

Theory and Application of Weibull Distributions to 1D Peridynamics for Brittle Solids

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Abstract: Peridynamics is a continuum mechanics modelling method, which is emerging as a solution for – in particular – the modelling of brittle fracture. The inherent variability of brittle fracture is captured well by the Weibull distribution, which describes the probability of fracture of a given material at a given stress. Recreating a Weibull distribution in peridynamics involves adjusting for the fact that the body is made up of a large number of bonds, and the distribution of strengths associated with these bonds must be different to the distribution of strengths associated with the peridynamic body. In the local case, where the horizon ratio, $m = 1$ is used, Weibull’s original simple size scaling gives exact results, but the overlapping nature of non-local bonds that occurs in higher m cases, typically used in the peridynamics literature (such as $m = 3$), causes a significant distortion of Weibull distributions. The cause of these distortions is spurious toughening and partial component failures as a result of the reduced localisation associated with larger horizon ratios. In order to remove these distortions, appropriate size scaling is used for the bonds, and a methodology that is capable of reflecting the heterogeneity of the material in the model, is proposed. The methodology described means Weibull parameters measured at specimen or component level can be reproduced for higher values of m .

1 Introduction

Peridynamics [1] is a non-local continuum mechanics formulation, claimed to be better suited to convenient modelling of fracture than classical continuum mechanics methods. The governing equations of peridynamics do not contain the spatial derivatives that cause breakdowns at discontinuities in classical continuum mechanics [2]. In the original (bond-based) peridynamics formulation the governing equations may be modelled explicitly as pair interactions, often as linear elastic bonds between material points, stretching across a finite distance called the horizon. The ratio between the horizon size and the typical distance between two nearest-neighbour material points is an important variable, referred to as the horizon ratio, m . Bond-based peridynamics suffers from limitations including constraints on material properties (notably Poisson’s ratio) and an inability to capture incompressibility in plastic deformations [3]. Although these problems are addressed by state-based peridynamics, this behaviour is not of interest in this work, so the simpler bond-based method is sufficient.

The non-local nature of peridynamics stems from a horizon ratio of $m > 1$, with a common use in the range of 3 - 4 material point spacings [4]. Increasing m significantly above such values causes excessive wave dispersion, and increases computational effort for little meaningful gain in accuracy. Using a smaller m can cause the direction of crack growth to be influenced by grid orientation [5] – i.e. one of the great advantages of peridynamics, which is its mesh independence, is then lost.

Peridynamics is particularly useful and well-used for simulation of brittle fracture [6–9], often of ceramic materials [10–12]. The theoretical fracture strengths of ceramic materials are much higher than experimentally observed values, because of their tendency to brittle fracture and inherent microscopic flaw distributions. Small flaws in ceramic objects act as stress raisers, and the lack of ductility inherent in ceramics renders blunting of these flaws highly improbable at most temperatures of application, and so the ultimate

result of this stress concentration is fracture [13]. Since these flaws are randomly sized and oriented, and their size and orientation affects the degree to which they raise stress in the material, ceramic materials have a distribution of possible fracture strengths. A commonly used distribution for describing the fracture strengths of ceramics and other brittle materials is the Weibull distribution [14–16]. Peridynamics is widely being used to model fracture of ceramics and glasses, and the fracture properties of ceramics are well described by a Weibull distribution. It therefore follows that is highly desirable to have a proper understanding and method to implement the Weibull distribution in peridynamics and this is important and necessary to the modelling of industrially relevant ceramic components, where design and verification is often based on approaches incorporating experimentally determined Weibull statistics, see e.g. NASA's approach to design and verification of ceramic components [17].

The typical linear elastic bond-based peridynamics formulation includes a single value for critical stretch (fracture strain) at which a bond fails [10,18,19]. This is usually sufficient to get representative crack patterns and even produces a Weibull output from a single valued input, presumably due to the inherent Weibull distribution of rounding errors in the computational implementation [20]. In other cases an arbitrary distribution has been applied to create some scatter [21,22]. This approach is generally used to avoid problems related to symmetry in the discretization, rather than in an attempt to recreate behaviour of real materials by implementing a known experimentally measured distribution. A similar effect can be achieved by randomly displacing material points by a small amount [23]. It has been shown that randomness and some degree of heterogeneity in peridynamic properties can have beneficial effects on fracture prediction capabilities [24]. Some work exists in the literature involving Weibull distributions in peridynamics, but methods that explicitly model defects [25] are not useful on scales where the mesh spacing needs to be much larger than such defects and removes advantages of the rather coarse and pseudo meshless nature of peridynamics.

