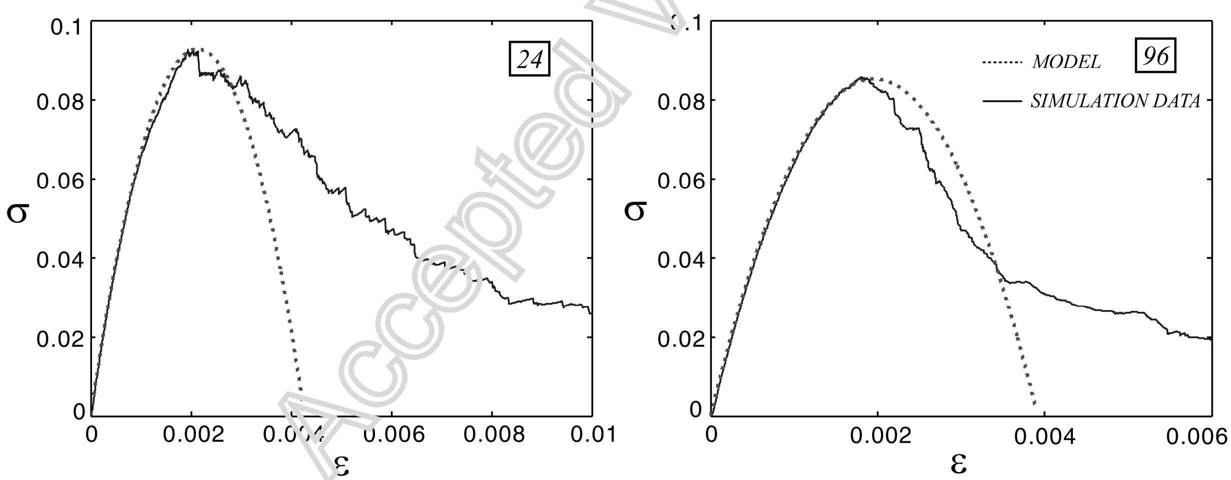

Fig.9. Mean response from simulation data (solid line) plotted *vs.* constitutive model Eq. (4) (dotted line) from the damage definition Eq.(12) for L =24,96. The model appears accurate up to the peak and, expectedly, deviates from simulations afterwards.

3.1.2. Step#2: post-peak region

The step#2 of the K-approach proceeds in an analogous manner but focuses exclusively on the post-peak data Δn vs. $\Delta\varepsilon$, with $\Delta n = n - n_p$ and $\Delta\varepsilon = \varepsilon - \varepsilon_p$. The best results are displayed in Fig.10 and are obtained for $\beta' = -0.54$, such that Eq.(10) can be rewritten as

$$\Delta n(\varepsilon, L) = L^{1.40}\ g'\left(\frac{\Delta\varepsilon}{L^{-0.60}}\right) \tag{18}$$

