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Ductile-to-brittle transition behavior using peridynamics simulations

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Abstract. The problem of the Size effect on the material's tensile strength becomes a particularly important point when a transition is made between the size of the structure tested in the laboratory and its actual size. Thus, the question of the validity of laboratory tests and the prediction of their behavior in engineering structures continue to be a topic in constant research. It is known that as the size of the tested sample increases, there is a change in the global behavior from ductile to brittle. Capturing this change is the key to knowing the real behavior of the sample and offering better predictions for the design of this type of structure. In this work, the application of the peridynamic (PD) theory is evaluated to predict the behavior of quasi-brittle material specimens of different sizes submitted the uniaxial tensile load. The potential of the numerical method shown that PD is a powerful tool capable of successfully representing the transition between global behaviors.

Keywords: size effect, peridynamic, quasi-brittle material.

1 Introduction

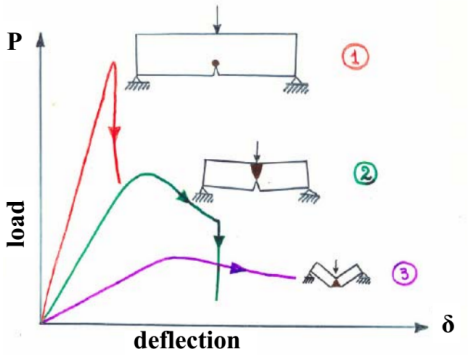
The problem of the scale effect in quasi-brittle materials such as rocks, concrete, ceramics and some fiber-reinforced polymers has become a topic of constant research due to the need for an adequate prediction of the mechanical behavior in large structures, based on laboratory test data, that is, on a scale generally smaller than the actual size of the structure [1]. Knowing whether the experimental results of these small-scale structures have wide applicability and practical significance for real structures has become one of the challenges faced by most researchers and designers.

Based on experimental studies, it is known that the scale effect in quasi-brittle materials is responsible for altering the mechanical *properties* of the material, such as tensile strength, fracture energy and critical deformation [2]. However, another registered phenomenon is the transition of the global behavior of the component or structure from ductile, in small samples, to brittle in large samples, as shown in Fig. 1, where three beam sizes of quasi-brittle material are presented in a three-point bending test and the respective classification of their behaviors. During the transition process the governing failure mechanism changes. While in ductile behavior, plasticity causes crack propagation to occur in a controlled manner after the peak load, in the fragile case the failure occurs due to the unstable crack propagation governed by fracture mechanics. In the transition zone, the rupture is stable initially and later unstable. This ductile-to-brittle transition can be described by a dimensionless parameter called stress brittleness number, N_P, propose by Carpinteri [3]. This parameter is a function of the material toughness K_c, the ultimate stress σ_u and the structure characteristic length Z, as shown in eq. (1):

$$N_P = \frac{K_c}{s_u \sqrt{Z}} \tag{1}$$

From eq. (1) the same material, but in different scales, will present different global behaviors depending on its characteristic size. In general, for $N_P \rightarrow 0$, a brittle behavior is expected and ductile when $N_P \rightarrow \infty$. Experimental results of van Vliet and van Mier [4] and Carpinteri and Ferro [5] analyzed by Kosteski et al. [6], show that for values of $N_P < 1$, there is a brittle behavior and for $N_P > 1.5$ a ductile behavior, with a transition zone between these values. However, the geometric shape of the tested structure, the slender ones and the boundary conditions can cause these values to change from case to case.

The complexity of the failure process in this type of materials makes numerical models an alternative to complement the results obtained in the laboratory and in the prediction of the behavior of large structures. One of the theories that has shown great potential in the representation of the fracture is Peridynamics (PD). Considered a recent theory, it was proposed by Silling [7] and has been gaining attention in recent years. In this work, the application of the peridynamic theory is evaluated to predict the behavior of specimens of rocks of different sizes submitted the uniaxial tensile load. The potential of the numerical method shown that PD is a powerful tool capable of successfully representing the transition between global behaviors.



