QUASI-STATIC NON-ORDINARY STATE-BASED
PERIDYNAMICS FOR THE MODELING OF 3D FRACTURE

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DISSEPTION

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Abstract

A majority of the efforts in modeling crack propagation have used continuum models built upon partial derivatives with respect to the spatial coordinates in the force and displacement relationship. These methods are inherently incompatible for modeling cracks because the partial derivatives are undefined at crack faces due to the discontinuous displacement field. Furthermore, these methods fall short on robustness and computational complexity when involving heterogeneous materials, crack initiation and crack branching, especially in a 3D setting. A recent addition to the list of numerical methods used in fracture mechanics, peridynamics is a particle-based continuum model that addresses some shortcomings of other methods.

In this work, a quasi-static linearly elastic implicit parallel implementation of the non-ordinary state-based peridynamics formulation is presented for both stationary and propagating cracks. Emphasis is placed on assessing the accuracy of the numerical scheme in the vicinity of the crack front and other sources of stress concentration. The near-tip solution is affected by the presence of zero-energy modes, particularly in regions of high strain gradients, caused by the nonlocal definition of the strains. A systematic comparative study is presented between the various methods introduced to address this numerical instability. The accuracy of the peridynamics scheme, including the impact of the grid spacing and configuration, is assessed through a detailed analysis of the near-tip stress and displacement fields and the extraction of key fracture parameters such as stress intensity factors and conservation integrals. This assessment includes a verification study based on the classical 3D penny-shaped crack problem and a validation study of a 3D notched fracture specimen. For the modeling of propagating cracks, the emphasis of the assessment study is placed on the ability of the method to predict crack path. To that effect, a variety of verification and validation problems corresponding to classical test geometries (double cantilever beam, four-point bend specimen and V-notched Brazilian disc) are simulated. Lastly, an analytical and numerical study linking peridynamics and cohesive zone modeling under Mode I, Mode II and mixed-mode loading is developed.
And whatever you do, in word or deed, do everything in the name of the Lord Jesus, giving thanks to God the Father through Him.

Colossians 3:17
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1 Introduction

1.1 Motivation

The numerical study of material failure and, in particular, the simulation of fracture events, is still to this day a very challenging problem as evidenced by the sheer volume of literature over the last few decades dedicated to the topic. Simulations of 3D crack propagation are often problematic theoretically when modeling heterogeneous, or anisotropic, or even orthotropic nonlinear materials commonly found in a wide range of applications, from aerospace to industrial engineering. Complications arise when predicting fracture in these types of materials due to the complexities of the near crack-tip fields and complex physical phenomena, due in part to, the deficiencies of classical fracture mechanics in accurately predicting the crack path. Often these types of materials are homogenized, or a complicated and computationally expensive multi-scale analysis is performed in order to capture the subscale processes driving the crack growth, such as micro-cracking ahead of the crack-tip.

While the constitutive behavior may be simpler for isotropic materials, the algorithmically complexity of modeling crack propagation in 3D is nonetheless still very challenging. This is especially true when cracks branch or when multiple cracks coalesce. This is because it is numerically difficult to track and accurately depict the crack surfaces and the ever-evolving boundary they create. Additionally, crack formation is another formidable challenge due to the fact that it is often a micro-scale process that classical fracture mechanics fails to predict. Peridynamics (PD) was conceived to address and lessen these difficulties when modeling complex fracture phenomenon.

1.2 Presentation of peridynamics

The PD theory was first introduced by Silling [1] as a continuum model for handling the spontaneous formation, propagation, branching and coalescing of discontinuities such as cracks. In PD, particles are influenced by other
particles separated over a finite distance referred to as the horizon; hence the method is classified as a nonlocal theory. The use of nonlocal elasticity for the study of fracture problems is not new; an early study by Eringen et al. [2] presented the nonlocal solution for the Griffith crack problem and showed that the use of nonlocal elasticity captured the physical nature caused by the geometrical discontinuity of the crack, namely the removal of the crack-tip stress singularity. This work led to a new stress-based fracture criteria incorporating the effects of the intermolecular forces as the dominant phenomenon around the discontinuities. As will be discussed in Section 1.3, many of the past nonlocal theories rely on averaging the strains or stresses within the neighborhood of a point and then differentiating the stress tensor in the equations of motion. For the interested reader, a thorough overview on the development of nonlocal theories and their applications is given by Bazant and Jirásek [3].

The first PD formulation introduced in the literature is the so-called “bond-based” formulation, in which the continuum is discretized by a grid of nodes interacting through pair-wise bonds. In this formulation, the response of a bond is independent of the other bonds. As a consequence, the bond-based PD scheme is limited to constitutive models with a Poisson’s ratio of 1/4. Nevertheless, the bond-based method has been and continues to be employed to study a wide variety of mechanical systems. Fracture and damage simulations have included the impact damage of composites [4, 5], fracture of plain and reinforced concrete structures [6, 7], fracture of membranes and fibers [8], and fracture of quenched glass [9]. At the nanoscale, PD has been used to model nanofiber networks and carbon nanotube-reinforced composites [10] as well as modeling nano-indentation of ultra-thin films in which the PD results compare favorably with those obtained using molecular dynamics and atomic force microscopy experiments [11].

A reformulation of the bond-based PD relations proposed by Silling and coworkers [12, 13] led to two new PD formulations referred to as ordinary state-based (OSB) and non-ordinary state-based (NOSB) PD. The state-based formulation introduces a force-vector state $T$ which maps a deformation-state into a force-state at all points within a volume of influence with no restrictions on the mapping function being linear or continuous [14]. Consequently, the state-based formulation eliminates the bond-based PD restriction requiring a Poisson’s ratio of 1/4 for isotropic linear elastic materials since the bond forces now depend on the collective deformation of the bonds in the volume of influence. The OSB formulation is an active area of research and has been used to model problems involving plastic [15]
and viscoelastic [16] constitutive models.

In contrast to its OSB counterpart, the NOSB PD formulation represents $T$ in terms of strain and stress tensors and consequently does not necessarily require co-linearity between the continuum points. The NOSB formulation therefore allows for classical continuum mechanics quantities, such as deformation gradient and stress tensor, to be used in constitutive models. This in turn allows for the incorporation of classical constitutive models into PD without the need to reformulate the constitutive laws in terms of the force-vector state $T$. Efforts to date using the NOSB formulation are relatively few and have focused mainly on the explicit formulation for dynamic simulations. In particular, Foster et al. [14] modeled rate-dependent plasticity for explicit dynamic Taylor impact tests of aluminum. Warren et al. [17] simulated transient dynamic fracture of a center cracked aluminum bar. Littlewood used the non-ordinary formulation to model fatigue crack growth of an elastic inclusion in a single elastic-viscoplastic crystal [18], and the dynamic fracture of an expanding steel tube was modeled using a classical mechanics elastic-plastic constitutive law [19]. Lastly, Tupek et al. [20] implemented a classical continuum damage model within the state-based formulation by modifying PD’s influence function according to the accumulated damage state, where the bonds are severed within a horizon in accordance with the damage law.

1.3 Comparison with other numerical methods

Various methods used in the modeling of LEFM, for both static cracks and arbitrary crack growth, have been proposed and a recent survey of the various state-of-the-art computational methods was recently published [21], which provides an excellent review of methods currently in use to model failure in brittle and quasi-brittle materials. Therefore, this section will not provide an in-depth presentation of these methods and is by no means an exhaustive review of these methods. This section will instead contrast the peridynamics method with other methods and will hopefully provide the reader with a better understanding as of how peridynamics relates to other popular methods. The reader should consult the aforementioned paper for a greater explanation of each method discussed in this section.

In terms of regularization of the boundary value problem (BVP), the peridynamics method is considered a strong nonlocal method, where the nonlocality is due to the state’s at a given material point dependence on the state of neighboring points. However, this is unlike other strong nonlocal
integral-type approaches where a material point’s state values are obtained by a weighted averaging over the spatial neighborhood and where those spatial neighbors represent “local” first or higher gradients of the state variables [3]. In contrast to strong nonlocal methods, gradient models can be classified as weakly nonlocal models [3], where the stress at a single point is expressed as a function of the strain and its gradients at that same point [22]. Cohesive Zone Modeling (CZM), originally introduced by assuming a plastic zone ahead of the crack-tip [23] and then by assuming the stresses ahead of the crack-tip vary with deformation [24], is another method used to achieve a well-posed BVP. The topic of CZM, which is often used in conjunction with the Finite Element (FE) method, and its relationship with peridynamics will be discussed further in Chapter 6.

One method of classifying the current computational methods used for fracture is whether the method ensures crack path continuity, thus forming a discrete crack with a continuous surface. The majority of the computational methods with underpinnings of the finite element method and most meshless methods, ensure crack path continuity and form discrete cracks. These various methods need a law that predicts both the orientation and the length of a crack segment’s propagation. For LEFM, the most popular fracture mechanics criteria are

- Maximum-stress criterion [25],
- Minimum-strain-energy-density criterion [26, 27, 28],
- Maximum-energy-release-rate criterion [25, 29],
- Local symmetry criterion [30].

Other methods for crack propagation prediction are [21]:

- Rankine Criterion — When the principal tensile stress exceeds the uniaxial tensile strength then a crack is introduced. Interestingly, for improved reliability, this criteria often uses a smoothing technique for the crack-tip stresses [31, 32] or crack normals [33, 34] to improve reliability, and thus introduces a nonlocal approximation to the stresses or the crack normals.

- Loss of material stability — Cracks form when the material stability is lost, dependent in the classical sense on the Legendre-Hadamard condition.
Global energy minimization criterion — The global energy is computed for different orientations of the crack, and the crack path that minimizes the global energy is selected.

In comparison to these methods, one of peridynamics fundamental premises and the main inspiration in its development is that auxiliary fracture criterion are not needed, but instead the cracks initiate and propagate naturally according to the fundamental equations.

Once the crack propagation length and direction are determined, the crack’s topology needs to be tracked. The current approaches for crack tracking are [21]: (1) local, (2) global, (3) level set methods. An in-depth review of these methods is presented by Rabczuk et al. [35]. Additionally, these methods must have a means to incorporate the discrete crack into the mesh. The most straightforward method is to do a global or local remeshing around the crack. However, this becomes difficult when multiple cracks form and coalesce. Alternatives to remeshing are: (1) eliminating elements crossed by a crack’s path by “deleting” the element, (element erosion, [36, 37, 38]), (2) enrichment of the displacement field to capture the discontinuous displacement field within a single element (embedded elements (EFEM), [39]) or introducing additional nodal parameters and using local partition of unity (extended finite elements (XFEM), [40, 41, 42]) and (3) by using overlapping elements (phantom node method [43]).

A popular alternative to the FEM-based methods is the use of meshless methods. As with the FEM, most of the meshless methods still require crack path continuity. However, one popular subset of the meshless methods for which a continuous crack is not required is the cracking particle method [44, 45, 46], for which the crack is represented by a set of cracked particles. In general, both FEM and mesh-free methods have difficulty, especially in 3D, modeling fracture when multiple cracks propagate and when those cracks eventually coalesce. Additionally, methods modeling discrete cracks commonly have a difficult time with predicting crack branching and crack nucleation [21].

The other class of computational methods in use today is smeared crack formulations where a finite band around the physical crack is assumed to be fully or partially damaged. In these methods, there is not necessarily a requirement for crack path continuity, and they usually lack the means to track the physical crack itself. Peridynamics falls into this category as the crack is over a region surrounding a material point. Another relatively new method that falls into this category are the variational approaches [47], also known as phase-field methods [48], where the crack trajectory follows the
path of least energy.

It should be noted that another popular meshless method, which is more of a point based method, used to model fracture is the smoothed particle hydrodynamics (SPH) method [49, 50]. Topologically, SPH is similar to peridynamics in the sense that there is no dependence on geometrical linkages (meshes or grids) in order to calculate spatial derivatives. However, in SPH, the partial differential equations are transformed into integral equations by the use of an interpolation function, giving a ‘kernel estimate’ of the field variables. Therefore, in SPH, the spatial derivatives operate on the interpolation kernel at a point instead of operating on the physical quantities [50]. Peridynamics, on the other hand, removes the partial differential operators completely by relying on integration over the difference in the displacements to find forces between material points.

As with peridynamics, the crack surfaces in SPH are not tracked explicitly. Furthermore, when modeling fracture using SPH, the damage state at each particle is determined, most commonly, by using a statistical flaw distribution function, and the amount of tensile force transmitted between particles is scaled depending on the damage at a particle [51, 50, 52]. In contrast, peridynamics’ interconnection between particles is handled by ‘bonds’, and the breaking of these bonds, which is predicted from the peridynamics fundamental equilibrium equations, dictates the definition of the crack. Hence, the damage state at a material point, i.e., ratio of broken to unbroken bonds, is a secondary indicator as to the crack’s location and is not the driving force in determining the crack trajectory.

In conclusion, nearly all these methods, local and standard integral-type nonlocal, use models that include partial derivatives with respect to the spatial coordinates in the force and displacement relationship between adjacent regions in the material. Therefore, these methods are inherently insufficient for modeling cracks because the partial derivatives are undefined along the crack faces where the displacement field is discontinuous. Hence, computational methods involving displacement gradients or higher-order spatial derivatives in a domain containing a crack must remove the discontinuous displacement field by either redefining the discretized body so that the crack lies on the boundary, or by using other techniques for evaluating the spatial derivatives on crack surfaces, as highlighted earlier. In contrast, the peridynamics formulation eliminates the spatial derivatives altogether by solely depending on an integral formulation of the force acting at a continuum point, resulting in equilibrium equations that are valid everywhere in the body. Furthermore, the overarching goal of the peridynamics method is to
eliminate the need for separate fracture mechanics criteria to model the fracture process as this process occurs as a result of solving the peridynamics equilibrium equations.

1.4 Thesis objectives and outline

This work will focus on a subset of fracture mechanics by considering only linear elastic material behavior for the bulk material and a small fracture process zone for which the assumptions of linear elastic fracture mechanics (LEFM) is a valid approximation. As noted in Section 1.2, the NOSB method is a relatively new formation and hence lacks a detailed investigation of the method for modeling fracture, leaving fundamental questions unanswered. To the author’s knowledge, with the exception of a qualitative dynamic simulation of a center notched specimen using a very coarse particle distribution in the seminal paper on the NOSB formulation [17], no quantitative fracture mechanics analysis has been performed using the NOSB formulation. Since it is the aim of this work to study the accuracy of the NOSB computational method for fracture, the effects of inertia and the associated complications of wave and crack interactions were eliminated so as to facilitate this goal. Therefore, this thesis

- Reviews the NOSB continuum formulation (Section 2.1.1),
- Develops a small-strain linearly elastic static implicit implementation of the NOSB PD formulation for static and propagating cracks (Section 2.1.2),
- Develops an efficient parallel implementation for both structured and unstructured grids composed of millions of particles (Section 2.2),
- Investigates and addresses zero-energy modes inherent in the nonlocal definition of the strains, especially in regions near the crack-tip where high gradients are present (Section 3.1),
- Details the ability of NOSB PD to capture key local fracture parameters commonly affiliated with non-propagating crack problems, including the stress intensity factor and the stress and strain concentrations around notches (Chapter 4),
- Investigates NOSB PD in predicting crack propagation and the effects of grid discretization on crack path predictions (Chapter 5),
• Provides an analytical and numerical study of the link between PD and cohesive zone modeling under Mode I, Mode II and mixed-mode loading (Chapter 6).
2 Formulation and Implementation

2.1 Formulation

In preparation for the derivation of the implicit non-ordinary state-based PD scheme, a brief review of the critical notations and the underlying PD theory is needed. Section 2.1.1 is a synopsis of the PD conventions introduced by Silling et al. [1] and a review of the continuum non-ordinary formation as presented by Warren et al. [17]. In Section 2.1.2, the discretized continuum equations presented in Section 2.1.1 are expanded for the implicit quasi-static formulation, and the numerical implementation is presented.