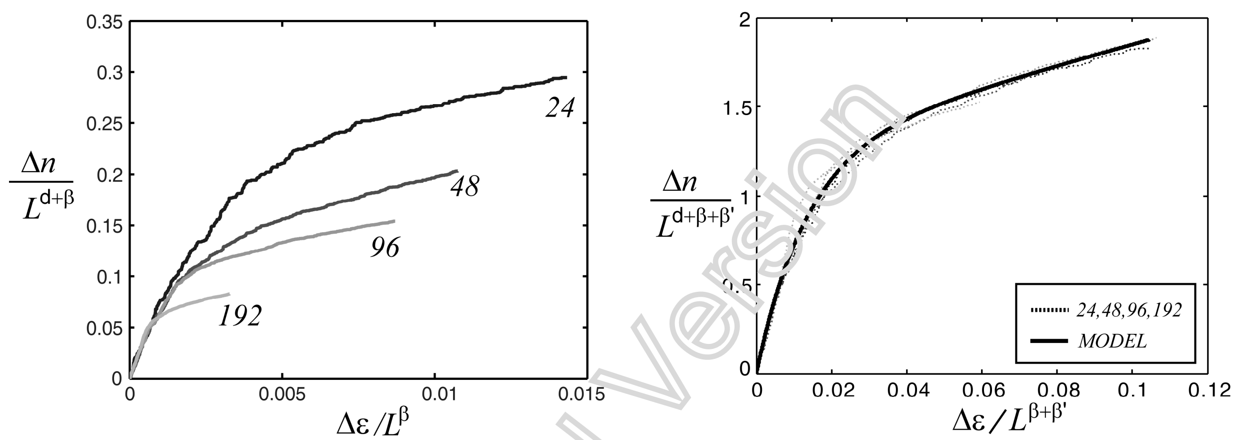

Fig.10. (a) Post-peak data after the transformation Eq.(9) and (b) results from step#2 of the K-approach bringing all datasets fall into one scale invariant function $g'(\Delta\varepsilon/L^{\beta+\beta'})$ for $\beta' = -0.54$ in Eq.(10).

The scaling function $g'(\Delta\varepsilon/L^{\beta+\beta'})$ is well approximated by the following analytical function (Fig. 10b - solid line)

$$g'(\Delta\varepsilon / L^{\beta+\beta'}) = a_1 \frac{\Delta\varepsilon}{L^{\beta+\beta'}} + b_1\left[1 - exp\left(-c_1 \frac{\Delta\varepsilon}{L^{\beta+\beta'}}\right)\right] \tag{19}$$

where the fitting parameters are ($a_1 = 6,\ b_1 = 1.25,\ c_1 = 75.2$) for our data. The latter ones are not independent and the two following conditions

$$a_1 + b_1 c_1 = \partial n / \partial\varepsilon\big|_{\varepsilon_p} \tag{20}$$

$$a_1 = \partial n / \partial\varepsilon\big|_{\infty} \tag{21}$$

can be imposed onto the scaled $\partial n / \partial\bar{\varepsilon}$ in order to:

1. to maintain a C^1 continuity with data pre-peak data from Eq.(14) and
2. to insure the correct asymptotic failure rate.

The terms on the right-hand side in Eqs.(20,21) are measurable from Fig.10b. Thus, since a_1 is imposed, only one free parameter is left and the pair $\{b_1, c_1\}$ is selected to optimize the data fit of Eq.(19). Combining Eqs.(18) and (19) yields the desired scaling law for the microcracks Δn in the propagation regime

$$\Delta n(\varepsilon, L) = L^d a_1 \Delta\varepsilon + L^{d+\beta+\beta'} b_1 \left[1 - exp\left(-c_1 \frac{\Delta\varepsilon}{L^{\beta+\beta'}}\right)\right] \quad (22)$$

Next, the determination of the damage parameter for the softening phase requires a model, similarly to Eq.(12) for step#1. Because damage is additive, the softening damage simply sums up to the amount previously cumulated up to the peak strain with the new increment

$$D(\varepsilon; L) = D_p + \Delta D(\varepsilon; L) \quad (23)$$

where $\Delta D = D - D_p$ and $D_p = 0.5$ from Eq.(17). To this purpose, we can recall and use the model developed by Rinaldi et al (2006) by seeking to identify the damage increment ΔD from normalizing Δn by an appropriate factor $X(L)$

$$\Delta D(\varepsilon, L) = \frac{\Delta n}{X(L)} \quad (24)$$

The determination of $X(L)$ is pursued through statistical methods to reach a "data driven" decision. According to standard ordinary least square (OLS) regression methods, the stress estimate $\hat{\sigma}_i$ in correspondence to ε_i and Δn_i at the generic i-th point of the stress response Eq.(4) was expressed as

$$\hat{\sigma}_i(\varepsilon_i, \Delta n_i, X) = E_0\left[0.5 - \Delta n_i / X\right]\varepsilon_i \quad , \quad (25)$$

where X is the target parameter to be estimated. Since this model is linear in $1/X$, the OLS method can be used to compute a minimum unbiased estimator $\hat{X}$ the minimization of the error function $Err(1/\hat{X}) = \sum_{i=1}^{Q}\left(\bar{\sigma}_i - \hat{\sigma}_i\right)^2$ over Q simulation points by setting $\partial Err / \partial \hat{X} = 0$ leads to

$$\hat{X}(L) = \frac{\sum_{i=1}^{Q} \bar{K}_0 \bar{\varepsilon}_i^2 \Delta n_i^2}{\sum_{i=1}^{Q} \left(\left[\left(1 - D_p\right) \bar{K}_0 \bar{\varepsilon}_i - \bar{\sigma}_i \right] \Delta n_i \bar{\varepsilon}_i \right)} \tag{26}$$