	Structural behaviour	Crack growth process
1	Brittle	Unstable
2	Ductile/Brittle	Stable/Unstable
3	Ductile	Stable

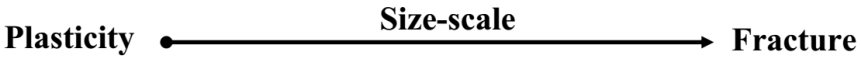


Figure 1. Illustration of the scale effect on beams of different sizes and their global behavior (adapted from [8])

2 Bond-Based Peridynamics Theory

Bond-based Peridynamics (BBPD) is the original version of peridynamics, later generalized as state-based Peridynamics (SBPD). PD was introduced by Silling [7] and its governing equations are in the form of integro-differential equations and can be written as:

$$\rho(\boldsymbol{x})\ddot{\boldsymbol{u}}(\boldsymbol{x},t) = \int_{H_x} \boldsymbol{f}(\boldsymbol{u}'-\boldsymbol{u}, \boldsymbol{x}'-\boldsymbol{x})dV_{x'} + \boldsymbol{b}(\boldsymbol{x},t) \tag{2}$$

where $\rho(\mathbf{x})$ is the density of the material point, $\ddot{\mathbf{u}}(\mathbf{x}, t)$ is the acceleration of the material point at time t; H_x is defined as the horizon which defines the range of interaction of the material point at x with other material points; $dV_{x'}$ is the volume of the materials points within the horizon (see Fig. 2a); $\boldsymbol{b}(\boldsymbol{x}, t)$ is the body load externally exerted on the material point at $\mathbf{x}$. $\boldsymbol{f}$ is the bond force between material points $\boldsymbol{x}$ and $\boldsymbol{x}'$ and it can be calculated as:

$$\boldsymbol{f} = cs\frac{y'-y}{|y'-y|} \tag{3}$$

where y = x + u is the position of the material point in the deformed configuration where u is the displacement and x is the position of the material point in the original configuration and c is the bond, for 3-D isotropic materials, the bond constant can be written as [9]:

$$c = 12E/\pi\delta_0^4 \tag{4}$$

In eq. (4), E and ν are material constants corresponding to elastic modulus and Poisson's ratio, respectively

and δ_0 is the radius of the horizon, considered a material property, as a characteristic length. This concept is discussed in detail in Nestor et al. [10]. This will allow, as will be shown below, to use a bilinear law as a constitutive relations. One of the most important parameters of BBPD is the stretch and it can be defined as:

$$s = \frac{\left|y' - y\right| - \left|x' - x\right|}{\left|x' - x\right|} \tag{5}$$

To model the quasi-brittle material behavior, the bilinear law proposed by Cabral et al. [10] is used to replace the classic uniaxial law of PD, Fig 1b. It is important to mention in this formulation the horizon (δ_0) is defined as a properties of the material and not of the model (δ'), which can be adopted as the convenience observing the increase in computational time when this value increases. Thus the bilinear law makes an equivalence between the energies with the material and computational horizon, making the law more flexible and allowing to change the global behavior of the material. For more information on the bilinear law and the calibration of the parameters, see Cabral et al. [10].

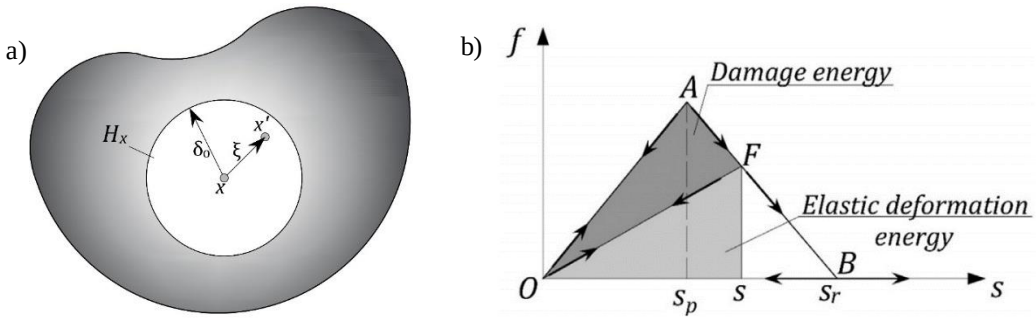


Figure 2. a) PD parameters [7], b) bilinear law and its relation with the involved energies in the loading process [10].