2.1.1 Continuum formulation

A continuum point at $\mathbf{x}$ in domain $\mathcal{B}$ interacts with its neighbors, i.e., those material points located within a distance called the horizon, $\mathcal{H}$, by means of bonds between continuum points (Fig. 2.1). The reference position vector state $\mathbf{X}$ is defined as

$$
\mathbf{X}(\xi) = \xi = \mathbf{x}' - \mathbf{x}.
$$

By operating on the bond $\xi$ between material points at $\mathbf{x}'$ and $\mathbf{x}$, the deformation vector state $\mathbf{Y}$ is the deformed state of the bond defined by

$$
\mathbf{Y}(\mathbf{x}' - \mathbf{x}) = \eta + \xi = (\mathbf{u}' + \mathbf{x}') - (\mathbf{u} - \mathbf{x}),
$$

where $\mathbf{u}'$ and $\mathbf{u}$ are the displacements at $\mathbf{x}'$ and $\mathbf{x}$, respectively, in the reference configuration and, thus, the relative displacement $\eta$ is

$$
\eta = \mathbf{u}' - \mathbf{u}.
$$

The nonlocal deformation gradient $\mathbf{F}$ at $\mathbf{x}$ is given by

$$
\mathbf{F}(\mathbf{x}) = \left[ \int_{\mathcal{H}} \omega(|\xi|) (\mathbf{Y} (\xi) \otimes \xi) \, dV_{\xi} \right] \mathbf{K}(\mathbf{x}),
$$

where $\omega$
where the shape tensor $\mathbf{K}(\mathbf{x})$ is defined as

$$
\mathbf{K}(\mathbf{x}) = \left[ \int_{\mathcal{H}} \omega(|\xi|)(\xi \otimes \xi) \, dV_{\xi} \right]^{-1},
$$

(2.5)

and physically represents the point distribution in the body $\mathcal{B}$, accounting for the partial horizons near the boundaries. The influence function $\omega$ can be chosen as a constant, meaning all points in $\mathbf{x}$’s horizon have equal influence, or as a non-constant function where the influence of each continuum point in the horizon is a function of the distance from $\mathbf{x}$. An influence function equal to zero indicates the bond $\xi$ between $\mathbf{x}'$ and $\mathbf{x}$ is broken.

The force state in terms of the stress tensor, $\sigma$, is shown to be [17]

$$
\mathbf{T} \langle \mathbf{x}' - \mathbf{x} \rangle = \omega \left( |\mathbf{x}' - \mathbf{x}| \right) [\sigma(\mathbf{F})]^T \mathbf{K}(\mathbf{x}) \xi,
$$

(2.6)

where, in this work, we consider the constitutive model $\sigma(\mathbf{F})$ in (2.6) as linearly elastic. The angle brackets denote the bond that the vector state operates on (e.g., $\mathbf{T}$ operates on the bond $\mathbf{x}' - \mathbf{x}$). The final system of the PD quasi-static equilibrium equations is from the Euler-Lagrange equation

$$
\int_{\mathcal{H}} \left\{ \mathbf{T}[\mathbf{x}] \langle \mathbf{x}' - \mathbf{x} \rangle - \mathbf{T}[\mathbf{x}'] \langle \mathbf{x} - \mathbf{x}' \rangle \right\} \, dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}) = 0,
$$

(2.7)

where $V_{\mathbf{x}'}$ is the volume associated with continuum point $\mathbf{x}'$ and $\mathbf{b}$ is an
external body force density field.

2.1.2 Discretization and numerical implementation

In a discrete system, the nonlocal deformation gradient, \( F(x_j) \), at a particle \( j \) can be expressed using Riemann sums over the total number of particles, \( m \), within the horizon, \( H \); as [17]

\[
F(x_j) = \left[ \sum_{n=1}^{m} \omega(|x_n - x_j|) (Y(x_n - x_j) \otimes (x_n - x_j)) V_n \right] K(x_j), \quad (2.8)
\]

where \( V_n \) is the volume associated with particle \( n \) in the horizon \( H_j \) of particle \( j \) and the discretized expression of the shape tensor (2.5) is

\[
K(x_j) = \left[ \sum_{n=1}^{m} \omega(|x_n - x_j|) ((x_n - x_j) \otimes (x_n - x_j)) V_n \right]^{-1}. \quad (2.9)
\]

Equation (2.8) represents the average value of the deformation gradient at location \( x_j \) associated with all the \( x_n \) points connected to \( x_j \).

For the implicit formulation, the system of equations is derived starting from Equations (2.8) and (2.9). Using the property,

\[
(\alpha u + \beta v) \otimes w = \alpha (u \otimes w) + \beta (v \otimes w), \quad (2.10)
\]

and substituting \( Y(x_n - x_j) = (u_n - u_j) + (x_n - x_j) \), the deformation gradient (2.8) takes the form

\[
F(x_j) = \left[ \sum_{n=1}^{m} \omega(|x_n - x_j|) (u_n - u_j) \otimes (x_n - x_j) V_n + \right.
\]

\[
\left. \sum_{n=1}^{m} \omega(|x_n - x_j|) (x_n - x_j) \otimes (x_n - x_j) V_n \right] \cdot K(x_j). \quad (2.11)
\]

Substituting (2.9) into (2.11), we get
\[ F(x_j) = \sum_{n=1}^{m} \omega \left( |x_n - x_j| \right) (u_n - u_j) \otimes (x_n - x_j) V_n. \]

\[ \left[ \sum_{n=1}^{m} \omega \left( |x_n - x_j| \right) (x_n - x_j) \otimes (x_n - x_j) V_n \right]^{-1} + I, \quad (2.12) \]

where \( I \) is the identity matrix. Introducing the displacement gradient, \( \nabla u = F - I \), yields

\[ \nabla u = F(x_j) - I = \sum_{n=1}^{m} \omega \left( |x_n - x_j| \right) (u_n - u_j) \otimes (x_n - x_j) V_n \cdot K(x_j), \quad (2.13) \]

where the shape tensor, \( K(x_j) \), is defined in (2.9). The small strain tensor,

\[ \varepsilon = \frac{1}{2} (\nabla u + (\nabla u)^T) = \frac{1}{2} (F - I + (F - I)^T) = \frac{1}{2} (F + F^T) - I, \quad (2.14) \]

evaluated at particle \( x_j \) is thus discretized as

\[ \varepsilon(x_j) = \frac{1}{2} \sum_{n=1}^{m} \omega \left( |x_n - x_j| \right) \left[ (u_n - u_j) \otimes (x_n - x_j) \right. \]

\[ \left. (x_n - x_j) \otimes (u_n - u_j) \right] V_n \cdot K(x_j). \quad (2.15) \]

Let us define the nodal displacement vector, \( U \), as

\[ U = \begin{bmatrix} u_1 & v_1 & w_1 & \cdots & u_m & v_m & w_m \end{bmatrix}^T, \quad (2.16) \]

where, by convention, the displacement components \( u_1, v_1 \) and \( w_1 \) are always reserved for point \( x_j \). The small strain tensor in vector notation then takes the form

\[ \varepsilon = \begin{bmatrix} \varepsilon_{11} & \varepsilon_{22} & \varepsilon_{33} & \varepsilon_{12} & \varepsilon_{13} & \varepsilon_{23} \end{bmatrix}^T = KNU, \quad (2.17) \]

where \( K \) and \( N \) are described by (A.2) and (B.5) in the Appendices A and B, respectively. The matrix of isotropic elastic moduli takes the usual form
\[ D = \frac{E(1 - \nu)}{(1 + \nu)(1 - 2\nu)} \begin{bmatrix}
  1 & \frac{\nu}{1-\nu} & \frac{\nu}{1-\nu} & 0 & 0 & 0 \\
  \frac{\nu}{1-\nu} & 1 & \frac{\nu}{1-\nu} & 0 & 0 & 0 \\
  \frac{\nu}{1-\nu} & \frac{\nu}{1-\nu} & 1 & 0 & 0 & 0 \\
  0 & 0 & 0 & \frac{1-2\nu}{2(1-\nu)} & 0 & 0 \\
  0 & 0 & 0 & 0 & \frac{1-2\nu}{2(1-\nu)} & 0 \\
  0 & 0 & 0 & 0 & 0 & \frac{1-2\nu}{2(1-\nu)} 
\end{bmatrix} , \quad (2.18) \]

where \( E \) and \( \nu \) respectively denote the Young’s modulus and Poisson’s ratio, leading to the following expression of the stress at location \( \mathbf{x} \):

\[ \mathbf{S} = \begin{bmatrix}
  \sigma_{11} & \sigma_{22} & \sigma_{33} & \sigma_{12} & \sigma_{13} & \sigma_{23} 
\end{bmatrix}^T = \mathbf{DKNU} . \quad (2.19) \]

To derive the matrix form of the force state \( \mathbf{T} \) described in Eqn. (2.6), let us capture the last term \( \mathbf{K}(\mathbf{x}) \cdot \xi \) in (2.6) by introducing the matrix \( \mathbf{Q} \) as

\[ \mathbf{Q} = \begin{bmatrix}
  Q_1 & 0 & 0 & Q_2 & Q_3 & 0 \\
  0 & Q_2 & 0 & Q_1 & 0 & Q_3 \\
  0 & 0 & Q_3 & 0 & Q_1 & Q_2 
\end{bmatrix} , \quad (2.20) \]

with

\[ Q_1 = \sum_{i=1}^{3} K_{1i} \xi_i \quad Q_2 = \sum_{i=1}^{3} K_{2i} \xi_i \quad Q_3 = \sum_{i=1}^{3} K_{3i} \xi_i , \quad (2.21) \]

where \( \xi_i \) is the component of the vector \( \xi \) in the \( i \)th coordinate direction and \( \mathbf{K} \) is the shape tensor (2.9). The final matrix form of the force state (2.6) is then

\[ \mathbf{T} (\mathbf{x}' - \mathbf{x}) = \omega (|\xi|) \mathbf{QDKNU} , \quad (2.22) \]

and the resulting system of equations for the \( q \) particles discretizing the body is obtained by combining (2.22) with the discretized form of quasi-static equilibrium equations (2.7) as

\[ \sum_{n=1}^{m} \left\{ \mathbf{T}[\mathbf{x}_j](\mathbf{x}_n - \mathbf{x}_j) - \mathbf{T}[\mathbf{x}_n](\mathbf{x}_j - \mathbf{x}_n) \right\} V_n + \mathbf{b}(\mathbf{x}_j) = 0 , \quad j = 1, 2, ..., q , \quad (2.23) \]

where \( m \) is the number of unbroken bonds to particle \( j \). In this work, for bodies discretized using a structured lattice of particles, the grid spacing between particles is designated as \( dq \).
2.2 Implementation

The 3D implicit NOSB PD formulation presented in Section 2.1 was implemented within \textit{Emu} [53], a peridynamics code in development at Sandia National Laboratories. \textit{Emu} is a parallel MPI-based Fortran code used principally in the study of explicit dynamic simulations. In extending its use for implicit quasi-static simulations as part of this project, the parallel solver packages \textit{Trilinos} [54] and \textit{PETSc} [55] were added to \textit{Emu} to solve the large system of equations formed by (2.23). The solver \textit{PETSc} was added to address memory issues present in the larger simulations since \textit{PETSc} allows for storing only the upper triangular half of the symmetric left-hand-side matrix. Additionally, the \textit{Trilinos} sub-package \textit{Zoltan} was added for partitioning the particles, and a recursive coordinate bisection (RCB) method was used where the particles are weighted by the number of bonds associated with each particle. A typical particle partitioning for a plate with a center hole is presented in Fig. 2.2. As an initial comparison to \textit{Emu}’s in-house partitioning algorithm, the RCB algorithm was implemented by repartitioning \textit{Emu}’s in-house partition, using \textit{Trilinos} package \textit{Isorropia}, before entering the solver. With the RCB algorithm, the solver efficiency improved to 98% on eight processors with 500,000 points. To ease the compilation of \textit{Emu} with these additional libraries, the build system \textit{CMake} was implemented.

\textit{Emu} is primarily written in Fortran 90, whereas \textit{Trilinos} is a C++ li-
Table 2.1: Serial timings using different solvers for solving an *Emu*-generated 10,000x10,000 system of equations.

<table>
<thead>
<tr>
<th>Solver</th>
<th>Preconditioner</th>
<th>Time (sec.)</th>
<th>Iterations</th>
</tr>
</thead>
<tbody>
<tr>
<td>CG</td>
<td>None</td>
<td>19.1</td>
<td>787</td>
</tr>
<tr>
<td>CG</td>
<td>Jacobi</td>
<td>15.9</td>
<td>659</td>
</tr>
<tr>
<td>CG</td>
<td>Order 1 Neumann series polynomial</td>
<td>23.6</td>
<td>544</td>
</tr>
<tr>
<td>CG</td>
<td>Order 1 least-squares polynomial</td>
<td>25.3</td>
<td>576</td>
</tr>
<tr>
<td>CGS</td>
<td>None</td>
<td>49.7</td>
<td>1057</td>
</tr>
<tr>
<td>TFQMR</td>
<td>None</td>
<td>53.1</td>
<td>1110</td>
</tr>
<tr>
<td>BICGSTAB</td>
<td>None</td>
<td>86.8</td>
<td>1825</td>
</tr>
<tr>
<td>LU</td>
<td>None</td>
<td>167.9</td>
<td>1</td>
</tr>
</tbody>
</table>

library, thus *Trilinos* Fortran wrappers had to be further developed and/or modified in order to work within *Emu*. The different solvers and preconditioners available within *Trilinos* were tested in serial using a 10,000x10,000 sparse, symmetric, positive definite coefficient matrix, and the timing results are presented in Table 2.1. The conjugate gradient with Jacobi preconditioning was the fastest of the ones tested and was used as the solver for all the simulations in this work.

Another challenge in the code development was addressing the memory issues within *Emu*. Since *Emu* was primarily an explicit peridynmaics code, the code’s memory usage did not take into account the substantial memory usage involved with the assembly and decomposition of the system of equilibrium equations. Additionally, the NOSB has effectually a horizon size twice that of the horizon of a single point due to the dependency on $F(x_j)$, increasing the bandwidth of the stiffness matrix. Thus, the code was restructured to remove approximately seventeen global arrays storing various lattice quantities. Current parallel architecture has between 1.0-1.5 GB per core, thus, disregarding all other memory usage within *Emu*, these global arrays limited the number of global particles to less than 10 million.