In this paper, the suitability of bond-based peridynamics for modelling material with a Weibull distribution of fracture strengths was investigated, using a 1D implementation of peridynamics for simplicity and computational efficiency. In a first part of the paper, direct application of the Weibull distribution is explored and it is shown that simple scaling following Weibull's original proposal gives exact results when the horizon ratio, $m = 1$. However, for higher values of m the process of randomisation of bond strengths drawn from the Weibull distribution is demonstrated to need modification to create a truly heterogeneous material, in which the onset of failure also leads to overall failure as inherent in the Weibull approach. This is discussed in a second part of the paper and a method is presented that can accurately implement an experimentally measured Weibull distribution into the peridynamics theory.

2 Methodology

2.1 1D Bond-Based Peridynamics

In 1D, bond-based peridynamics consists of an array of material points separated by [in this work] a constant distances, R . The material points interact with each other through linearly elastic bonds, with each material point interacting with every other material point in its horizon.

In bond based, peridynamics, the relative elongation of a bond (sometimes referred to as the ‘bond strain’), s_{ij} , linking material points i and j , with initial separation ξ_{ij} , and relative displacement η_{ij} , is given by:

$$s_{ij} = \frac{|\xi_{ij} + \eta_{ij}| - |\xi_{ij}|}{|\xi_{ij}|} \quad (1)$$

In 1D, the parameters in (1) can be treated as scalars. Setting the initial separation to be equal to the length of the bond, l_{ij} , gives

$$s_{ij} = \frac{\eta_{ij}}{l_{ij}} \quad (2)$$

The pairwise force in the bond is found by multiplying the bond elongation by the bond elastic stiffness (sometimes referred to as the micro-modulus), c_{ij} , which is frequently a function of the horizon size and initial separation.

$$f_{ij} = c_{ij}s_{ij} \quad (3)$$

The number of bonds, connecting a single material point to material points on the left-hand side of the material point being considered, is given by the horizon ratio, m , defined as the ratio of the horizon, H and material point spacing R :

$$m \equiv \text{int} \left(\frac{H}{R} \right) \quad (4)$$

Hence the total force acting on the material point, j , under consideration due to material points on the left of it, F_j^L , will be:

$$F_j^L = \sum_{i=1}^m c_{ij}s_{ij} \quad (5)$$

Assuming that all of bonds have the same bond elastic stiffness, c_B , gives:

$$F_j^L = \sum_{i=1}^m c_B s_{ij} \quad (6)$$

If the sample is undergoing a homogeneous strain, ε_0 , the distance between two neighbouring material points will be a constant Δ , and this distance will increase by Δ for every material point further away. Hence the total force acting on the material point under consideration due to material points on the left of it will be:

$$F_j^L = \sum_{i=1}^m c_B \frac{\eta_{ij}}{l_{ij}} = \sum_{i=1}^m c_B \frac{\varepsilon_0 l_{ij}}{l_{ij}} = \sum_{i=1}^m c_B \varepsilon_0 \quad (7)$$

$$F_j^L = m c_B \varepsilon_0 \quad (8)$$

Alternatively, the force to the left however is also equal to the elastic stiffness of the global body, c_0 , multiplied by the strain. Equating this to (8) gives:

$$m c_B \varepsilon_0 = c_0 \varepsilon_0 \quad (9)$$

And therefore:

$$c_B = \frac{c_0}{m} \quad (10)$$

This reduction in the elastic stiffness of the overlapping bonds compared to the section of the material being model avoids spurious stiffening of the sample. The elastic stiffness of the body will of course depend upon its dimension and the elastic modulus.

2.2 Interpreting Weibull in 1D Peridynamics

Weibull developed his distribution because he noticed that the normal distribution struggled to fit data of weak materials with a large spread in strength. In such cases the probability of failure for zero applied stress is not zero, and a second problem is that it is difficult to account for the size dependence of strength of ceramics using the standard normal distribution [14]. To address the latter problem, he considered a chain of N links and realized that for the correct choice of distribution (an exponential function), predicting the strength of the chain from the strength of the links would be simple. Indeed, if the probability of failure, $P_{f,link}$, at an applied force, F , for a single link can be calculated using F_0 , the characteristic force at which $P_{f,link} = \sim 63\%$, and w , the Weibull modulus, which describes the spread of possible failure forces:

$$P_{f,link} = 1 - \exp\left(-\left[\frac{F}{F_{0,link}}\right]^w\right) \quad (11)$$