The critical condition is reached when s is equal to or greater than s_r Fig. 1b, equal to:

$$s_r = K_r s_p, \qquad K_r = s_0 d_0 / s_p d' \tag{6}$$

where K_r makes the relationship between the maximum linear stretch (s_p) and the critical stretch in the bi linear law (s_r), see Fig. 1b. s_p can be estimated, when experimental results are available, as the strain in which the structure loses its linearity. In (4) s_0 is the critical stretch of the bond. This parameter is the same in the classic uniaxial law, and for 3D case, can be defined in terms of the macroscopic fracture energy G_f:

$$s_0 = \sqrt{5G_f / 6E\delta_o} \tag{7}$$

In the PD model, G_f is assumed to have a Weibull probability distribution given by:

$$p(G_f) = 1 - \exp[-(G_f / b)^g] \tag{8}$$

being β and γ the scale and shape parameters, respectively. Such parameters can be computed through the coefficient of variation CV_{Gf} defined as the ratio between the standard deviation s_{Gf} and the mean value of the specific fracture energy G_f. However, a spatial correlation function for G_f needs to be defined. The correlation lengths *Lcx*, *Lcy*, *Lcz* along the three directions *x*, *y* and *z*, respectively. Details may be found in Friedrich et al. [11] and Puglia *et al*. [12].

3 Model description

To evaluate the response of peridynamics in the study of the scale effect in capturing the ductile-brittle transition, a set of plates of quasi-brittle material is simulated. The plates are subjected to a uniaxial tensile test,

fixing the lower part and applying a prescribed displacement in the upper region. Figure 3 shows the configuration of the board, its relative dimensions and the boundary conditions.