The effects of the horizon size on the serial execution time and memory usage was also studied using different options and coding practices when using *Trilinos*. The various options compared were:

- **summing** or appending the new entries into the coefficient matrix,
- **building a graph of the column layout**, indicating non-zero entries for each row,
- **sending multiple rows to the assembly routine** instead of a send-
The finalizing operation consists of Trilinos functions: globalAssemble, optimizeStorage, and initializeParameterList. A considerable decrease in memory was achieved using the options specified in bold, which allowed for a successful simulation using a horizon $\delta/dq = 3$ without running out of memory. The evolution of the residual of the conjugate gradient solver using a Jacobi preconditioner versus the number of iterations is presented in Fig. 2.3 for a system with 79,212 d.o.f., showing a converged solution in under 600 iterations.

A serial comparison between the solver packages Trilinos and PETSc was also done for a lattice of 10,404 particles and using the optimal Trilinos, (Table 2.3). A nice feature in PETSc is the ability to split the finalizing of the left and right hand sides of the system of equations, i.e., to exchange global entries. This allows one to overlap the communication with computation by first looping over the particles on a partition boundary and then looping over the interior particles, which requires no communication between processors. Similarly to Trilinos, preallocated storage for the coefficient matrix was used in PETSc and a Jacobi (i.e., diagonal scaling) preconditioning was
Table 2.2: Horizon size effects on execution time and memory using Trilinos with different assembling and solver options. The lattice size for entries in bold was 10,404 particles and those entries listed in parentheses had 13,284 particles. A substantial memory savings was achieved using various options within Trilinos.

<table>
<thead>
<tr>
<th>Horizon Size, δ/dq</th>
<th>Assembling and Finalizing (sec.)</th>
<th>Solution (sec.)</th>
<th>Total Time (sec.)</th>
<th>Peak Memory (GB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.0</td>
<td>56.9 (29.8)</td>
<td>27.9 (7.6)</td>
<td>113 (45)</td>
<td>0.436 (3)</td>
</tr>
<tr>
<td>2.5</td>
<td>230.5 (288.6)</td>
<td>32.0 (32.0)</td>
<td>297 (308)</td>
<td>0.644 (10.9)</td>
</tr>
<tr>
<td>2.8</td>
<td>253.8 (865.4)</td>
<td>42.9 (42.9)</td>
<td>335 (912)</td>
<td>0.823 (12.8)</td>
</tr>
<tr>
<td>3.0</td>
<td>358.6 (Failed)</td>
<td>43.6 (--)</td>
<td>446 (--)</td>
<td>0.9 (20.1+)</td>
</tr>
</tbody>
</table>

Table 2.3: Comparison of the horizon size effects on execution time and memory using PETSc (in bold) and Trilinos (in parentheses) for a lattice size of 10,404 particles. The execution time between the two solvers is about equivalent, with PETSc on average faster in execution time and using less memory due to storing only half of the symmetric coefficient matrix.

<table>
<thead>
<tr>
<th>Horizon Size, δ/dq</th>
<th>Assembling and Finalizing (sec.)</th>
<th>Solution (sec.)</th>
<th>Total Time (sec.)</th>
<th>Peak Memory (MB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.0</td>
<td>40.2 (56.9)</td>
<td>16.2 (27.9)</td>
<td>82 (113)</td>
<td>257 (446)</td>
</tr>
<tr>
<td>2.5</td>
<td>173.1 (230.5)</td>
<td>23.6 (32.0)</td>
<td>230 (297)</td>
<td>358 (660)</td>
</tr>
<tr>
<td>2.8</td>
<td>177.2 (253.8)</td>
<td>23.3 (42.9)</td>
<td>234 (335)</td>
<td>433 (843)</td>
</tr>
<tr>
<td>3.0</td>
<td>270.8 (358.6)</td>
<td>27.4 (43.6)</td>
<td>338 (446)</td>
<td>443 (942)</td>
</tr>
</tbody>
</table>

used, together with a conjugate gradient iterative solver. The execution time between the two solvers is about equivalent, with PETSc on average faster in execution time for both the assembling and solution of the system. PETSc also uses less memory due its ability to store only half of the symmetric coefficient matrix.

Once the serial performance was optimized, the parallel performance of Trilinos was measured on RedSky located at Sandia National Laboratories (Table 2.4 and Fig.2.4). RedSky is based on SUN X6275 blades, with 2.93 GHz dual socket/quad core Nehalem X5570 processors and 12 GB RAM per computer node (1.5 GB per core). The optimum number of particles per core was determined to be around 15,000 and the maximum number of particles per core, before exceeding the on-board memory, was around 32,000 for a horizon δ/dq = 2, and less for larger horizons.
Figure 2.4: Scalability performance on RedSky where the problem size was increased with the number of cores. Eight cores was considered as the baseline.

Table 2.4: Parallel performance on RedSky. Around 15,000 particles per core was considered to be optimal and used for most simulations.
Additional *Emu* software changes included using a kd-tree data structure [56] for quick searching of points in the horizon, and making the data structure local to each processor’s lattice, both resulting in 4x speedup. The global particle numbering was changed to be continuous on each processor to avoid using *PETSc*’s ‘Application Ordering’ routines because they are not scalable when used in parallel. For post-processing of the results, each of the solver’s processors creates its own output file using the *Silo* I/O library from the Lawrence Livermore National Laboratory (http://wci.llnl.gov/codes/silo) and HDF5 (http://www.hdfgroup.org/HDF5). The visualization software *VisIt* (http://wci.llnl.gov/codes/visit) then automatically combines each processor’s lattice and plots the results.

The initial lattice generation is done in serial within *Emu* as a preprocessing step and is the current limiting factor in determining the size of the lattices. *Emu* also has a limited number geometrical primitives (blocks, spheres, cylinder, etc) for describing the geometry. Hence, a supporting project was started in the summer of 2011 by Jacob Clifton, an undergraduate in Electrical Engineering, to develop a means to take a CAD model (generated using Patran, AutoCad, or Pro-E) and generate a partitioned lattice for the *Emu* solver. The first step involves creating a triangular surface mesh and storing the mesh in Polygon File Format (.ply) by either importing the model into Blender (www.blender.org) or transforming a Patran neutral file into a PLY format (a utility program was created to accomplish this) and making sure the surface mesh is ‘water tight’ (i.e., contains no holes). A point cloud is then created using a uniform lattice and testing whether a lattice point is located inside the polyhedron defined by the triangular surface mesh. The preprocessing code incorporated Liu’s *et al.* point containment algorithm [57] as implemented in source code available at http://ptinpoly.pbworks.com. The discretization procedure for a bracket is shown in Fig. 2.5. Once the point cloud was generated, the points were partitioned and each processor’s input file was created containing a point’s coordinates, volume and material id. It should be noted that, this initial implementation does not reduce a boundary point’s cubic volume when the cube intersects the surface mesh. The process is fairly fast in generating *Emu* input files when starting from the PLY description, and, as expected, the more complicated the CAD model (i.e., the longer the number of surface triangles), the longer the point containment algorithm takes (Fig. 2.6). The resulting input files were tested qualitatively using an eye-bolt geometry where the bottom of the eye-bolt has fixed displacement and a point load is applied at the inner apex of the eye (Fig. 2.7).
Figure 2.5: Point model generation from (a) CAD model, (b) to surface triangulation and (c) to point cloud for using a uniform arrangement points.

Figure 2.6: Total time needed to generate *Emu* input files (starting from a PLY description) for various surface triangulations and geometries.
(a) Displacement loading conditions.  
(b) Surface triangulation. 

(c) Displacement magnitude. 
(d) Stress $\sigma_{yy}$.

Figure 2.7: Eye-bolt under tension using a lattice generated from a CAD model.
3 Fundamental Numerical Characterization

3.1 Zero-energy modes

The NOSB formulation has inherent stability issues associated with the presence of zero-energy modes. To understand their origin [58], let us consider a NOSB material model with a spherically symmetric influence function \( \omega(\xi) = \omega(|\xi|) \) and an interior point \( x \) (i.e., points a distance \( \delta \) from any boundary or interface) with deformation state \( Y_x \) and deformation gradient tensor \( F \) defined by (2.4). While holding all other points fixed, let us further displace point \( x \), resulting in an additional vector \( u' \). The new deformation state is given by

\[
Y'(\xi) = Y(\xi) - u'
\]  

for any bond \( \xi \) (Fig. 3.1). The approximate deformation gradient tensor \( F' \) for this new deformation state (3.1) is

\[
F' = F - u' \otimes \left( \int_{\mathcal{H}} \omega(|\xi|)\xi dV_\xi \right) K^{-1},
\]

where the integral in (3.2) vanishes because \( \mathcal{H} \) is in the interior of a sphere, and thus \( F' = F \). This suggests that the existence of zero-energy modes in the non-ordinary PD theory is due to the weak coupling of each point to its own family. The primary methods used in this thesis for controlling the zero-energy modes are investigated in Section 3.1.1. Additionally, a fourth method based on stabilization of the zero-energy modes was studied in Section 3.1.4.

3.1.1 Methods of zero-energy mode control

In the following discussion, three methods for zero-energy mode control are considered. The basic idea behind these three methods is to introduce a force state, \( T_{ZE} \), in addition to the force state present at \( x \), as

\[
T[x](x' - x) = \omega(|\xi|) [\sigma(F)]^T \cdot K(x) \cdot (x' - x) + T_{ZE}[x].
\]
• Method I – Supplemental Interconnected Springs. This method simply introduces supplemental linear springs with spring constant $C_I$ between a particle and all the particles belonging to its horizon. The force state arising from the supplemental bonds is then

$$\mathbf{T}_{ZE}[\mathbf{x}] \langle \mathbf{x}' - \mathbf{x} \rangle = C_I \omega(|\mathbf{\xi}|) (u(\mathbf{x}') - u(\mathbf{x})). \quad (3.4)$$

• Method II – Average Displacement State. In this method $[58]$, a zero-energy mode control term based on the averaged displacement over all the particles in the horizon is added to the force state $\mathbf{T}[\mathbf{x}] \langle \mathbf{x}' - \mathbf{x} \rangle$ as

$$\mathbf{T}_{ZE}[\mathbf{x}] \langle \mathbf{x}' - \mathbf{x} \rangle = C_{II} \int_{\mathcal{H}_x} \omega(|\mathbf{\xi}|) \mathbf{\eta} dV_{\mathbf{x}'} . \quad (3.5)$$

The zero-energy control term in (3.5) is then discretized as

$$C_{II} \int_{\mathcal{H}_x} \omega(|\mathbf{\xi}|) \mathbf{\eta} dV_{\mathbf{x}'} \approx C_{II} \sum_{n=1}^{m} \omega(|\mathbf{\xi}|) [u(\mathbf{x}_n) - u(\mathbf{x}_j)] V_n . \quad (3.6)$$

• Method III – Penalty Approach. The final method $[18]$ (Fig. 3.2) uses a penalty term added to the force state, where the penalty force is proportional to the difference between the actual position of a point in the current (deformed) configuration and the position predicted by the deformation gradient $\mathbf{F}$ at point $\mathbf{x}$:

$$\mathbf{T}_{ZE}[\mathbf{x}] \langle \mathbf{x}' - \mathbf{x} \rangle = -C_{III} \left( \frac{18K}{\pi \delta^4} \right) \mathbf{h} \cdot (\mathbf{\xi} + \mathbf{\eta}) \frac{(\mathbf{\xi} + \mathbf{\eta})}{\|\mathbf{\xi} + \mathbf{\eta}\|^2} \Delta V_{\mathbf{x}} \Delta V_{\mathbf{x}'} ; \quad (3.7)$$

where the hourglass vector is defined as $\mathbf{h} = (\mathbf{F} - \mathbf{I}) \mathbf{\xi} - \mathbf{\eta}$ and $K$ is the bulk modulus.
3.1.2 3D illustration: bar under tension

In this section, a bar under tensile loading is used to qualitatively investigate the first zero-energy mode control method mentioned in Section 3.1.1. The material properties of the bar are $E = 1\,\text{GPa}$, and $\nu = 0.25$. The length $L$ of the bar is eight times the width $b$ of the square cross-section (Fig. 3.3). The points satisfying $x \leq 0$ are placed on rollers with $u_x$ fixed. Rigid body motion is prevented by setting all three displacements ($u_x$, $u_y$ and $u_z$) at point $(0, 0, 0)$ to zero.

The first study determines the amount of energy introduced by the background springs compared to the total strain energy in the bar (termed the strain energy ratio) for three lattice spacing, $dq$, using a cubic lattice, a hexagonal close-packed lattice and a horizon of $\delta/dq = 2.20$. The strain energy ratio using a lattice spacing of $dq/L = 32, 80, 160$ is summarized in Table 3.1, and the effects of the zero-energy control on the axial displacements are presented in Fig. 3.4. The spring stiffness constant $C_I$ is expressed in terms of the bond-based material micromodulus [59]

$$c = \frac{18K}{\pi\delta^4},$$  \hspace{1cm} (3.8)

where $K$ is the bulk modulus. Minimizing the effects of the zero-energy modes, as measured by the deviation from the analytical solution, requires a large energy stored in the springs for the cubic lattices, however, it is interesting that the hexagonal lattice arrangement requires less energy stored.
Figure 3.3: 3D geometry of a bar under tension with loading along the longitudinal axis of the bar.

<table>
<thead>
<tr>
<th>$C_I/c$</th>
<th>$dq/L=32$</th>
<th>$dq/L=80$</th>
<th>$dq/L=160$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Cubic</td>
<td>Cubic</td>
<td>Hexagonal</td>
</tr>
<tr>
<td>0.01</td>
<td>0.03</td>
<td>0.07</td>
<td>.009</td>
</tr>
<tr>
<td>0.05</td>
<td>0.05</td>
<td>0.08</td>
<td>.032</td>
</tr>
<tr>
<td>0.10</td>
<td>0.10</td>
<td>0.10</td>
<td>.06</td>
</tr>
<tr>
<td>0.25</td>
<td>0.25</td>
<td>0.19</td>
<td>–</td>
</tr>
</tbody>
</table>

Table 3.1: Strain energy ratio between the ‘background spring’ energy and the total strain energy in the bar.

in the background springs to minimize the error. The hexagonal lattice arrangement shows a larger deviation in the regions where the boundary conditions are applied compared to the cubic meshes (Fig. 3.4c).

The effects of varying the background spring stiffness as a function of radius from the center of the horizon has been studied next. The chosen cubic lattice spacing is $dq/L = 160$, and the spring stiffness values considered are: (i) a constant $C_I/c = 0.1$, (ii) a linearly varying stiffness $C_I/c = C_I/c(1-r/\delta)$, and (iii) a stiffness that is very rigid near the horizon’s center $C_I/c = C_I/c/(r/\delta)$. Varying the stiffness either has a detrimental effect when less stiffness is used (i.e., the linearly varying case), or shows little benefit over a constant spring stiffness when using a stiffness that is more resistant toward the center of the horizon (Fig. 3.5). Similarly, the last case investigates using a constant spring stiffness in a smaller region of the horizon $C_I/c = 0.01$. A negative effect on zero-energy control is observed for all cases when the applied region is less then $\delta$ (Fig. 3.6).
Figure 3.4: Zero-energy control effects on axial displacement using different lattice arrangements and background spring stiffness values $C_I$. 