The probability of failure of a chain consisting of N links is then given by:

$$P_{f,chain} = 1 - \exp\left(-N \left[\frac{F}{F_{0,link}}\right]^w\right) = 1 - \exp\left(-\left[\frac{F}{F_{0,chain}}\right]^w\right) \quad (12)$$

From (12), it follows that the characteristic force for the chain can be obtained from that of the links from:

$$F_{0,chain} = \left(\frac{1}{N}\right)^{1/w} F_{0,link} \quad (13)$$

It is clear that the characteristic force for chains will be lower than that for single links, while the Weibull modulus is a material property and invariant under a change of size of the system. In terms of the characteristic stresses of a measured sample ($\sigma_{0,Sample}$) and of peridynamic bonds ($\sigma_{0,Bond}$) this translates as:

$$\sigma_{0,Sample} = \left(\frac{1}{N}\right)^{1/w} \sigma_{0,Bond} \quad (14)$$

or, more usefully:

$$\sigma_{0,Bond} = N^{1/w} \sigma_{0,sample} \quad (15)$$

Hence, since 1D peridynamics with horizon ratio, $m = 1$ is in fact completely analogous to the chain and its links, it is straightforward to derive the bond strengths from a Weibull distribution for the sample and vice versa. Nevertheless, an example will be treated below to illustrate this. All that needs to be done is to assign a bond strength to each of the bonds by random drawing out of the Weibull distribution. In practice this is implemented in our computer program by drawing a random number between 0 and 1 for each bond, and assuming it represents a probability of failure, P_f . Using the Weibull equation, these numbers were converted into strength values i.e. a critical stress at which the bond was considered to have failed. Once failed the bond has no stiffness and carries zero force.

2.3 Modelling Strategy

A framework for a 1D model of a tensile test, with bond strengths determined so as to replicate a Weibull distribution was constructed, with each model described by the following variables:

- The number of material points, N , and their spacing, dx to describe the length of the model.
- Weibull parameters: shape parameter (or modulus), w , and characteristic strength, $\sigma_{0,sample}$. These values define the Weibull distribution for the sample that the model is intended to recreate, i.e. obtained by testing a large number of samples.
- Probability of failure, P_f , values randomly assigned to each bond, with a uniform distribution, 0-1.
- Non-Weibull properties of the object such as its dimensions and elastic modulus, E .
- The horizon ratio, m , defined as the ratio between horizon size and material point spacing.

This model was then placed under tensile stress by moving the material point at one end in explicit increments, while keeping the other end fixed. Extension was increased until fracture was detected, and the peak stress was recorded as the fracture stress.

To calculate the Weibull properties of the model, a number of tests were performed with bond strengths randomly calculated according to a given set of parameters. The probability of failure for a given sample may be obtained using its rank x , and the total number of samples, X using

$$P_F = \frac{x}{X + 1} \quad (16)$$

The two-parameter Weibull cumulative probability distribution equation is given by (17), in which w is the shape parameter and σ_0 the scale parameter:

$$P_f = \exp - \left(\frac{\sigma}{\sigma_0} \right)^w \quad (17)$$

The cumulative probability distribution equation can be rearranged so that the equation now takes the form $y = mx + c$:

$$\ln \left(\ln \left(\frac{1}{1 - P_f} \right) \right) = w(\ln(\sigma)) - w(\ln(\sigma_0)) \quad (18)$$

Plotting these data and performing a least-squares regression was used to determine the Weibull parameters displayed by the model.

3 Results & Discussion

3.1 The importance of scaling

Before any discussion of the correct way to implement fracture distributions in peridynamics can begin it is important to demonstrate the flaws in the naïve, intuitive methods of doing so. The three test cases at the beginning of this section are used to do this, by attempting, in three different ways detailed in Table 1, to recreate a Weibull distribution of modulus 6 and a characteristic stress of 1000 MPa. The first two cases deal with a local ($m = 1$) model. In the first case, the bond strengths were assigned by directly drawing from the distribution of the sample strength, whereas in the second, the bond strength distribution was determined by the scaling according to (15). Case 3 examines the effects of increasing horizon size to introduce non-locality. In each case, the characteristic strength of the sample was 1000 MPa and the modulus 6.00.