The estimates from Eq.(26) are displayed in Fig.11 with circles (note that extra data for L={72,120} are also used for validation purposes) and reveals that the function $X(L)$ is well approximated by regression line

$$X(L) = a_2 L + b_2 \ , \tag{27}$$

with $a_2 = 65$ and $b_2 = -1038$, and a coefficient of determination ($R^2 = 0.997$). Such a result fully solves our problem, with Eqs.(24) and (27) delivering the desired scaling relations for the average constitutive model in the softening regime, which for very large L (such that $1038 << 65L$) can be reasonably approximated as

$$\Delta D(\varepsilon, L) = \frac{\Delta n(\varepsilon, L)}{a_2 L} \tag{28}$$

which intuitively means that the number of microcracks roughly scales with the size of the lattice in the fracture propagation regime. By substituting Eq.(22), we finally obtain the analytical expression

$$\Delta D(\varepsilon, L) = \frac{L^d a_1 \Delta\varepsilon + L^{d+\beta+\beta'} b_1 \left[1 - \exp\left(-c_1 \frac{\Delta\varepsilon}{L^{\beta+\beta'}} \right) \right]}{a_2 L} \tag{29}$$

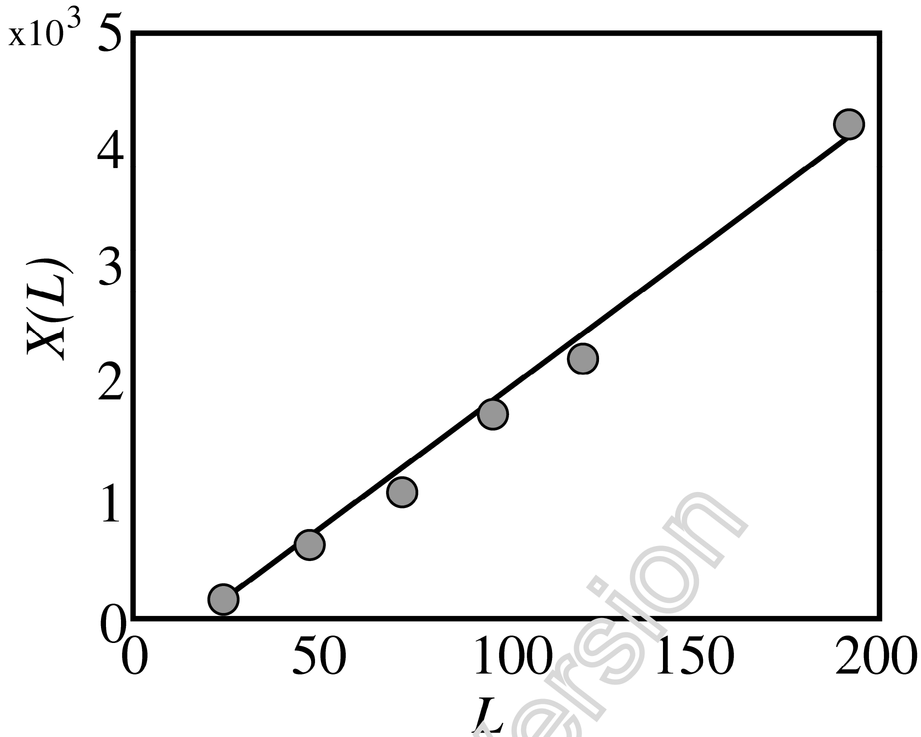

Fig.11. Comparison of *X(L)* estimated from Eq.(26) vs Eq. (27) from average data Δn (circles).

The application of Eq.(29) is shown in Fig.12a, where the model (4) now matches simulation for most of the damage process. The scaling law (29) provides a convenient smooth analytical relation for $\Delta n(\varepsilon, L)$ but is clearly a trade-off between the need of having an average estimate of the microcracks number valid for any lattice size and the inevitable loss of "details" characterizing each individual curve, as made evident in Fig.12b when actual numerical data for n, N_P, and Δn are used directly in Eq.(28).Yet, the difference between the estimate of Δn from scaling (118) and the real value from simulations never exceeded 10% for any lattice size, which confirms the robustness of the K-approach.