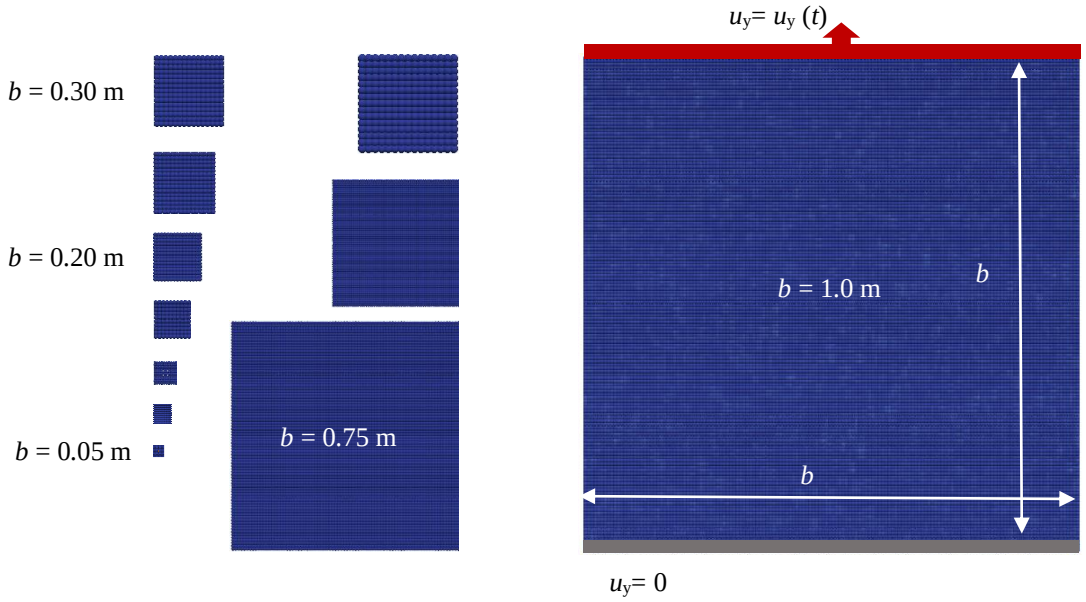


Figure 3. Relative plate dimensions and boundary conditions applied

In order to simulate the plane strain state, in all cases the displacement of material points in the normal direction to the plane of the plate is restricted. As the peridynamics model used is three-dimensional, in all cases the thickness (t) is equal to $3dx$. The length b of the plates varies from 0.05 to 1 m. All cases are simulated with a spacing between material points (dx) equal to 0.005 m. Table 1 shows the basic dimensions of the samples, while Tab. 2 indicates the properties of the material used as well as the parameters that define the bilinear law. It is important to note that the fracture energy G_f is constant within the bilinear law for all cases, that is, it does not change with the size of sample. Thus, G_f is considered in this case an average value among all sizes. To obtain representative statistical results, 4 simulations were performed for each case.

Table 1. PD models dimensions

Plate	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**
***b* (m)**	0.05	0.075	0.10	0.15	0.20	0.25	0.30	0.40	0.50	0.75	1.00
Points	10	15	20	30	40	50	60	80	100	150	200

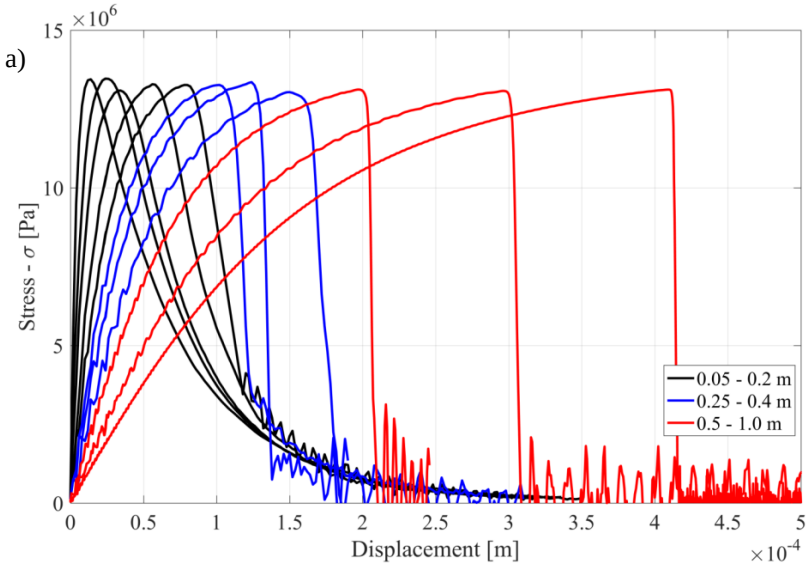
Table 2. Material properties and PD parameters

Material properties	**Valor**
E (Modulus of elasticity)	75 GPa
ρ (Density)	2700 kg/m^3
ν (Poisson ratio)	0.25
G_f (Frature energy)	1300 N/m
PD parameters	
dx	0.005 m
δ_0	0.45 m
δ' (3.015dx)	0.015075
K_r	57
s_p	1.29 10^{-04}
CV$_{Gf}$ (Coefficient of variation)	120%
$Lcx = Lcy$	dx/2

4 Results and discussion

Figure 4 shows a representative curve for each simulated sample size in terms of nominal stress vs global displacement. All samples were tested until complete rupture, or until the nominal stress reaches 2% of the maximum nominal stress (σ_u). In Fig. 4 it is clear the ductile, brittle behavior and the transition region between them, which characterizes the structural effect scale. Thus, in Fig. 4 the plates were classified into three zones according to their global behavior: ductile for $b \leq 0.2$ m (black lines), brittle for $b \geq 0.5$ m (red lines) and samples between these values represent the transition zone between ductile and brittle behavior (blue lines). According to van Vliet and van Mier [4], the change in behavior is related to the stable propagation of crack in the plates classified as ductile and the instability recorded in larger samples, which results in a brittle fracture.