(a) Cubic lattice with $dq/L = 80$.

(b) Cubic lattice with $dq/L = 160$.

(c) Hexagonal lattice with $dq/L = 80$. 

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Figure 3.5: Effects of using spatially varying background spring constant $C_I$ with horizon radius on zero-energy modes.

Figure 3.6: The effects of using a constant background spring stiffness $C_I$ in only a sub-region of the horizon.
3.1.3 1D illustration: "singular" bar

In this section, we study the effects of the zero-energy mode controls described in Section 3.1.1, particularly in regions where large deformation gradients are present in the solution fields. For simplicity, we consider the simple 1D problem of a bar with a spatially varying stiffness, fixed at one end and with a force applied at the opposite end. To model these boundary conditions using PD, we impose the boundary conditions over a volume at each of the bar’s ends: For \( x \leq 0 \), we impose fixed displacement conditions over an extended volume \( a \) of the bar (Fig. 3.7), and, at the opposite end \( x \geq L \), we apply a body force density over a lengthened volume \( b \) of particles, resulting in a total traction \( \sigma \) at \( x = L \).

In order to emulate a crack singularity in this simpler 1D setting, a variable Young’s modulus along the axis of the bar is adopted as

\[
E(x) = \begin{cases} 
E^0 = \sigma/\alpha & x \leq L/2 \\
\sigma \left( \alpha + \frac{\beta}{2\sqrt{L} \sqrt{x/L-1/2}} \right)^{-1} & x > L/2 
\end{cases}
\]  

(3.9)

The analytical (local) solution for the axial displacement \( u \) and strain \( \varepsilon \) along the bar is

\[
u(x) = \begin{cases} 
\frac{\alpha x}{L} & x \leq L/2 \\
\frac{\alpha x}{L} + \frac{\beta}{\sqrt{L}} \sqrt{x/L - 1/2} & x > L/2 
\end{cases}
\]  

(3.10)

\[
\varepsilon(x) = \begin{cases} 
\alpha & x \leq L/2 \\
\alpha + \frac{\beta}{2\sqrt{L} \sqrt{x/L-1/2}} & x > L/2 
\end{cases}
\]  

(3.11)

In the simulations presented hereafter, the adopted parameters are as follows: applied traction \( \sigma/E^0 = 0.01 \), particle spacing \( dq/L = 0.0005 \), \( a/dq = 4 \) and \( b/dq = 12 \). In the absence of zero-energy control, the axial displacement and strain obtained along the bar show large instabilities as the horizon size increases, as apparent in Fig. 3.8. The smallest horizon possible, i.e., the
horizon containing only the particles immediately to the left and right of \( x \), minimizes the effects of zero-energy modes. However, for crack propagation problems, such a small horizon is not applicable since breaking a bond results in the inverse of the shape tensor (2.9) becoming undefined.

In the simpler 1D case, methods I and III are conceptually very similar except for the definition of the constants, \( C_I \) and \( C_{III} \), as both methods apply a supplemental force along each bond. Therefore, we mainly focus our comparative study on methods I and II by varying the values of the constants \( C_I \) and \( C_{II} \) for a fixed horizon \( \delta/dq = 2 \). To quantify the impact of zero-energy control, we define the L_2 norm of the relative displacement error as

\[
e_u = \sqrt{\frac{\int_B (u^{num} - u^{local})^T (u^{num} - u^{local}) dB}{\int_B (u^{local})^T (u^{local}) dB}}, \tag{3.12}
\]

where the numerical (PD) and exact displacements are \( u^{num} \) and \( u^{local} \), respectively. Similarly, we introduce the energy error norm as

\[
e_E = \sqrt{\frac{\frac{1}{2} \int_B (\varepsilon^{num} - \varepsilon^{local})^T (\sigma^{num} - \sigma^{local}) dB}{\frac{1}{2} \int_B (\varepsilon^{local})^T (\sigma^{local}) dB}}, \tag{3.13}
\]

where \( \varepsilon \) and \( \sigma \) respectively denote the axial strain and stress. It should be noted that, for the definition of the error, the solution associated with the classical (local) theory of elasticity is adopted as the reference solution. Since the PD formulation is nonlocal, we expect the error to approach zero only for vanishing values of the horizon size [60]. As shown in Fig. 3.9, which presents the dependence of the two error norms on the zero-energy mode control coefficient, the error associated with the PD solution decreases with increasing values of the coefficient, reaching a minimum before increasing for very high values of the coefficient, for which the correction term starts to dominate the solution and affect the effective stiffness of the material.

In addition to improving the overall accuracy and stability of the solution, zero-energy control reduces the displacement instability present especially in high gradient regions close to the source of singularity. Achieving a smooth displacement field devoid of numerical instabilities in the crack-tip region is critical in crack propagation simulations since bond breakage laws usually involve the stretching of individual bonds [8]. The axial displacement and stress distributions obtained with the optimum value \( C_{II} dq^2/E^o = 5e13 \) are plotted in Fig. 3.10 as a function of the distance to the ‘crack-tip’, showing substantial smoothing of the numerical solution and good comparison with
Figure 3.8: Impact of zero-energy modes, for various sizes of the horizon, $\delta$, on the axial displacement (3.8a) and strain (3.8b) distributions in the absence of zero-energy mode control.
Figure 3.9: Effect of zero-energy mode control constant, $C_{I,II}$, on the L2-norm of the displacement and energy solution for the singular bar problem, indicating an optimum value for eliminating the sporadic oscillations without adversely affecting the overall solution.

the analytical (local) solutions (3.10) and (3.11). Although the two methods compared in Fig. 3.9 have similar impact on the precision of the PD solution, method II is used in the remainder of the manuscript since it has a greater range of optimum values of the control parameter $C_{II}$. Furthermore, for fully 3D problems, method II has a limited effect on the material properties when the coefficient is chosen at the optimum value, while method I tends to introduce an extra stiffness, and hence energy, into the system.

For method III, if the analytical displacement field (3.10) is imposed everywhere in the domain then there should be no zero-energy modes and the penalty vector $h$ should be zero. However, around areas of high gradients, such as the pseudo crack-tip, there are non-zero penalty forces $h$ present (Fig. 3.11). Therefore, method III tends to smooth out high gradient regions around the crack-tip, regardless of the presence of zero-energy modes. However, for the case when the Young’s modulus is considered constant, the displacement is regularized, resulting in a stress field that converges to the local solution and the penalty force $h$ at each interior point goes to zero (Fig. 3.12a and Fig. 3.12b respectively).
Figure 3.10: Displacement and strain distribution obtained using method II for zero-energy mode control, with an optimum constant value ($C_I d q^2 / E^o = 5e13$), where the origin for the spatial coordinate $r$ is located at the “crack-tip” ($x/L = .5$).

Figure 3.11: The analytical strain (solid blue curve), the NOSB strain computed from the analytical displacement fields (red squares) and method III’s summation of penalty forces $h$ over all the bonds in each particle’s horizon (black circles). Even though no zero-energy modes are present, there are still non-zero penalty forces present in areas of high gradients.
Figure 3.12: 1D bar with a constant Young’s modulus, under tension and using Method III zero-energy control. (a) The stress field is regularized and converges to the local solution as $C_{III}$ is increased and (b) the magnitude of the penalty force $h$ at each interior point goes to zero.
3.1.4 Stabilized penalty zero-energy control

In developing a nodally integrated tetrahedral element, Puso and Solberg [61] supplemented the energy form with a stabilized term that penalizes the difference between the nodal averaged strain and the element strains

\[
\int_\Omega \varepsilon : D\varepsilon da \to \sum_{I}^N V_I \varepsilon_I : D\varepsilon_I + \sum_{I=\text{elem}(\Omega_I)}^\alpha \frac{V_e}{4} (\varepsilon_I - \varepsilon_e) : \tilde{D}(\varepsilon_I - \varepsilon_e),
\]  

(3.14)

where \(0 \leq \alpha \leq 1\) is the stabilization term, \(\tilde{D}\) is a positive-definite material tensor, \(V_e\) is the volume of the tetrahedral finite element and \(\varepsilon_I\) and \(\varepsilon_e\) are the nodal and element strains, respectively. Further simplification of (3.14) yields,

\[
\sum_{I}^N V_I (\varepsilon_I : D - \alpha \tilde{D}) \varepsilon_I + \sum_{I=\text{elem}(\Omega_I)}^\alpha \frac{V_e}{4} \varepsilon_e : \tilde{D} \varepsilon_e. \tag{3.15}
\]

A similar idea can be implemented in NOSB peridynamics by using the nodal strains at \(x'\) as the element strain,

\[
\int_\Omega \varepsilon : D\varepsilon da \to \sum_{n=1}^m V_n \varepsilon_n : D\varepsilon_n + \sum_{n=\text{nodes}(H_n)}^m \alpha V_n V_e (\varepsilon_n - \varepsilon_e) : \tilde{D}(\varepsilon_n - \varepsilon_e)
\]

\[
= \sum_{n=1}^m V_n \varepsilon_n : (D - \alpha \tilde{D}) \varepsilon_n + \sum_{n=\text{nodes}(H_n)}^m \sum_{n=1}^{m'} \alpha V_n V_e \varepsilon_e : \tilde{D} \varepsilon_e \tag{3.16}
\]

where \(\varepsilon_e\) is the strain at \(x'\) and \(m'\) is the number of particles in the horizon at \(x'\). Using the NOSB discretized form of the force state,

\[
\mathbb{T}[x_j] < x_j - x_n > = \sum_{n=1}^m \omega(|\xi|) \underbrace{QDKNU}_{\varepsilon_j} V_n, \tag{3.17}
\]

and adding a term to penalize the difference between the nodal strains at particle \(j\) and the averaged strain for points within particle \(j\)'s horizon gives,
Figure 3.13: Geometry and boundary conditions for a bar under tension.

Figure 3.14: Effects of the stabilization term $\alpha$ on suppressing the zero-energy modes using the stabilized penalty formulation.

\[ T[x_j] < x_j - x_{n_i} > = \sum_{n=1}^{m} \omega (|\xi|) QDKNUV_n + \]

\[ \alpha \sum_{n=1}^{m} \omega (|\xi|) Q\tilde{D}V_n(\sum_{e \in nodes(H_n)} \sum_{e \in nodes(H_n)} KNU) \]  \( \text{(3.18)} \)

For an isotropic elastic material, Puso et al. recommend an optimal choice for lamé constants $\lambda$ and $\mu$ as

\[ \hat{\mu} = \mu, \quad \hat{\lambda} = min(\lambda, 25\mu) \]  \( \text{(3.19)} \)

The formulation was tested in one dimension for a uniform bar under tension (Fig. 3.13) where $E = 1\text{GPa}$, $\nu = 0.25$, $L/dq = 300$ and $\delta/dq = 3$. While the relative error in the displacement was decreased with increasing stabilization parameter $\alpha$, the displacement variation from point to point could not be minimized (Fig. 3.14), which would cause problems in fracture simulations as detailed in Chapter 5. Therefore, this method was rejected in favor of the preferred zero-energy control methods outlined in Section 3.1.
3.2 Effects of key numerical parameters

Even though the recommended situation when using NOSB are for fracture problems and other problems having a displacement discontinuity, the method still must be able to solve the underlying elasticity problem. Since the behavior in bending plays an important role in many validation and verification fracture problems, a study in bending performance is studied in Section 3.2.1. Many of the validation examples in this thesis compare to the classical local solutions, so the convergence rate to the local solution as a function of grid spacing and horizon is investigated in Section 3.2.2.

3.2.1 Three point bending test

A three point bend test (Fig. 3.15) is used for determining the convergence rate in bending as a function of lattice density. The material properties of the beam are $E=38\times10^9$ GPa, $\nu = 0.18$, and the geometry is $L=800$ mm, $h=10$ mm and $b=2.5$ mm. At the top of the beam, a body force density was applied over a small volume at $L/2$ such that the resulting force $F$ is 515 N. The analysis assumes plane stress conditions, a cubic lattice and $\delta/dq = \sqrt{2}.$

In order to put the accuracy and convergence rates into perspective, a FE analysis is performed using 3-node constant strain triangles (CST). The deflection at $L/2$ on the bottom of the beam is monitored and compared to the local analytical solution. Both NOSB and FE solutions roughly converge to the analytical solution at the same rate, and the accuracy is slightly less in NOSB for the coarser PD grids. Therefore, NOSB captures bending as well as CST. Additionally, just as there was an optimum value of zero-energy control constant $C_{II}$ for a bar under tension (Section 3.1.3), there is also an optimum value under bending for different grid spacings (Fig. 3.17).
Figure 3.16: Convergence rate in bending of the NOSB method compared to a FE analysis using constant strain triangles.

Figure 3.17: Effect of zero-energy mode control constant, $C_{II}$, on the maximum deflection solution for a beam under three point loading, indicating an optimum value for eliminating the sporadic oscillations without adversely affecting the overall solution.
3.2.2 Convergence study

Any acceptable numerical method should have a solution that converges or tends to the exact local or exact nonlocal solution. In PD, given a domain discretized by \( m \) particles, three types of convergence can be defined [60]: 

- \( m \)-convergence, where the horizon size \( \delta \) remains fixed as \( m \to \infty \), 
- \( (\delta m) \)-convergence, where the horizon decreases with decreasing \( m \), but where \( m \) increases equally fast or faster than \( \delta \) decreases, and 
- lastly \( \delta \)-convergence, where \( \delta \to 0 \) with \( m \) fixed or increasing. In this study, we investigate \( \delta m \)- and \( \delta \)-convergence since we are interested in comparing the PD solution to the classical local model. We also assume \( \omega (|x' - x|) = 1 \) for all bonds.