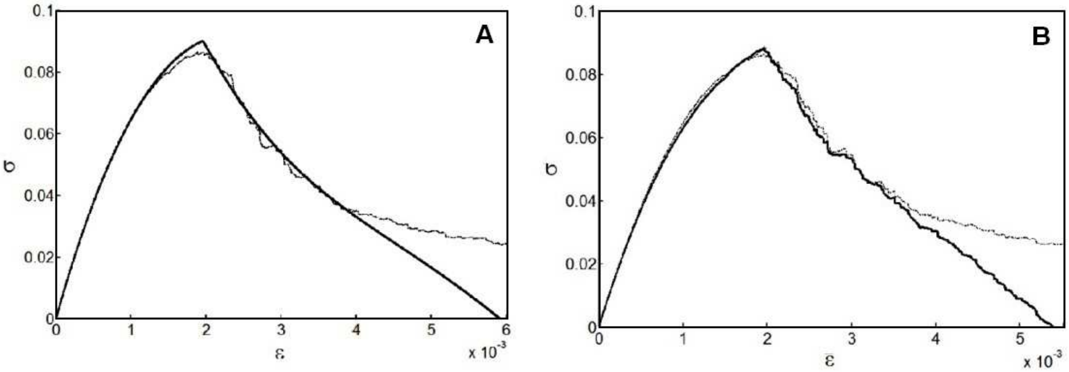

Fig.12. Complete model fit to average data for N =96 from (A) analytical expression (29) vs. and (A) scaling model (28), where actual numerical data for n , N , and Δn are used directly.

Also the parameter $X(L)$ contributes to the accuracy of the model. In fact, as shown by the four randomly picked replicates of $L = \{24, 48, 96, 192\}$ in Fig.13, the model (28) dramatically improves and captures the damage response from individual simulations by using the exact value for $X(L)$ ("o" marks in Fig.11), thus further confirming the choice of damage parameter and scaling laws.

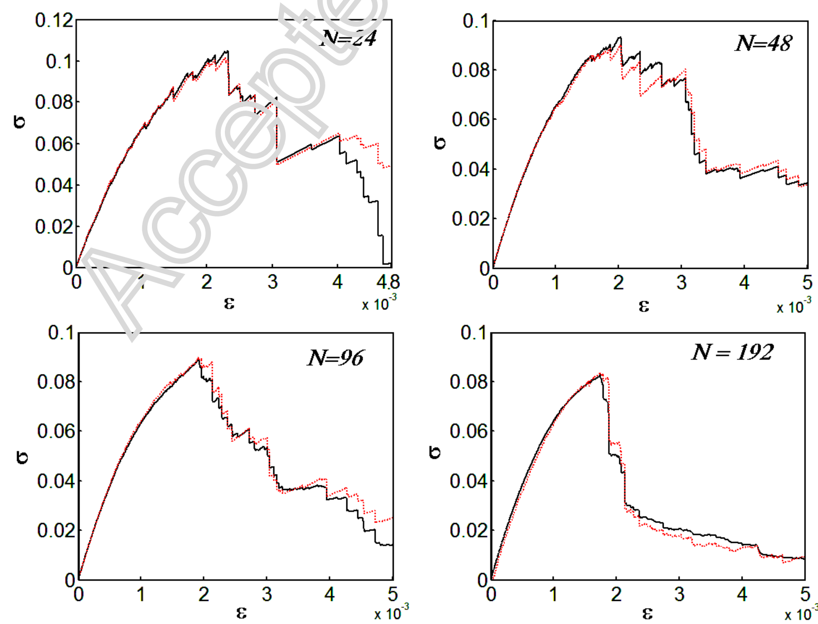

Fig. 13. Responses of scaling model Eq.(17) and (28) from the "K-approach" (dotted line) vs. original simulation data (solid line) for 4 random replicates for $L = \{24, 48, 96, 192\}$.