a)



b)

b [mm]	σ_u [MPa]	CV [%]	N_p
50	13.91	4.31	3.18
75	13.73	1.33	2.63
100	13.30	1.22	2.35
150	13.34	1.03	1.91
200	13.37	2.31	1.65
250	13.27	0.38	1.49
300	13.27	1.01	1.36
400	13.18	1.16	1.18
500	13.23	0.72	1.06
750	13.16	0.60	0.87
1000	13.07	0.88	0.76

Figure 4. a) Displacement versus stress and b) Mean values of peak stress, coefficient of variation (*CV*) and stress brittles number (N_p)

Figure 4b shows the mean value of the maximum nominal stress and the coefficient of variation for each sample size. In addition, the brittleness number proposed by Carpinteri (N_p) is presented, considering $Z = b$ and the mechanical properties used in the simulations, Tab. 2.

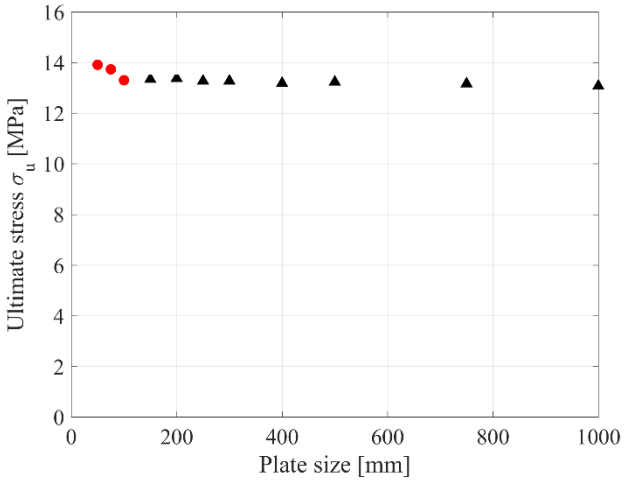


Figure 5. Ultimate global stress versus place size

Also in Fig. 4b, different gray scales indicate the samples in the zones previously classified in Fig. 4a. Comparing the results, it is possible to identify a good correlation of the behavior presented by the curves and the values predicted by the Carpinteri brittleness number. When $N_p \leq 1$, the brittle behavior is evidenced by an abrupt down in the stress curve. On the other hand, when $N_p > 1.5$ a controlled behavior of the stress curve shows a ductile rupture.

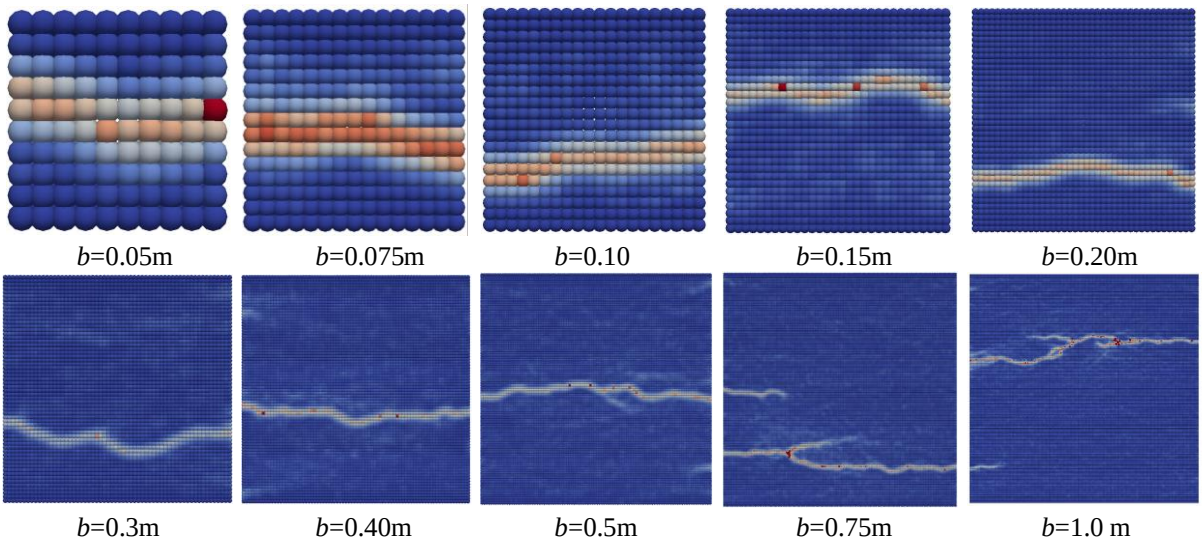


Figure 6. Damage distribution and rupture configuration of specimens of various sizes