The same geometry and boundary conditions as those described in Section 3.1.3 are used in this convergence study. The number of particles over which the boundary conditions are applied is always kept fixed at \( a/dq = 4 \) and \( b/dq = 12 \), with the grid spacing defined as \( dq = L/m \). For the \( (\delta m) \)-convergence, the grid spacing is divided by two \( (dq = (.5)^n dq^o) \) at every convergence iteration \( n \), while the horizon size decreases at the same rate, with two \( \delta/dq \) ratios: \( \delta/dq = 1 \) and \( \delta/dq = 2 \). In the \( \delta \)-convergence study, the grid spacing again decreases as \( dq = (.5)^n dq^o \), whereas the horizon size decreases at a slower rate of \( \delta = (.75)^n \delta^o \) where \( \delta^o \) is the starting horizon size at \( n = 0 \). At each convergence increment, the optimum value of \( C_{II} \) minimizing the displacement error (3.12) was chosen with the optimum values plotted in Fig. 3.18 for each nodal refinement. For both types of convergence, the optimum \( C_{II} \) value increases with increasing mesh size, where the magnitude of \( C_{II} \) increases roughly linearly with the number of degrees of freedom, \( m \). As also apparent in Fig. 3.18, the \( \delta m \)-convergence shows first-order convergence independent of the horizon size, whereas the \( \delta \)-convergence shows approximately half the rate of convergence.
Figure 3.18: Relative error in the PD displacement solution (lines) for δm- and δ-convergence, and dependence of the optimum value of the zero-energy mode control parameter $C_{II}$ (vertical bars) on the grid spacing and horizon size.
Non-propagating Cracks and Stress Concentration

4.1 Near-tip solution for 2D stationary crack

4.1.1 Extraction of J-integral and stress intensity factors

We now focus our attention on the extraction of some of the key parameters that define the near-tip fields in linearly elastic fracture mechanics (LEFM): the J-integral and stress intensity factors. While a nonlocal expression of the conservation J-integral compatible with the (bond-based) PD formulation has been derived using the infinitesimal virtual extension approach [62], we adopt hereafter the classical expression given by [63]

$$J_m = \int_{\Gamma} \left( U n_m - \sigma_{ij} n_j \frac{\partial u_i}{\partial x_m} \right) d\Gamma \quad (m = 1, 2), \quad (4.1)$$

where $U$ is the strain energy density, $n_m$ are the components of the unit normal vector to the contour $\Gamma$ surrounding the crack-tip, $\sigma_{ij}$ are the stress components, and $u_i$ are the displacement components. Within the theory of LEFM, the J-integral components are related to the stress intensity factors $K_I$ and $K_{II}$ characterizing the near-tip stress field by

$$J_1 = \frac{K_I^2 + K_{II}^2}{E^*}, \quad J_2 = \frac{2K_IK_{II}}{E^*}, \quad (4.2)$$

where $E^* = E$ for plane stress and $E^* = E/(1 - \nu^2)$ for plane strain. The computation of the J-integral used in this study is similar to that used in the Material Point Method [64], which relies on the mid-point rule:

$$J_m = \sum_{p=1}^{n_p-1} \left( F_m^{(p)} + F_m^{(p+1)} \right) \frac{l_p}{2} \quad (m = 1, 2), \quad (4.3)$$

where $l_p$ is the length of segment between points $p$ and $p+1$ and $F_m^p$ denotes the integrand at point $p$,

$$F_m^{(p)} = U^{(p)} n_m - \sigma^{(p)}_{ij} n_j \frac{\partial u_i^{(p)}}{\partial x_m}, \quad (4.4)$$
with the displacement gradient at each point given by (2.13). A rectangular path for a uniform lattice or an alpha-shape (i.e., a generalized convex hull) path for irregular lattices (with all paths going through the particles), and with the crack-tip at its center chosen for the line integral, as schematically shown in Fig. 4.1. The path was chosen to be at least five horizons from the crack-tip.

4.1.2 Crack-tip fields in plane stress Mode I

To investigate the ability of the PD solver to capture the near-tip displacement and stress fields regardless of the orientation of the underlying lattice, we perform the analysis shown schematically in Fig. 4.2, where a circular plate of diameter $2a$ and thickness $0.023a$, and with a radial crack of length $a$, is subjected to displacement boundary conditions along its entire circumference corresponding to the K-field solution [65]:

$$
\begin{align*}
\begin{cases}
    u_x \\
    u_y
\end{cases}
    &=
    \frac{K_I}{2\mu}\sqrt{\frac{r}{2\pi}}
    \begin{cases}
    \cos\left(\frac{\theta}{2}\right)\left[\kappa - 1 + 2\sin^2\left(\frac{\theta}{2}\right)\right] \\
    \sin\left(\frac{\theta}{2}\right)\left[\kappa + 1 - 2\cos^2\left(\frac{\theta}{2}\right)\right]
    \end{cases},
\end{align*}
$$

(4.5)

where the polar coordinates $(r, \theta)$ are defined at the crack-tip (Fig. 4.2), $\mu = E/(1+\nu)$ is the shear modulus, and $\kappa = (3-\nu)/(1+\nu)$ for plane stress. In the numerical studies, the adopted material properties are $E = 1\, GPa$ and $\nu=0.25$, and the loading amplitude is specified by prescribing $K_I = 1\, MPa\sqrt{m}$, with the displacement boundary conditions (4.5) applied over the region $(a \leq r \leq a + 2\delta)$ along the circumference. As illustrated in Fig. 4.2, the lattice orientation with respect to the plane of the crack is
Figure 4.2: Geometry and boundary conditions used for the analysis of near-tip solution under Mode I. The angle $\theta_m$, i.e., the orientation of the uniform lattice, is varied to study the influence of the lattice orientation with respect to the crack plane on the solution.

denoted by $\theta_m$. A hexagonal mesh arrangement is used as this lattice configuration shows a lower sensitivity to zero-energy modes than other lattice arrangements (regular and random). The other simulation parameters are: $a/dq = 100$, $\delta \approx dq\sqrt{2}$ and $C_{11}dq^2/E = 5.3e11$, with the zero-energy mode control only applied in a vicinity $3\delta$ around the crack.

To quantify the numerical error on the computed value of the stress intensity factor $K_I$, we define the relative error measure $\left| K_I^{\text{num}}/K_I^{\text{local}} - 1 \right| \times 100\%$ (Table 4.1). Three separate studies are performed. In the first one (corresponding to Case (a) in the table), the accuracy of the J-integral computation described in the previous section is assessed by imposing at every lattice point in the circular domain the 'exact' (based on LEFM theory) expression of the near-tip displacement field (4.5) and the stress K-field given by

$$
\begin{align*}
\sigma_{xx} = K_I \sin \left( \frac{\theta}{2} \right) \\
\sigma_{yy} = K_I \cos \left( \frac{\theta}{2} \right) \\
\sigma_{xy} = K_I \left( 1 - \sin \left( \frac{\theta}{2} \right) \sin \left( \frac{3\theta}{2} \right) \right).
\end{align*}
$$

As shown in the first row of Table 4.1, the associated error on the extracted value of $K_I$ is very small for all lattice orientations, thereby verifying the algorithm used to compute the J-integral. In the second study (corresponding
\[
|K_{I}^{\text{num}}/K_{I}^{\text{local}} - 1| \ast 100% \quad \theta_m \\
\hline
(a) J\text{-integral numerical} & 0.0012 & 0.0029 & 0.0023 & 0.0029 \\
(b) Partial PD solution & 0.046 & 0.13 & 0.24 & 0.056 \\
(c) Full PD solution & 0.14 & 0.32 & 0.033 & 0.16 \\
\hline
\]

Table 4.1: Relative error in Mode I stress intensity factor vs. mesh orientation, \(\theta_m\). Case (a): The near-tip displacement (4.5) and stress (4.6) fields are applied everywhere in the domain. Case (b): The near-tip displacement fields are imposed in the domain and the PD solver is used to calculate the resulting strain and stress solution. Case (c): The near-tip displacement solution is only applied along the outer boundary of the circular domain.

to Case (b) in the table), only the K-field displacement solution (4.5) is applied at every lattice point in the domain, while the nonlocal PD formulation is used to compute the strains and the stresses in the domain, allowing us to quantify the contribution of the nonlocal nature of the strain definition on the extracted value of \(K_I\) (whose reference value is, once again, taken from the local theory of elasticity). As shown in Table 4.1, while more substantial than in the first study, the error in this case is still relatively small. In the last study, the PD solver is used to compute the displacement and stress field in the circular domain, with the K-field displacements applied along the boundary as indicated above. As indicated in Case (c) of the table, the error in the computed value of \(K_I\) remains small for all values of \(\theta_m\), showing the ability of the PD scheme to capture quantitatively the near-tip fields, irrespective of the mesh orientation. Because cracks are defined as regions where bonds have completely broken, coupled with the fact that the bond orientation also changes with \(\theta_m\) with respect to the crack plane, the crack-tip location is slightly dependent on \(\theta_m\). This contributes to the variability between Cases (b) and (c), especially at \(\theta_m = 45^\circ\), where the PD crack length is not exactly that used in the ‘exact’ solution.

The effect of the horizon size on the precision of the near-tip solution is shown in Fig. 4.3, which presents the \(\delta\)-dependence of the \(L_2\)-norm of the displacement and energy error for the four lattice orientations. While the error norms show a monotonic increase with the horizon size, the solution appears to be insensitive to the lattice orientation. The larger difference in the strain energy density is primarily associated with the region located directly around the crack-tip, as the location of the crack-tip is only known within a distance \(d_\varphi\) since the crack does not go through particles but rather is represented by broken bonds between particles. Additionally, when enforce-
ing the analytical local displacement field (4.5) everywhere in the domain, the resulting $\sigma_{yy}$ is relatively independent of the horizon size (Fig. 4.4).

Details on the computed values of the crack opening displacement $\Delta_y$ (Fig. 4.5a) and of the $u_y$ displacement and $\sigma_{yy}$ stress solutions along $\theta = 60^\circ$ (Fig. 4.5b) confirm the lack of dependence on $\theta_m$. The full-field $\sigma_{yy}$ near-
tip solution presented in Fig. 4.6 clearly shows the stress concentration captured by the PD solver. Other visualizations of the full-field solutions are presented in Fig. 4.7 for the displacements $u_x$ and $u_y$ obtained for $\theta_m = 0^\circ$, and in Fig. 4.8 for the stress fields $\sigma_{xx}$ and $\sigma_{yy}$.

Figure 4.5: Details of the near-tip solution obtained with $\delta/dq = \sqrt{2}$ and $C_{II}dq^2/E = 5.3e11$: (a) Effect of lattice orientation angle, $\theta_m$, on the crack opening displacement, $\Delta_y$, and comparison with the asymptotic solution. (b) Displacement, $u_y$, and stress $\sigma_{yy}$ along a line at $\theta = 60^\circ$, showing the ability of the PD scheme to capture the near-tip gradients irrespective of the lattice orientation.
Figure 4.6: Full $\sigma_{yy}$ stress field in the vicinity of the crack-tip.
Figure 4.7: Displacement fields (a) $u_x$ and (b) $u_y$ under Mode I loading, $K_I = 1 \, MPa\sqrt{m}$ and $\theta_m = 0^\circ$. 
Figure 4.8: Stress fields (a) $\sigma_{xx}$ and (b) $\sigma_{yy}$ under Mode I loading, showing the ability of the PD scheme to capture the stress concentration at the crack-tip.
In contrast to the bond-based formulation where the micromodulus function affects the elastic stiffness \[60\], the material properties for the NOSB PD formulation are not derived from the influence function, \( \omega (|\xi|) \). In the NOSB formulation, \( \omega (|\xi|) \) controls the influence of the force state for points within the horizon, which can have an overall effect on the accuracy of the method. Past NOSB studies \[17, 14\] assumed the influence function to be constant within the horizon, resulting in a discontinuity at \( \pm \delta \). However, other forms of the influence function can be used, ranging from a linear decay to an exponential decay with respect to \( \xi \). The error in the displacement for the various \( \omega (|\xi|) \) functions and horizon sizes is presented in Fig. 4.9. The effects are overall quite small, only varying less than half a percent in the relative error. The \( \omega (|\xi|) \) function showing the smallest error (Option (3) in Fig. 4.9) corresponds to a nearly constant influence in the vicinity of the observation point \( x \) and increasing influence for points nearer to the outer limits of the horizon.

![Figure 4.9: Effects of influence function, \( \omega (|\xi|) \), on the displacement error for various sizes of the horizon, \( \delta \).](image)

<table>
<thead>
<tr>
<th>Influence Function Type</th>
<th>Displacement, Relative Error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. ( \omega (</td>
<td>\xi</td>
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<tr>
<td>2. ( \omega (</td>
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<td>5. ( \omega (</td>
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<td>6. ( \omega (</td>
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<tr>
<td>7. ( \omega (</td>
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</tr>
<tr>
<td>8. ( \omega (</td>
<td>\xi</td>
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**4.1.3 Crack-tip fields in plane strain Mode I**

With the exception of the analysis assuming plane strain and using a single layer of particles through the thickness, the same plate geometry as in Sec-
Figure 4.10: The regional extents of Method II’s zero-energy control. If a particle has any broken bonds, then all points within a radius of \(2\delta\) of that point have a non-zero \(C_{II}\).

Section 4.1.2 is used to study the near field crack-tip displacements and stresses in a circular plate with a crack having a length of \(a\). The material was the same as well, with a Young’s modulus of \(E = 1\) GPa and \(\nu = 0.25\). The \(K_I\) and applied local continuum analytical displacements (4.5) are the same as the plane stress case (Section 4.1.2) with the exception that \(\kappa = (3 - 4\nu)\). A hexagonal mesh arrangement was used, and the other simulation parameters were \(dq = .005\) (37,742 particles) and \(\delta \approx dq\sqrt{2}\). Instead of applying the zero-energy (ZE) control for a fixed region around the crack-tip, as was done in Section 4.1.3, it is applied only in a surrounding region containing particles with broken bonds (Fig. 4.10); in these regions, \(C_{II}dq^2/E = 5.3e11\). This approach becomes necessary when cracks propagate because determining the region where bonds are breaking is easier than determining where the crack-tip is located. When comparing the \(u_y\) displacement and the \(\sigma_{yy}\) stress to the local analytical solution, both capture the local solution well, and there is minimal difference between applying the ZE control everywhere in the domain versus limiting it to only regions having broken bonds as shown in Fig. 4.11.

4.1.4 Crack-tip fields in plane strain Mode II

The same geometry presented in Section 4.1.2 is used to investigate the ability of the PD solver to capture the near-tip fields when subjected to a
Figure 4.11: Mode I plane strain near-tip displacement, $u_y$, and stress $\sigma_{yy}$ along a line at $\theta = 30^\circ$ and the difference between using zero-energy control everywhere in the domain versus limiting it to only regions having broken bonds, i.e., near the crack.