Table 1 - Parameters describing the Weibull distributions of the bonds and the resulting data for case 1, 2, and 3

		Case 1	Case 2	Case 3
Distribution of bond strength	σ_0 (MPa)	1000	2154	2154
	w	6.00	6.00	6.00
Horizon Ratio, m		1	1	3
Scaling		None	<i>Bond</i>	<i>Volume</i>
Resulting distribution	σ_0 (MPa)	473	995	1860
	w	4.60	6.76	11.20

In case 1 (see Figure 1a), clearly the outcome was still a Weibull distribution of sample strengths but with a characteristic strength much reduced compared to the 1,000 MPa value required/expected for the sample. In contrast, in case 2, this problem disappears as the appropriate bond scaling technique was used (see Figure 1(b)). Although this is a simple result, in line with the theory, it is nonetheless important. Using fracture strength distributions assigned to bonds in peridynamics is not uncommon [21,22] but rarely is the issue addressed. Moreover, the simple examples illustrates that in a local formulation of peridynamics, in which failure is caused by failure of a single bond, the modelling methodology reproduces a key assumption underpinning the Weibull approach namely that once a single flaw is activated, the entire body fails.

However, using such a small horizon ($m = 1$) is not favoured within peridynamics as it strips away the non-locality that is peridynamics' core function.

Increasing the m to a value of 3, typical value in the literature [4], produces very poor results (Figure 1(c)) even when using a scaling function modified from (15) to include the effects of the size of bonds relative to the sample. It should be noted that when scaling the Weibull distribution, that there are m overlapping bonds between each material point. All other aspects of bond strength selection are unaffected by the increase in m .

The source of this distortion was made obvious upon examining the stress-strain graphs in the $m = 3$ case (Figure 1(d)). There were several occurrences of partial failures of the model, characterised by a significant decrease in stress that did not lead to ultimate failure. Instead, stress was allowed to reaccumulate (at a lower stiffness) until an eventual fracture and decrease in stress down to zero. These models clearly did not fail when the first bond failed. Instead, the samples tested displayed behaviour analogous to a crack propagating and then being arrested, allowing the material to stay whole, while reducing stiffness. This behaviour is characteristic of some materials such as that of low-temperature ferritic steel fracture toughness tests, and is termed “pop-in”[28]. The characteristic of the model, which produced this behaviour was the homogeneity with which the strengths were distributed. Weak bonds occupied the same space as stronger bonds, due to the overlapping inherent in the non-local method. It was therefore possible for a weak bond to fail, while the bonds around it carried the increased stress, preventing a fracture. This behaviour is not analogous to any phenomenon present in wholly brittle fracture, so if brittle behaviour is to be reproduced, whilst implementing a known Weibull distribution, a new approach to bond strength distribution is needed.

3.2 Localisation of failure for $m > 1$

Accepting that greater heterogeneity in fracture strength is desired, thus providing a better model of brittle fracture, so attention turns to how to introduce this heterogeneity. The bonds do not have a location attributed to them, but they exist between two material points that do. By assigning random values for probability of failure to the material points instead of the bonds, a spatially heterogeneous distribution of strengths was created. Strength values at material points are not useful to the model during calculation, however. Strain (and therefore stress) occurs in the bonds, and failure is determined to have occurred in a bond when the stress in it is greater than its fracture strength. It is therefore necessary to define the strength of the bonds as a function of the “strength” values associated with the material points around them. This section will focus on describing that function as a set of rules through four further example cases 4-7 for which the parameters are given in Table 2. As before, the characteristic strength of the sample was 1000 MPa and the modulus 6.00.

Table 2 - Parameters describing the Weibull distributions of sample, the bonds and the resulting data for cases 4-7. The characteristic strength of the sample was 1000 MPa and the modulus 6.00.

		Case 4	Case 5	Case 6	Case 7
Distribution of bond strength	σ_0 (MPa)	2154	2154	2154	2154
	w	6.00	6.00	6.00	6.00
Method		Connected Material Points	Average Intersect	Extreme Ends	Extreme Intersect
Resulting Sample Distribution	σ_0 (MPa)	1412	1432	1221	1008
	w	11.30	13.40	8.14	6.20

It is important to note that using this method of interpreting Weibull in peridynamics (regardless of how material point strengths are converted to bond strengths) has an effect on the scaling function. In the naïve interpretation in case 3, the increase in critical stress is a function of the difference in volume between a bond and the overall object. For the simple case, where $m = 1$, with probability of failure values directly applied to the bonds, this produced satisfactory results. In the process of moving the probability of failure values to the material points, the sampling of the Weibull distribution was changed. Instead of sampling once for each bond, now the distribution is sampled once per material point. This means that the sampling is now independent of m , and the size of any individual bond. The volume ratio is now of material points to the object, and the ratio may be replaced by a value equal to the number of material points in the sample.