3.1.3. Summary of the procedure

In summary the "Krajcinovic approach" proposed herein consists of a two-steps scaling procedure encompassing the following:

1. Collection/simulation of *σ-ε* and *n-ε* for several samples and over a sufficiently large *L* range (recommended 2 orders of magnitude) ;
2. Compute averages curves per each *L*;
3. Subdivide the datasets in pre-peak and post-peak data;
4. Apply scaling Eq.(9) to the all data for the sake of scaling peak points into one;

   →*I check point:* IF NOT POSSIBLE, THEN STOP

5. Compute approximate relations for $n(\varepsilon;L)$, ε_p and D_p (the later one being scale-invariant);
6. Identify a suitable model/definition for the damage parameter in the fracture initiation regime;
7. Apply scaling Eq.(10) to the softening data seeking to transform the remaining of the data;

   →*II check point:* IF NOT POSSIBLE, THEN STOP

8. Compute approximate relations for $\Delta n(\varepsilon;L)$ and ΔD_p;
9. Identify a suitable model/definition for the damage parameter in the fracture propagation regime;
10. Validate the results of the scaling law and of the choice of D by comparing Eq.(4) vs. the initial datasets of simulations or experiments

4. CONCLUSIONS

For quite a few decades, lattice models have been focused on the investigation of finite-size scaling and on the formulation of physical/rational models of damage. They have appealed specially to the community of physicists and mathematicians active in statistical physics who have seized the opportunity to investigate failure in heterogeneous systems by the same approaches developed for phase transitions and chaos. However, the K-approach developed here from lattice data is an heuristic scaling procedure bears the potential to evolve from science to a practical tool for the engineering community, being (i) based on the physics of the fracture initiation process underlying the damage in quasi-brittle-system and (ii) being transferable in principle also to experimental data, provided that the number of microcracking events is tracked along with the stress response. Approximate analytical expressions are readily deduced from scaled data and shown to yield robust stress vs. strain constitutive relations. Yet, this method has to be benchmarked against the current mainstream approached described in the introduction, contributing to the ongoing debate about size-effects modeling and control in quasi-brittle system.

5. APPENDIX: LATTICE MODEL

Fracture initiation in quasi-brittle materials has proved to be an elusive subject that has been approached by a continuum and discrete angle for over 20 years now. By a continuum standpoint, a substantial amount of work has been produced. The consideration of at least two length scales (see Fig. 14) poses an intrinsic difficulty for first displacement gradient continuum damage model (CDM), more suited to capture macroscopic effects (e.g. Chambolle et al, 2009, 2010; Contrafatto and Cuomo, 2002, 2005, 2006; Del Piero and Truskinovsky, 2009; Rinaldi and Placidi 2013), and micropolar elasticity (e.g. Altenbach et al. 2010; Diebels and Geringer, 2013; Diebels and Scharding 2011; Eremeyev, 2005; Forest et al. 2001; Forest, 2009) or higher displacement gradients (e.g. Diebels and Ebinger, 2005; Ebinger, Steeb, Diebels, 2005; Alibert, Seppecher and dell'Isola, 2003; Seppecher, Alibert, Dell'Isola, 2011) are required to capture damage localization (e.g. Sunyk and Steinmann, 2003; Yang and Misra, 2010).

Conversely, the problem can be approached from the bottom length scale using discrete microstructural models. These are a convenient and increasingly popular alternative pursued by many research groups besides those already cited (e.g. Curtin and Scher, 1990; Jagota and Bennison, 1995; Van Mier et al. 2002; Mastilovic, 2008, Rinaldi et al. 2008; Miguel et al. 2010) for they are well suited for multiscale problems. They can incorporate several microstructural features into the model by using statistical information that can be measured directly and, without making extensive assumptions, are capable of scaling the material response to the macro level. In this class, considerable attention has been drawn by lattice models, which provide simple representations of complex systems, such as the disordered microstructures of ceramics, concrete and other quasi-brittle polycrystalline materials. Contrarily to a classical CDM, lattice models resolve individual grain boundaries and are convenient for study of brittle damage by intergranular cracking. Van Mier and coworkers (2002), for example, showed the agreement between simulated tensile tests and actual tests for concrete using lattice models of the microstructure. Some effort has been progressively devoted to bridge across discrete and continuum approaches, in the attempt to reconcile the two. For example, Rinaldi and Placidi (2013) established the connection between the present lattice models and 2nd gradient CDM by analyzing a case study that reveals such a consistency. The present paper is the complement to the latter work, addressing size effects and providing the continuum scaling laws discussed in the body text.