Displacement boundary condition corresponding to the K-field solution in Mode II $[65]$

\[
\begin{bmatrix} u_x \\ u_y \end{bmatrix} = \frac{K_{II}}{2\mu \sqrt{2\pi r}} \begin{bmatrix} \sin \left( \frac{\theta}{2} \right) \left[ \kappa + 1 + 2\cos^2 \left( \frac{\theta}{2} \right) \right] \\ -\cos \left( \frac{\theta}{2} \right) \left[ \kappa - 1 - 2\sin^2 \left( \frac{\theta}{2} \right) \right] \end{bmatrix},
\]

where the polar coordinates $(r, \theta)$ are defined at the crack-tip (Fig. 4.2), $\mu = E/(1 + \nu)$ is the shear modulus and $\kappa = (3 - 4\nu)$ for plane strain. In the numerical studies, the adopted material properties are $E = 1$ GPa and $\nu = 0.25$, and the loading amplitude is specified by $K_{II} = 1\, MPa\sqrt{m}$. A hexagonal lattice arrangement is used as the lattice configuration. The other simulation parameters are: $a/dq = 100$, $\delta \approx dq\sqrt{2}$ and $C_{II}dq^2/E = 5.3e11$, with the zero-energy control only applied in a vicinity $3\delta$ around the crack. The full field shear stress $\sigma_{xy}$ shows the capture of the stress concentration at the crack-tip (Fig. 4.12). Quantitatively, the displacement and stress ahead of the crack-tip along a line radiating out from the crack-tip at $\theta = 30^\circ$ (Fig. 4.13), shows good agreement compared to the local analytical displacement (4.7) and stress K-fields $[65]$

\[
\begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{xy} \end{bmatrix} = \frac{K_{II}}{\sqrt{2\pi r}} \begin{bmatrix} \sin \left( \frac{\theta}{2} \right) \left( 2 + \cos \left( \frac{\theta}{2} \right) \cos \left( \frac{3\theta}{2} \right) \right) \\ \sin \left( \frac{\theta}{2} \right) \cos \left( \frac{\theta}{2} \right) \cos \left( \frac{3\theta}{2} \right) \\ \cos \left( \frac{\theta}{2} \right) \left( 1 - \sin \left( \frac{\theta}{2} \right) \sin \left( \frac{3\theta}{2} \right) \right) \end{bmatrix}.
\]

51
Figure 4.12: Full $\sigma_{xy}$ stress field under Mode II loading.

Figure 4.13: PD (symbols) and local analytical (solid line) displacement $u_x$ and stress $\sigma_{yy}$ along a line at $\theta = 30^\circ$ under Mode II loading with $\delta/dq = \sqrt{2}$ and $C_{11}dq^2/E = 5.3e11$, showing the ability of the PD scheme to capture the near-tip gradients.
4.2 3D numerical examples

4.2.1 3D – Penny-shaped crack in a cylindrical bar

For the first example, consider a circular cross-section bar of radius \( b \) and length \( L \) with a penny-shaped crack of radius \( a \) located at the midpoint of the bar \( (z = 0) \), with its normal parallel to the bar axis. The end of the cylindrical bar at \( z = L/2 \) is subjected to a uniform axial tensile traction \( \sigma_\infty = 1.33 \) MPa, and, at the opposite end \( (z = -L/2) \), the displacement \( u_z = 0 \). Taking advantage of symmetry, only one-quarter of the bar is modeled, with symmetry boundary conditions \( u_x = 0 \) and \( u_y = 0 \) applied in the \( xz- \) and \( yz- \) planes, respectively. The adopted dimensions and material properties for the bar are \( L = 2b \), \( E = 10 \) GPa and \( \nu = 0.32 \). For the analysis that follows, the horizon size is \( \delta = \sqrt{2}dq \), \( C_{II}dq^2/E = 4.2 \times 10^7 \) and a hexagonal grid with a particle spacing of \( dq/b = 5 \times 10^{-3} \) is used to accurately capture the curvature of the crack and the circumference of the bar, resulting in a grid of approximately 21 million particles.

The non-dimensional stress intensity factor for a long cylindrical bar of finite radius \( b \), with a centered penny-shaped crack of radius \( a \) is given approximately by [66]

\[
\frac{K_I}{\sigma_\infty \sqrt{\pi a}} \simeq \frac{b^2}{b^2 - a^2} \sqrt{\frac{b-a}{b}} \left[ \frac{2}{\pi} \left( 1 + \frac{1}{2} \frac{a}{b} - \frac{5}{8} \frac{a^2}{b^2} \right) + 0.268 \frac{a^3}{b^3} \right].
\tag{4.9}
\]

To extract the SIF \( K_I \), the J-integral technique described in Section 4.1.1 is used. The path is chosen to be far away from the crack-tip where the stresses are more accurate. The path of the line integral is a square in the \( xz- \) plane having a side length of \( 30 \times dq \), with the exception of \( a/b = 0.95 \), for which the contour length was chosen as \( 16 \times dq \). The stress intensity factor predicted by the analytical approximation and PD solutions for various crack radii are compared in Fig. 4.14 showing excellent agreement for the whole range of adopted \( a/b \) values.

Focusing on the near-tip displacement and stress solutions, we adopt the case \( a/b = 0.25 \) as an approximation for the penny-shaped crack in an infinite domain, for which the LEFM crack opening displacement solution is

\[
\Delta_z(r) = \frac{4(1-\nu)\sigma_\infty \sqrt{a^2 - r^2}}{\pi \mu},
\tag{4.10}
\]

while the stress \( \sigma_{zz} \) in the region \( r > a \) and \( z = 0 \) is given by
Figure 4.14: Stress intensity factor vs. penny-shaped crack radius \(a\) in a circular cross-section bar of radius \(b\). The analytical solution is given by (4.9).

\[
\frac{K_I}{\sigma \sqrt{\pi a}} = \text{Analytical}
\]

As shown in Fig. 4.15, the agreement between numerical and reference solutions is very good despite the finite nature of the computational domain, with the relative error in the maximum crack opening displacement on the order of 3.6%. In Fig. 4.16, the full \(\sigma_{zz}\) field around the penny shaped crack is depicted, where all particles having a value \(\sigma_{zz} \sqrt{a}/K_I < .8\) are hidden so as to view the 3D contours around the crack-tip. The artifacts around the circumference of the crack are due to the visibility of particles at different depths inside the volume due to the hexagonal nature of the nodal arrangement.

\[
\sigma_{zz} = \frac{2\sigma_{\infty}}{\pi} \left( \cos^{-1} \frac{a}{r} + \frac{a}{\sqrt{r^2 - a^2}} \right).
\]  

(4.11)
Figure 4.16: $\sigma_{zz}$ stress field in the vicinity of the crack-tip: (a) cross-sectional slice, (b) isolated points around crack, demonstrating PD’s ability to capture the stress concentration around the crack-tip for a 3D analysis.
4.2.2 3D – Double edge notch specimen under tension

The last example is a validation of the ability of the NOSB PD scheme to capture 3D stress concentrations around notches. In the experiment described in [67], a flat bar with circular notches in the mid section was loaded under tension (Fig. 4.17), and strain gauges were placed at key locations around the notches. The bar was made of 2024-T4 Aluminum alloy with $E = 73$ GPa and $\nu = .32$. Making use of symmetry, only one-quarter of the specimen is modeled. The top ($y = 100$ mm) of the specimen has a body force density applied along the top layer of particles ($y = 100$ mm) equivalent to an applied traction, $\sigma_\infty$, of 14.5 MPa, and the bottom ($y = -100$ mm) is placed on rollers. The geometry is discretized using a little over 20 million particles in a hexagonal arrangement and with a horizon size of 1.7 times the mesh spacing of 0.25 mm.

Fig. 4.18 compares the PD solution and experimental measurements for the $\sigma_{ii}$ (no sum) stress distributions along the face ahead of the notch ($y = 0$ mm, $z = 15$ mm) and along the base of the notch ($x = 22.5$ mm, $y = 0$ mm). The numerical solution on the $xy$-face shows excellent agreement in capturing the stress concentration at the notch, with some influence seen near the center line where symmetric boundary conditions are imposed. Along the base of the notch, the numerical solution for $\sigma_{yy}$ and $\sigma_{zz}$ captures the increasing trend from the outer edge to the mid-point, but the numerical values are lower than those measured in the experiment. One possible cause of the discrepancy is the curvature (Fig. 4.17, inset) not being entirely smooth, but flat at the base of the notch. One way to improve the solution would be to use adaptive refinement [68] around the notch to capture its full curvature, which would eliminate the current need for large numbers of particles throughout the entire domain.

A standard linear elastic finite element analysis of the double edge notch specimen was also performed in order to establish a baseline for the numerical results. Due to the symmetry of the problem, only an eighth of the specimen was modeled using 44,588 10-node tetrahedral elements (231,162 degrees of freedom), with a high concentration of the elements around the notch (Fig. 4.19). As shown in Fig. 4.20, the finite element method naturally offers the ability to focus the mesh in regions of high stress concentrations, yielding a numerical solution able to capture the stress field near the notch with a substantially smaller number of degrees of freedom (Fig. 4.20). It is clear that, in the absence of crack propagation, the finite element method is more efficient than the PD scheme at capturing stress concentra-
Figure 4.17: Aluminum alloy 2024-T4 notched specimen loaded under axial tension (dimensions in mm) [67]. The inset shows the particle arrangement around the notch tip and the resulting discrete curvature of the notch.

Figure 4.18: Comparison of the PD solution and the experimental data [67] for the $\sigma_{ii}$ stresses in the vicinity of the notch.
Figure 4.19: Finite element model of the notched specimen using 44,588 10-node tetrahedral elements (231,162 degrees of freedom).

tions. As emphasized in the introductory section, the PD scheme has been introduced primarily to simulate crack propagation, and the present study demonstrates that, although not optimal for non-propagating crack problems, the method is able to capture regions of stress concentration where crack initiation is likely to occur.
Figure 4.20: Comparison of PD, FE and the experimental data [67] for the $\sigma_{ii}$ stresses in the vicinity of the notch.
5 Propagating crack

5.1 Non-ordinary state-based modeling of quasi-static fracture

The criteria used to break the bonds between particles is a key component in PD because it is the fundamental way in which discontinuities, such as cracks, are defined. A critical component of any bond failure criteria is the ability to relate the PD quantities to key classical measurable fracture parameters, i.e., the fracture toughness $G_c$. The first bond failure criterion introduced in [59] is the ‘bond stretch’ criterion which is based on a critical value $s_c$ of the bond stretch $s$

$$s = \frac{|\xi + \eta| - |\xi|}{|\xi|} = s_c,$$  \hspace{1cm} (5.1)

where $\xi$ and $\eta$ have been defined in (2.1) and (2.3), respectively. This value can be related to the fracture toughness $G_c$, i.e., the total energy per unit of fracture surface needed to completely separate two halves of the horizon. In terms of the critical bond stretch (5.1), Silling et al. [59] considered the work required to break a single bond

$$w_0(\xi) = \int_0^{s_c} g(s) \eta d\eta = \int_0^{s_c} g(s)(\xi ds), \hspace{0.5cm} \xi = \|\xi\|.$$  \hspace{1cm} (5.2)

Assuming a stiffness $c$ of the bond (3.8) and a linear function for $g(s) = cs$, the integration of (5.2) simplifies to

$$w_0(\xi) = \int_0^{s_c} cs(\xi ds) = \frac{cs^2\xi}{2}.$$  \hspace{1cm} (5.3)

Therefore, the work $G_c$ required to break all the bonds per unit fracture area is (Fig. 5.1)

$$G_c = \int_0^\delta \int_0^{2\pi} \int_0^\delta \int_0^{\cos^{-1}z/\xi} \left(\frac{cs_0^2\xi}{2}\right) \xi^2 \sin \phi d\phi d\xi dz,$$  \hspace{1cm} (5.4)

leading to
Figure 5.1: Geometrical representation of the integration bounds (5.4) for a horizon containing a bisecting fracture plane used in the ‘bond stretch’ and ‘energy density’ criteria. The total work to break all the bonds connecting point A to all points B in the spherical cap is the integration over all these connections for each point A along the line z.

\[ G_c = \frac{\pi c s^2 \delta^5}{10}. \]  

(5.5)

Alternatively, since the NOSB formulation incorporates classical continuum mechanics definitions, Warren et al. [69] proposed two criteria using these classical definitions. By averaging the Lagrangian strain tensor between \( x \) and \( x' \), i.e., \( E_{IJ}(x,x') = \frac{(E_{IJ}(x) + E_{IJ}(x'))}{2} \), the first criteria is based on the equivalent strain \( E_{eq}(x,x') \) obtained from the second invariant \( I_2' \) of the averaged deviatoric strain tensor \( E_{IJ}' = (E_{IJ}(x,x') - 1/3 E_{KK}(x,x') \delta_{IJ}) \) and expressed as

\[
E_{eq}(x,x') = \sqrt{\frac{4}{3} I_2'} = \sqrt{\frac{2}{3} E_{IJ}'(x,x') E_{IJ}'(x,x')}
\]

\[
= \left\{ \frac{2}{9} \left[ (E_{11}(x,x') - E_{22}(x,x'))^2 + (E_{22}(x,x') - E_{33}(x,x'))^2 + (E_{11}(x,x') - E_{33}(x,x'))^2 \right] + \frac{4}{3} \left[ E_{12}(x,x')^2 + E_{13}(x,x')^2 + E_{23}(x,x')^2 \right] \right\}^{1/2}. \quad (5.6)
\]

The failure criterion for the bond is then expressed as

\[ E_{eq}(x,x') > E_{eq}^{critical}(x,x'). \]  

(5.7)
The second method introduced in [69] uses the averaged value of the volumetric strain $E_{\text{vol}}(x, x')$ in the principal directions:

$$E_{\text{vol}}(x, x') = I_1 + I_2 + I_3$$

$$= E_{11}(x, x') + E_{22}(x, x') + E_{33}(x, x')$$

$$+ E_{11}(x, x')E_{22}(x, x') + E_{22}(x, x')E_{33}(x, x')$$

$$+ E_{11}(x, x')E_{33}(x, x') + E_{11}(x, x')E_{22}(x, x')E_{33}(x, x').$$  (5.8)

The second criterion then takes the form:

$$E_{\text{vol}}(x, x') > E_{\text{vol}}^{\text{critical}}(x, x').$$  (5.9)

Warren et al. [69] used the equivalent strain $E_{\text{eq}}(x, x')$ criteria to study qualitatively dynamic fracture in a center notched plate.

Lastly, a state-based PD energy density based failure criteria has been developed by Foster et al. [70] relating the critical energy density $w_c$ in a bond to the fracture energy. Similar to the integration used in the stretch based criteria, the total strain energy of all the bonds, each with an energy density $w_c$, crossing the fracture plane is (Fig. 5.1)

$$G_c = \int_0^\delta \int_0^{2\pi} \int_0^{\cos^{-1}\frac{z}{\xi}} w_c \xi^2 \sin \phi d\phi d\xi dz.$$  (5.10)

Integrating (5.10) and solving for $w_c$ gives

$$w_c = \frac{4G_c}{\pi \delta^4},$$  (5.11)

which relates the critical energy density to the fracture toughness. A bond’s energy density is a function of the stress state $\mathbf{T}$ and the displacement difference between the particles:

$$w_\xi = (\mathbf{T}[x_j] \langle x_n - x_j \rangle - \mathbf{T}[x_n] \langle x_j - x_n \rangle) \cdot (u_n - u_j),$$  (5.12)

and the bond fails if $w_\xi > w_c$.

The numerical algorithm for bond failure is fairly straightforward (Fig. 5.2). At each load step, the system of equations (2.23) are solved for the displacements. If the fracture failure criteria for bond $\xi$ is met, the influence
BONDS FAIL?

\[ n \langle \phi(x) \rangle - n \langle \phi(x) \rangle \langle T \rangle - \phi(x) - n \langle \phi(x) \rangle \langle T \rangle = 1 \sum_{m} \phi \sigma = 1 \phi \sigma \]

SOLVE SYSTEM OF EQUATIONS FOR DISPLACEMENTS

\[ \sum_{n=1}^{m} \langle T(x) \rangle \langle x_n - x_j \rangle - \langle T(x) \rangle \langle x_n - x_j \rangle W_n + b(x_j) = 0, \quad j = 1, 2, ..., q \]

LOAD STEP
Increment displacement or force loading

BONDS FAIL?
Use bond failure criteria

YES

BREAK BONDS

Figure 5.2: Algorithm for breaking bonds, the solution is considered at equilibrium when bonds have ceased breaking, triggering the next load step.

function (Section 2.1.1) for that bond, \( \omega(\xi) \) is set to zero, essentially removing any influence between \( x \) and \( x' \). This process is repeated until bonds no longer break, and the simulation progresses to the next load step. Additionally, although not implemented in this work, the updating and factorization of the stiffness matrix during each bond failure iteration step can be improved by only updating the parts of the stiffness matrix that change as a result of bond failure instead of reforming the entire matrix, as is currently done. Although there are not any issues with numerical instability in the implicit formulation, using large load increments can lead to non-physical catastrophic fractures which will lead to gross errors in the solution. In practice, the load step in this work was arrived at through numerical experimentation. However, the robust approach would be to incorporate an adaptive load stepping scheme that would decrease and repeat the previous load step if too many bonds are broken. What would constitute ‘too many broken bonds’ would depend on the problem and be left to the analyst to adjust accordingly.
5.2 Mode I double cantilever beam

The first verification study uses a double cantilever beam (DCB) test to investigate crack initiation and propagation. The dimensions of the beam are \( L = 0.6 \text{ m} \), initial crack length \( a_0 = 0.2 \text{ m} \), \( h = 0.025 \text{ m} \), \( b = 0.01 \text{ m} \) (Fig. 5.3) and the material properties are \( E = 1 \text{ GPa} \), \( \nu = 0.25 \) and \( G_c = 0.0624 \text{ J/m}^2 \).