Figure 5 shows the maximum nominal stress x plate length graph, where some points were discarded due to the non-correlation with the others, which may be a result of the low level of discretization in these cases. Note that there is no scale effect on the tensile strength. Global parameters of the model such as the boundary conditions and the distribution of the mechanical properties of the material (G_f in this case) can change this scenario, and studies on this will be carried out in other works.

Figure 6 shows an example of the final rupture configuration for each sample. Clearly as the size b increases and the plate shows a fragile behavior, most of the registered damage is concentrated around the main crack, characterizing the concentrated damage. On the other hand, in samples of more ductile behavior, the damage is distributed first, and only afterwards the localization occurs, with the damage being distributed throughout the body. This behavior is more evident in samples of b = 0.05 m and 0.075 m.

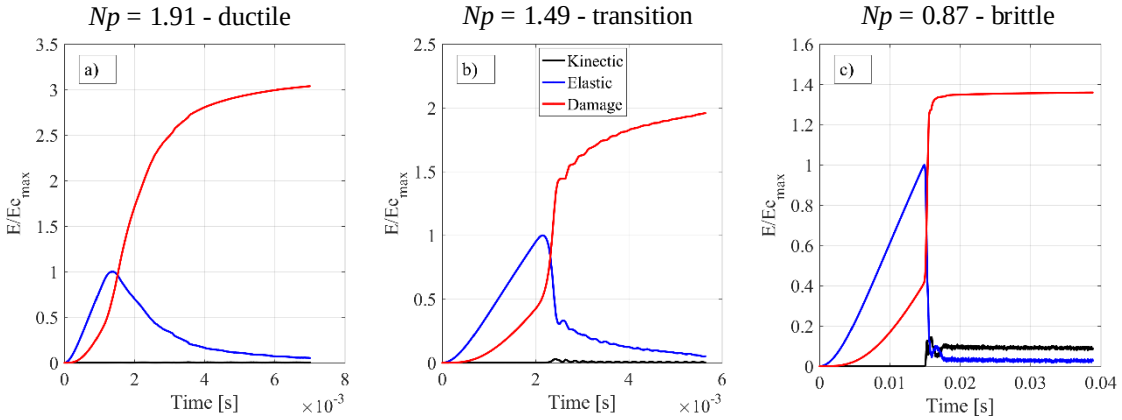


Figure 7. Evolution of the energies involved during the fracture process for the different classified behaviors

Figure 7 shows the energy balance observed during the damage process for three different behaviors. The

energies are normalized in relation to the maximum elastic energy of each case. Note that in the fragile behavior, Fig. 7c, the kinetic energy increases rapidly at the moment of rupture and the unstable damage process occurs. In this case, its maximum peak coincides with the peak of elastic energy. In the other cases, the kinetic energy remains close to zero, since the damage happens in a stable way. It is still possible to identify that as the ductile - brittle behavior changes, the ratio between the maximum energy dissipated by the damage and the maximum elastic energy decreases as N_p decreases. In the transition, Fig. 7b, there is a mixture of ductile and brittle behaviors, with a significantly higher damage energy value than elastic energy, however, this damage energy increases more abruptly, as seen in the brittle case.

5 Conclusions

In this work, we evaluated the PD in the prediction of the structural scale effect, through the transition from ductile-to-brittle behavior. When we evaluated the ultimate stress, there was no significant change, but many factors of the model must still be analyzed, such as the boundary conditions, sample format, random field, among others, to better understand the phenomenon. The results obtained for different sizes of simulated rock samples show that the overall mechanical behavior is in accordance with the brittleness number (N_p) prediction. PD proved to be a potential tool for the study of the scale effect, which makes it a good alternative to complement experimental data.

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