The details of the specific 2-D lattice model used in our discussion and presented in prior work (Rinaldi and Krajcinovic, 2007, Mastilovic and Krajcinovic, 1999) are briefly recalled here for convenience. The lattice is made of a disordered network of springs with finite strength, providing a first order approximation for the materials microtexture, the morphology of which can be represented by a random Voronoi froth and its dual Delaunay lattice. A Voronoi polygon represents a grain of ceramic, a concrete aggregate or a granule of clastic rock whereas a bond in the Delaunay lattices is representative of corresponding interface cohesion.

The lattice encapsulates both morphological and mechanical types of information at lower computational expense. Each grain of the polycrystalline material maps into a node in the lattice, while each lattice link marks a grain boundary and is a linear spring of stiffness $k_{(ij)}$ and finite tensile strength $f^{*+}_{(ij)}$ (or positive elongation $\Delta u^{*+}_{(ij)}$) that transmits the force between adjacent i-th and j-th generic grains ($i,j = 1..N_0$, such that $i \neq j$ and $N_0 = \#$ nodes) [2]

$$f_{ij}(\mathbf{u}_\mathrm{i}, \mathbf{u}_\mathrm{j}; t, t_0) = \begin{cases} k_{ij}(\mathbf{u}_\mathrm{j} - \mathbf{u}_\mathrm{i}) \cdot \mathbf{r}_\mathrm{ij} = k_{ij}\Delta u_{ij}(t) & (\Delta u_{ij}(t) < 0 \ \ or \ \ 0 < \Delta u_{ij}(t_0) < \Delta u^{*+}_{ij}, \forall\, t_0 \in [0,t]) \\ 0 & (\Delta u_{ij}(t) > 0 \ and \ \exists\, t_0 \in [0,t] \ such \ that \ \Delta u_{ij}(t_0) = \Delta u^{*+}_{ij}) \end{cases} \quad (30)$$

(not a tensor)[2]

The springs behave as decohesive elements that break under tensile load when a "random critical strain" is reached previously at any time point t_0 between 0 and the current time t, thus reproducing the intergranular cracking process of brittle materials such as concrete or ceramics.

For the data in this paper the following assumptions apply:

- the links have equal stiffness $k_{ij} = k$ (=100) and equal length ℓ_0 (=1) breaking at a tensile strain $\varepsilon^*_{ij} = \Delta u^{*+}_{ij} / \ell_0$,
- no healing is allowed,
- the (mechanical) disorder is inserted in this lattice by sampling the failure tensile strains from a uniform distribution $p_f(\varepsilon)$ in the interval $\left[0,\ 10^{-2}\right]$.

Damage is introduced in the network by the rupturing of the links, which are removed progressively from the system. Broken links remain active in compression if load reversal occurs in the course of deformation to account for crack closure. The lattice is geometrically distorted since the equilibrium link lengths are normally distributed within the range $\alpha_l \bar{\lambda} \le \lambda \le (2 - \alpha_l)\bar{\lambda}$ with $\alpha_l = 0.1$ (if $\alpha_l = 1$ all grains are perfect hexagons).

Quasi-static displacement-controlled uniaxial tensile tests are simulated on different lattice sizes L by means of a molecular dynamics solver based upon the Verlet's algorithm. Each simulation is carried on incrementally up to the threshold of failure by applying small displacement steps and by computing the equilibrium configuration at each step.

For the sake of the advocated similarity between the lattice and the fiber bundle model (FBM), the latter one consists of an ensemble of parallel and non-interacting links of equal stiffness k connected by rigid bus bars at the ends, the damage parameter of which is $D = \int p_f(\varepsilon) d\varepsilon$ (Rinaldi 2011). Under the conditions of uniform sampling distribution in our simulations, it is readily

[2] The index notation ε_{ij} refers to the ij-th link has end nodes i and j, not to be confused with second order tensors, as customarily reserved in solid mechanics.

obtained $D= \varepsilon/0.01$, according to which the stress response (4) is a parabola and Dp=0.5, as stated in Eq(16).

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