The analytical expression for the opening \( \Delta \) as a function of crack length \( a \) is

\[
\Delta = 2a^2 \sqrt{\frac{G_c}{3Eh^3}} \frac{1 + (3(1 + \nu)/5)(h/a)^2}{\sqrt{1 + ((1 + \nu)/5)(h/a)^2}}. \tag{5.13}
\]

where the crack opening displacement (COD) = \( 2\Delta \). The reaction force as a function of crack length is

\[
P = \frac{bh}{2a} \sqrt{\frac{G_c Eh}{3(1 + ((1 + \nu)/5)(h/a)^2)}}. \tag{5.14}
\]

The PD simulation uses the bond stretch criteria, where \( s_c \) is computed from (5.5), and the cubic lattice spacing is \( dq/\delta = \sqrt{2} \). Two snapshots showing the progression of the crack and the resulting crack-tip stress concentration are shown in Fig. 5.4. The PD solver is able to resolve the crack-tip stress concentration as the crack propagates. However, the load step must be sufficiently small in order to resolve the crack-tip stress concentration at each load step since breaking a very large number of bonds per load step leads to dissipation of the stress concentration. This dissipation will eventually cause the crack path to artificially branch or fragment. In comparison to the analytical solution for crack extension per COD load step, the crack starts to propagate at the predicted analytical COD and grows at the correct length per COD increment (Fig. 5.5a). The reaction force also shows favorable agreement with the analytical solution (Fig. 5.5b).

The DCB experiment is well suited for studying delamination or adhesive failure because the interface between the two materials is often weaker than the bulk material, keeping the crack path straight. On the other hand, in
Figure 5.4: DCB crack propagation and stress concentration at the crack-tip. The PD solver is able to capture the stress concentration in the vicinity of the advancing crack front.
Figure 5.5: Evolution of the (a) crack length and (b) reaction force for the DCB problem. The PD results are denoted with symbols, while the solid curve denotes the analytical solution.
the case of a solid material where a crack has been physically introduced, the crack path has the tendency to kink out of the plane due to inevitable anti-symmetry of the force or initial crack. Therefore, it is often advantageous to add a side groove to the specimen in order to keep the crack planar [71]. A numerical option is to add axial compression in order to make it unfavorable for the crack to kink out of plane. This technique was first tested by applying a compressive axial force without an applied COD (Fig. 5.6). The expected result from LEFM is that no stress concentration should occur at the crack-tip. However, in the PD simulations, a small stress concentration does occur at the crack-tip (Fig. 5.7) due to the nonlocal definition of the strains. If an opening displacement \( \Delta \) and an axial compressive force is applied, the results start to deviate from the analytical expression (Fig. 5.8a). As the compressive stress is increased, the crack starts to propagate sooner than predicted by LEFM which in turn affects the reaction force (Fig. 5.5b). This is due to the overstretching of the bonds around the crack-tip, and hence they fail at a lower value of the COD, and the crack propagates at a faster rate than it should.

Figure 5.6: DCB with only compressive forces applied.
Figure 5.7: Induced stress concentrations at the crack-tip due to an axial compressive load, $F = 1929$ N.
Figure 5.8: Evolution of the (a) crack length (symbols) and (b) reaction force (symbols) compared to the analytical solution (solid line) for a DCB specimen under various levels of axial compression.
5.3 Double notched split cantilever beam under mixed Mode II/III loading

In this section, a split cantilever bending test is simulated, and the crack front profile is compared to the experimental results presented by Suemasu et al. [72]. The test rig and specimen geometry are presented in Fig. 5.9, with the center cracked cantilever portion loaded vertically and the outside cantilever beams simply-supported. The specimen consists of three acrylic plates glued together everywhere along the interface except at the locations of the initial cracks. As shown in [72], the applied vertical load causes both a Mode II and Mode III component.

The NOSB model uses a cubic lattice with a lattice spacing $dq = 0.5 \, \text{mm}$ and a horizon size $\delta/dq = 2$. Other material parameters are: $E = 2.9 \, \text{GPa}$, $\nu = 0.39$, $s_c = 0.41608$ and the interface strength is assumed to be one-percent of the bulk material strength. The displacement-controlled vertical loading is applied in steps of 0.1 mm. As shown in Fig. 5.10, the NOSB crack front profiles compare favorably with the experimental results, capturing the forming of the crack front’s curvature and then maintaining the curved profile as the crack propagates.
Figure 5.10: Crack profile snapshots of the double notched split cantilever beam test. (a) Experimental crack front profile where the darker regions are intact material, and the lighter area denotes the crack region\cite{72}. (b) Series of snapshots highlighting the NOSB damage predictions, where the colors correspond to the damage (i.e., the ratio of broken to unbroken bonds) of the particles showing good agreement with the experimental profiles.
Figure 5.11: Mixed-mode geometry, loading and boundary conditions for three-point-bend specimen.

5.4 Three-point-bend with offset loading

The next example is a three-point-bend experiment with a notch that is offset from the vertical loading. The mixed-mode fracture experiments were performed using concrete by Galvez et al. [73] with the geometry and loading conditions presented in Fig. 5.11. The material parameters for concrete are: $E = 38$ GPa, $\nu = 0.18$ and $G_c = 69$ J/m$^2$. A body force density over a region of size 4x1 particles centered at 50 mm to the right of the initial crack was applied such that the resulting force $q = 515$ N.

The NOSB analysis uses a cubic lattice with $dq = 2$ mm, $\delta/dq = 2$, is conducted in plane stress and the critical bond stretch criterion is the analysis adopted. The predicted crack path by PD falls within the experimental crack trajectory envelope (Fig. 5.12). The surrounding area where the body force density was applied was not allowed to fail in order to prevent damage initiation at the applied load. Thus, the crack cannot reach the top surface of the beam.
5.5 Sharp V-notched Brazilian disc

The last example also models arbitrary crack path prediction under mixed-mode loading, but this section studies the effects of the lattice orientation on crack path trajectory. The validation experiments were conducted by Ayatollahi et al. [74]; they loaded PMMA sharp V-notched Brazilian discs under a compression load $P$ which varied with angle $\beta$ (Fig. 5.13). The dimensions of the disc are $D = 80$ mm, $d = 40$ mm and $\alpha = 30^\circ$, and the material properties are $E = 1$ GPa, $\nu = 0.25$ and $G_c = 0.0624$ J/m$^2$. For $\alpha=30^\circ$, the experiments were performed for loading angles ($\beta$) equal to 0°, 5°, 10°, 15° and 22.5°. The notch mode mixity parameter is defined as [74]

$$M_v^e = \frac{2}{\pi} \tan^{-1} \left\{ \frac{-p \cos (p\theta_0) + \frac{\sin(\omega_p/2)}{\sin(\omega_q/2)} \cos (q\theta_0)}{m \sin (m\theta_0) - \frac{\sin(\omega_m/2)}{\sin(\omega_q/2)} \sin (n\theta_0)} \right\}$$

(5.15)

where $\omega = 2\pi - \alpha$, $m = 1 + \lambda_1$, $n = 1 - \lambda_1$, $p = 1 + \lambda_2$, $q = 1 - \lambda_2$, $\lambda_1, \lambda_2$ are eigenvalues that depend on $\alpha$, and

$$\sigma^I_{\theta\theta} (\theta = 0) = \frac{m \sin (\omega_m/2)}{n \sin (\omega_n/2)} - 1,$$

(5.16)

$$\sigma^{II}_{r\theta} (\theta = 0) = 1 - \frac{q \sin (\omega_p/2)}{p \sin (\omega_q/2)}.$$  

(5.17)

The PD analysis assumed plane strain conditions and used a hexagonal
Figure 5.13: V-notched Brazilian disk under compression load $P$. The notch angle $\alpha$ was fixed at $30^\circ$, and $\theta_m$ is the lattice rotation angle about the center of the specimen and with respect to the $x$-axis.

lattice arrangement with a lattice spacing of $dq = 0.1$ mm. The bond stretch criteria is used with a critical stretch $s_c = 2.5$. The displacement magnitude under pure mode I ($\beta = 0^\circ$) loading and lattice rotation $\theta_m = 22.5^\circ$ shows a symmetric displacement magnitude (Fig. 5.14a) and stress $\sigma_{xx}$ (Fig. 5.14b) field. For a propagating crack, the predicted crack trajectory is compared to the experimental envelope for various lattice orientations in Fig. 5.15. The insets show all the unbroken bonds (in yellow) between particles and a crack when all the bonds have failed in a plane. lattice bias is observed to various degrees depending on the mode-mixity and how aligned the predicted path crack is to the lattice. For example, at $M_e = .3$ the experiment predicts a crack angle of $60^\circ$, and when $\theta_m = 60^\circ$ the PD predicted crack fails within this envelope. However, for the other lattice orientations, the predicted angles fall outside the experimental envelope.
Figure 5.14: (a) Displacement magnitude and (b) $\sigma_{xx}$ under pure mode I ($\beta = 0^\circ$) loading and lattice rotation $\theta_m = 22.5^\circ$. No lattice bias in the solutions fields are observed.
Figure 5.15: Crack trajectory for different degrees of mode-mixity. The insets show the crack path predictions at various lattice orientations and mode-mixity.
Cohesive zone modeling (CZM) is a well established and researched method for modeling fracture. Independently introduced in the early sixties by Dugdale [23] and Barrenblatt [24] to address the issue of the singularity of the crack tip field, CZM places ahead of the crack a nonlinear region governed by a cohesive failure law between the tractions resisting crack opening and the resulting displacement jump across the fracture surface. The approach regained a lot of attention two decades ago with the development of the cohesive finite element method, which incorporates the cohesive failure law in the constitutive response of interfacial (cohesive) elements placed between conventional (volumetric) finite elements [75, 76, 77, 78]. The cohesive finite element method has achieved remarkable success in the simulation of spontaneous crack propagation when the crack path is known a priori, such as in the failure of interfaces [79, 80, 81]. However, when the numerical method is used to model arbitrary crack growth, care must be exercised to address lattice dependency effects [82, 83, 84]. Nevertheless, CZM continues to be a valuable analysis tool in the study of fracture.

A key premise of the relation between the critical stretch $s_c$ and the fracture toughness $G_c$ outlined in Section 5.1 is the disregard for the failure process taking place in breaking the bonds; only the final state of complete bond failure is considered. However, for cohesive modeling, this process is modeled by considering the stretch $s$ of every bond, which is now a function of the crack face separation. Therefore, each bond will reach the critical stretch, $s_c$, at different crack opening displacement levels, resulting in a traction-separation law. The cohesive traction-separation laws in PD are investigated in the next sections for normal opening (Sections 6.1 and 6.2), tangential opening (Section 6.3) and mixed-mode loading (Section 6.4).

### 6.1 Analytical PD-based normal cohesive law

To derive analytically the normal traction-separation law described by PD, let us assume that a horizon is traversed by a fracture plane, which is then displaced normal to the crack surface by an opening distance $\Delta_n$ (Fig. 6.1).
Defining $\xi = \|\xi\|$ and $\eta = \|\eta\|$, the length of the stretched bond, $\overline{AC}$, of segment $\overline{AB}$ is

$$\overline{AC} = \sqrt{\xi^2 + \Delta_n^2 + 2\xi\Delta_n \cos \phi}. \quad (6.1)$$

The stretch $s_{AC}$ of segment $\overline{AC}$ is thus given by

$$s_{AC} = \frac{\overline{AC}}{\xi} - 1 = \sqrt{1 + 2 \left(\frac{\Delta_n}{\xi}\right) \cos (\phi) + \left(\frac{\Delta_n}{\xi}\right)^2} - 1. \quad (6.2)$$

Finding bonds which have exceeded the critical stretch, $s_c$, is achieved by setting $s_{AC}$ (6.2) equal to $s_c$, i.e,

$$\sqrt{1 + 2 \left(\frac{\Delta_n}{\xi}\right) \cos (\phi) + \left(\frac{\Delta_n}{\xi}\right)^2} - 1 = s_c, \quad (6.3)$$

and solving (6.3), for $\xi$,

$$\xi_c = \frac{\Delta_n \left(\cos (\phi) + \sqrt{\cos^2 (\phi) + 2 s_c + s_c^2}\right)}{s_c \left(2 + s_c\right)}. \quad (6.4)$$

Thus, all bonds with a length less than $\xi_c$ described by (6.4) have failed. Assuming a bond stiffness $c$, the force magnitude in segment $\overline{AC}$ is...
\[ \| \mathbf{T}_{AC} \| = c \frac{\eta}{\xi} = cs = c \left[ \sqrt{1 + 2 \left( \frac{\Delta_n}{\xi} \right) \cos(\phi) + \left( \frac{\Delta_n}{\xi} \right)^2} - 1 \right]. \] (6.5)

The components of the total force acting on the fracture surface per unit of fracture area due to all the bonds connecting points \( A \) located below the fracture plane \( (0 \leq z \leq \delta) \) to their counterpart points \( B \) in the spherical cap above the fracture plane are then

\[ T_x = \int_0^\delta \int_{\theta_1}^{\theta_2} \int_{\phi_1}^{\phi_2} \int_{\xi_1}^{\xi_2} \left( \| \mathbf{T}_{AC} \| \sin \phi \cos \theta \right) \xi^2 \sin \phi \, d\xi \, d\phi \, d\theta \, dz, \] (6.6)

\[ T_y = \int_0^\delta \int_{\theta_1}^{\theta_2} \int_{\phi_1}^{\phi_2} \int_{\xi_1}^{\xi_2} \left( \| \mathbf{T}_{AC} \| \sin \phi \sin \theta \right) \xi^2 \sin \phi \, d\xi \, d\phi \, d\theta \, dz, \] (6.7)

\[ T_z = \int_0^\delta \int_{\theta_1}^{\theta_2} \int_{\phi_1}^{\phi_2} \int_{\xi_1}^{\xi_2} \left( \| \mathbf{T}_{AC} \| \cos \phi \right) \xi^2 \sin \phi \, d\xi \, d\phi \, d\theta \, dz, \] (6.8)

where the fracture surface is in the \( xy \)-plane and \( z \) is normal to the crack surface. The force magnitude \( \| \mathbf{T}_{AC} \| \) in each bond is independent of \( \theta \), and evaluating the \( d\theta \) integral, with the bounds \( \theta_1 = 0 \) and \( \theta_2 = 2\pi \), results in the \( T_z \), referred to hereafter as the normal traction \( T_n \), being the only non-zero component:

\[ T_x = (\sin 2\pi - \sin 0) \int_0^\delta \int_{\phi_1}^{\phi_2} \int_{\xi_1}^{\xi_2} \left( \| \mathbf{T}_{AC} \| \sin \phi \right) \xi^2 \sin \phi \, d\xi \, d\phi \, dz = 0, \] (6.9)

\[ T_y = (\cos 2\pi - \cos 0) \int_0^\delta \int_{\phi_1}^{\phi_2} \int_{\xi_1}^{\xi_2} \left( \| \mathbf{T}_{AC} \| \sin \phi \right) \xi^2 \sin \phi \, d\xi \, d\phi \, dz = 0, \] (6.10)

\[ T_z = T_n = 2\pi \int_0^\delta \int_{\phi_1}^{\phi_2} \int_{\xi_1}^{\xi_2} \left( \| \mathbf{T}_{AC} \| \cos \phi \right) \xi^2 \sin \phi \, d\xi \, d\phi \, dz. \] (6.11)