The initially intuitive method to convert strengths at material points to strengths of bonds is to simply average the two strength values at the two ends of a bond (case 4), and use this average as the strength value for the bond. This method utilises the strength values at all material points. It also groups weak bonds together to some degree, which is important in removing the partial failure behaviour observed in Figure 1(d) However this averaging method produced poor results (see Figure 2(a)) with only a small improvement relative to the basic method. The reason for this is that it is still possible for strong bonds to exist in the same space as weak bonds. A long bond bridging -for example- 3 inter-material point spacings, may be stronger than the shorter bonds that exist entirely within its length. There is no relationship between the strengths of these two bonds, since they do not connect to any of the same material points.

It is necessary, then, to consider not just the material points at the ends of a bond, but all of the material points in between. Making the strength of a bond equal to the average of the strengths associated with all of

the material points it intersects reduces the possible difference in strength between long bonds and the short bonds (case 5), which exist in partially the same space as them. This improved averaging method still produced very steep gradient, high strength Weibull distributions compared to the desired input (see Figure 2 (b)). This error was attributed at least in part to the fact that the process of averaging values distorts the Weibull distribution. Very low-strength and high-strength bonds are highly unlikely, since they would require a sequence of low or high-strength material points. Every time the values are averaged they are pushed towards the centre of the distribution of possible strengths removing the distribution tails. The very high-strength bonds are of little to no importance to fracture, but removing the low strength bonds has two effects. Firstly, a decrease in the likely range of strength values (i.e. an increase in Weibull modulus) and secondly, an increase in the likely fracture strength of the model (i.e. an increase in the characteristic strength). Both of these effects are visible in the results.

In order to remove the bias towards moderate strength values for the bonds, a replacement for averaging was devised. Since the low-strength bonds are the most important in fracture, it is necessary that low-strength material points have a large impact on the strength of the bonds around them. To avoid simply replacing one bias with another, it is important that these low strengths are counter-balanced by high strength material points also having a large influence on the bonds around them. From these criteria, the “extreme” rule was devised (case 6). Using the “extreme” rule, a bond takes on the exact strength value of whichever material point (of those which are being considered for it: either the material points at either end; or all the material points it intersects) is most extremely weak or strong. Mathematically, “extremeness” was defined as the difference between probability of failure and 0.5. For example, if the material points being considered for a bond have probability of failure values of 0.05 and 0.9, the bond would have the strength corresponding to a probability of failure of 0.05, since that is further from 0.5 than 0.9 is.

Using the “extreme” method produces poor results when used in conjunction with initial “connected material points” method, (see Figure 2 (c)) but using it with the intersect method (case 7) produces excellent results (see Figure 2 (d)). It appears at face value to be somewhat arcane, but has good parallels to both real brittle materials and to more basic applications of Weibull peridynamics, however. In real brittle materials, there is a split between material around flaws, which may be considered weak, and material far away from flaws, which may be considered strong. There is very little material in reality that is analogous to a moderate fracture strength, and this is represented well in the model in this form. The basic application of Weibull in peridynamics (i.e. the $m = 1$ model described in section 2.2) works very well, and the combination of the extreme rule and the intersect rule functions to make the non-local model ($m = 3$) behave in the same way. Schematics describing each of the methods are shown in Figure 3.

It should be noted that this method is not presented as the only solution to the problem. Using a simpler minimum intersect method (where bonds take on the lowest P_f value of the material points associated with it) also produces good results. In 1D, there are likely other methods for which this is true. The extreme intersect method is presented most prominently in this work as it is believed that its ability to preserve a truer representation of the original distribution will be useful when scaling up to more useful 2D and 3D peridynamics models.

4 Conclusions

1. Randomising the properties of bonds in a peridynamic model affects the properties of that model in potentially unexpected ways (reduction in fracture stress and very narrow fracture stress distribution), and it is necessary to understand these effects when applying fracture distributions in peridynamics to recreate realistic Weibull behaviour.
2. The three key parts of the successful recreation of a given measured Weibull distribution in 1D peridynamics, producing brittle fracture behaviour, are:
 - a) properly size scaling the Weibull distribution to correct for the differences in size between a bond, a material point, and a sample.
 - b) randomising strength of material points, and using the more extreme values to calculate bond strengths, in order to recreate the strength distributions found in real materials.
 - c) using the intersect method outlined to properly concentrate weak bonds and create true heterogeneity
3. Practical applications of peridynamics will almost always involve two or three dimensions. The method presented is inherently one dimensional, and cannot be directly translated into higher dimensions. In any attempt to recreate the results obtained using the method outlined for 1D here in 2D or 3D, it would be important to avoid overlap between strong and weak areas or volumes.

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