The integration bounds in (6.9)-(6.11) change depending on the number of broken bonds, which is itself dependent on the crack opening displacement \( \Delta_n \) and critical stretch \( s_c \).
6.1.1 Case 1 – No bonds have reached critical stretch

Assuming no bonds have reached the critical stretch $s_c$, from Fig. 6.1, the bounds of integration are

$$
\begin{align*}
\phi_2 &= \cos^{-1} (z/\delta) \quad \xi_2 = \delta \\
\phi_1 &= -\cos^{-1} (z/\delta) \quad \xi_1 = z/\cos\phi.
\end{align*}
$$

(6.12)

To get the components of the force in the deformed configuration, i.e., the force components of vector $AC$, the angle $\phi$ with respect to $AC$ is

$$
\phi = \sin^{-1} \left( \frac{\xi \sin \phi}{\sqrt{\xi^2 + \Delta_n^2 + 2 \xi \Delta_n \cos \phi}} \right).
$$

(6.13)

Using the property $\cos(\sin^{-1} \phi) = \sqrt{1 - \phi^2}$, we get

$$
\cos \phi = \sqrt{1 - \left( \frac{\xi \sin \phi}{\sqrt{\xi^2 + \Delta_n^2 + 2 \xi \Delta_n \cos \phi}} \right)^2}.
$$

(6.14)

Substituting (6.14) into (6.11) gives the final form of the traction component normal to the crack surface,

$$
T_n = 2\pi \int_0^\delta \int_{\phi_1}^{\phi_2} \int_{\xi_1}^{\xi_2} \left( \|T_{AC}\| \sqrt{1 - \left( \frac{\xi \sin \phi}{\sqrt{\xi^2 + \Delta_n^2 + 2 \xi \Delta_n \cos \phi}} \right)^2} \right) \xi^2 \sin \phi \, d\xi \, d\phi \, dz,
$$

(6.15)

where $\|T_{AC}\|$ is described by (6.5). All the integrals are evaluated numerically using the Romberg integration function, a successively higher-order generalization of Simpson’s rule [85].

6.1.2 Case 2 – Bonds have exceeded the critical stretch

Case 2 handles the situation when any of the bonds crossing the fracture plane have exceeded the critical stretch. The integration bounds have to be split into two different cases, Case 2A and Case 2B, due to the drastic changes in the integration regions.

Case 2A – $\xi_c$ is less then the horizon size $\delta$

Case 2A corresponds to the situation when $\xi_c$ (6.4) is less then the horizon size $\delta$ at $\phi = 0$ and $z = 0$ (Fig. 6.2a)
Using spherical coordinates centered at point $A$, the integration needs to be split into three different regions $R_1$, $R_2$ and $R_3$ (Fig. 6.2 ). The colored regions are those where bonds have not failed. The bounds of integration for region $R_1$ (Fig. 6.2a) for the traction forces $(T_n)^{R_1}$ (6.15) are

\[ z_2 = z_c, \quad \phi_2 = \cos^{-1}\left(\frac{z}{\delta}\right), \quad \xi_2 = \delta \]
\[ z_1 = 0, \quad \phi_1 = \frac{z\sqrt{\Delta_n(\Delta_n+2z_s(2+s_c))}}{\Delta_n(\Delta_n+2z)}, \quad \xi_1 = \frac{z}{\cos\phi}, \quad (6.17) \]

where the angle $\phi_1$ is associated with point $a$, which is the intersection of the curves $ab$ and $ac$ (6.4), i.e., solving for $\phi$ in

\[ \frac{\Delta_n}{s_c(2+s_c)} \left( \cos\phi + \sqrt{\cos^2\phi + 2s_c + s_c^2} \right) = \frac{z}{\cos\phi}. \quad (6.18) \]

The bounds of integration for region $R_2$ (Fig. 6.2a) for the traction forces
Case 2B – \( \xi_c \) is greater than the horizon size \( \delta \)

Case 2B corresponds to larger values of \( \Delta_n \) for which \( \xi_c \) given by (6.4) is larger than the horizon size \( \delta \) at \( \phi = 0 \) and \( z = 0 \) (Fig. 6.3). Again using spherical coordinates, the integration needs to be split into two different regions, \( R_1 \) (Fig. 6.3) and \( R_4 \) (Fig. 6.3), where the bounds of integration for \( R_1 \) are the same as in the previous case (6.17). For region \( R_4 \), the bounds of integration for the traction forces \( (T_n)_{R_4} \) (6.15) are

\[
\begin{align*}
\text{Case 2B} & \quad \xi_c > \delta.
\end{align*}
\]
Figure 6.4: Analytical traction-separation law for normal opening. The area under the curve is the fracture toughness $G_c$ (5.5).

The resulting evolution of the normal traction $T_n$ as a function of the $\Delta_n$ is presented in Fig. 6.4. The area under the traction-separation curve is the fracture toughness $G_c$, which is found to be in excellent agreement (within 0.006%) with the expression (5.5) found earlier. The PD-based cohesive law has a profile typical of some of the polynomial and exponential relations adopted in the literature [75, 76]. Note that the critical value of the displacement jump corresponding to the maximum value of the normal cohesive traction is approximately $0.76/\delta s_c$. Using the semi-analytical method described above, it would be possible to solve the inverse problem and derive the bond failure relation that leads to a desired cohesive failure law, thereby allowing for a direct link between some of the cohesive failure laws available in the literature and the PD CZM.
6.2 Numerical approximation of PD-based cohesive law

Whereas Section 6.1 derived the ‘analytical’ cohesive law by essentially considering an infinite number of points A and points B, this section explores the effects of using a finite number of particles on approximating the analytical traction-separation law in normal opening (Fig. 6.4). The first particle arrangement is a cubic lattice (Fig. 6.5ab) using grid spacings $dq/δ$ equal to 0.5, 0.25, 0.125 and .0625. The second particle arrangement is a random grid (Fig. 6.5c) created by using the tetrahedron’s centroid in an unstructured lattice as the particle coordinates, and the particle’s volume is set equal to the tetrahedron’s volume. To model the progressive opening of the crack, the hemispherical cap is displaced rigidly by $Δ_n$ and the bottom half’s line of points are all held fixed. The other simulation parameters are: $c = 1.0 \text{kN/mm}^6$, $δ = 1.0 \text{mm}$ and $s_c = 0.1 \text{mm}$. The traction on the fracture surface $dq^2$ highlighted in red (Fig. 6.5d) is

$$ T_n = \sum_{j=1}^{M} \sum_{i=1}^{N_j} cs_i (dq)^3_i (dq)^3_j, \quad (6.22) $$

where $M$ is the total number of particles below the spherical cap and $N_j$ is the number of particles in the horizon of particle $M$. For the random arrangement of particles, $dq$ was assumed to be the average distance between all the particles, which is a reasonable approximation as the global edge lengths of the tetrahedron are fairly uniform throughout the lattice.

Looking first at the cubic particle arrangement, the traction-separation law is presented in Fig. 6.6 as a function of particle refinement. The cohesive traction converges to the analytical solution described in Section 6.1 as the grid is refined. The discretization effects are clearly evident for the coarser arrangements, leading to an overestimation of the maximum traction $T_n^{max}$ by roughly 30% and the fracture toughness by roughly 10% (Table 6.1). As the grid spacing is reduced, the error quickly drops. A typical peridynamics simulation would use a discretization of the order $dq/δ \gtrsim 0.33$ since the simulation would be prohibitively expensive for lower values of $dq/δ$.

Next is the cohesive traction using a random particle arrangement (Fig. 6.7). The effects of the coarser arrangement are again evident. However, the randomness of the bonds appears to help the convergence of $G_c$ as evident in Table 6.2 where, for fewer degrees of freedom, the relative error in $G_c$ is less than for the cubic arrangement. On the other hand, the relative error in $T_n^{max}$ is larger than that found in the cubic arrangement.
Figure 6.5: Lattice arrangements for the study of normal opening cohesive traction laws using a discretized domain.

<table>
<thead>
<tr>
<th>$dq/\delta$</th>
<th>Degrees of freedom</th>
<th>$T_n^{max}$ relative error</th>
<th>$G_c$ relative error</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5</td>
<td>39</td>
<td>30.8%</td>
<td>11.3%</td>
</tr>
<tr>
<td>0.25</td>
<td>633</td>
<td>3.5%</td>
<td>8.3%</td>
</tr>
<tr>
<td>0.125</td>
<td>2895</td>
<td>1.9%</td>
<td>2.8%</td>
</tr>
<tr>
<td>0.0625</td>
<td>24471</td>
<td>0.31%</td>
<td>0.9%</td>
</tr>
</tbody>
</table>

Table 6.1: The relative error of the critical strain energy release rate, $(G_c/G_c^{exact} - 1)100\%$, as a function of grid spacing for a cubic arrangements of particles.
Figure 6.6: Cohesive traction-separation law obtained numerically for different particle spacings in a cubic arrangement compared to the exact solution (6.15).

Figure 6.7: The cohesive traction versus the crack opening displacement using different particle spacings in a random arrangement compared to the exact solution (6.15).
Table 6.2: The relative error of the critical strain energy release rate, as a function of the degrees of freedom, for a random arrangements of particles.

<table>
<thead>
<tr>
<th>Degrees of freedom</th>
<th>$T_{n}^{\max}$ relative error</th>
<th>$G_{c}$ relative error</th>
</tr>
</thead>
<tbody>
<tr>
<td>78</td>
<td>55.3%</td>
<td>4.3%</td>
</tr>
<tr>
<td>180</td>
<td>35.8%</td>
<td>5.1%</td>
</tr>
<tr>
<td>780</td>
<td>5.0%</td>
<td>4.4%</td>
</tr>
<tr>
<td>2406</td>
<td>2.2%</td>
<td>1.6%</td>
</tr>
<tr>
<td>6774</td>
<td>1.6%</td>
<td>0.31%</td>
</tr>
</tbody>
</table>

6.3 PD-based tangential cohesive law

In this section, the traction law for tangential opening is investigated. Assume a horizon is traversed by a fracture plane which is then displaced tangential to the crack surface an opening distance $\Delta_{t}$ (Fig. 6.8). The length of the stretched bond, $\overline{AC}$, for segment $\overline{AB}$ is

$$\overline{AC} = \sqrt{\Delta_{t}^{2} + \xi^{2} + 2\Delta_{t}\xi \sin(\phi) \sin(\theta)},$$

and the stretch $s$ of segment $\overline{AC}$ is

$$s_{\overline{AC}} = \frac{\overline{AC}}{\xi} - 1 = \sqrt{1 + 2 \left( \frac{\Delta_{t}}{\xi} \right) \sin(\phi) \sin(\theta) + \left( \frac{\Delta_{t}}{\xi} \right)^{2}} - 1, \quad (6.23)$$

which can be either tensile or compressive (Fig. 6.9). The bond, $\xi$, at which the critical stretch, $s_{c}$, is exceeded is obtained by setting (6.23) equal to $s_{c}$,

$$\sqrt{1 + 2 \left( \frac{\Delta_{t}}{\xi} \right) \sin(\phi) \sin(\theta) + \left( \frac{\Delta_{t}}{\xi} \right)^{2}} - 1 = s_{c}, \quad (6.24)$$

and solving (6.24) for $\xi$

$$\xi_{c} = \frac{\Delta_{t} \left( \sin(\phi) \sin(\theta) + \sqrt{\sin^{2}(\phi) \sin^{2}(\theta) + 2 s_{c} + s_{c}^{2}} \right)}{s_{c} \left( 2 + s_{c} \right)}. \quad (6.25)$$

Depending on $s_{c}$ and $\Delta_{t}$ (6.4), all bonds with a length less then $\xi_{c}$ have failed. Additionally, in contrast to the normal opening analysis (Section 6.1), $\xi_{c}$ is also dependent on $\theta$.

The magnitude of the force in segment $\overline{AC}$ is
Figure 6.8: Tangential opening, $\Delta_t$, of the fracture surface.

Figure 6.9: Shear opening stretch between points on plane $z/\delta \simeq 0$ and a point located at $z/\delta = 0.75$ for an opening displacement $\Delta_t/\delta = 0.5$ showing both tensile and compressive stretches.

\[
\|\mathbf{T}_{AC}\| = \frac{c}{\xi} = cs = c \left[ \sqrt{1 + 2 \left( \frac{\Delta_t}{\xi} \right) \sin(\phi) \sin(\theta) + \left( \frac{\Delta_t}{\xi} \right)^2} - 1 \right].
\]

(6.26)

The components of the total force acting on the fracture surface per unit of fracture area due to all the bonds connecting points $A$ to points $B$ in the spherical cap are

\[
\mathbf{T}_x = \int_0^\delta \int_{\theta_1}^{\theta_2} \int_{\phi_1}^{\phi_2} \int_{\xi_1}^{\xi_2} (\|\mathbf{T}_{AC}\| \sin \phi \cos \theta) \xi^2 \sin \phi \, d\xi \, d\phi \, d\theta \, dz = 0, \quad (6.27)
\]
\[ T_y = T_t = \int_0^\delta \int_{\phi_1}^{\phi_2} \int_{\xi_1}^{\xi_2} (\| T_{AC} \| \sin \phi \sin \theta) \xi^2 \sin \phi \, d\xi \, d\phi \, d\theta \, dz, \quad (6.28) \]

\[ T_z = \int_0^\delta \int_{\theta_1}^{\theta_2} \int_{\phi_1}^{\phi_2} \int_{\xi_1}^{\xi_2} (\| T_{AC} \| \cos \phi) \xi^2 \sin \phi \, d\xi \, d\phi \, d\theta \, dz. \quad (6.29) \]

Note that, unlike in the tensile case, \( T_z \) is not identically zero, which leads to some normal component during the shear failure process.

The final expression of the shear traction \( T_t \) tangential to the crack face, in the direction of the displacement \( \Delta_t \), is thus

\[ T_t = \int_{\theta_1}^{\theta_2} \int_{z_1}^{z_2} \int_{\phi_1}^{\phi_2} \int_{\xi_1}^{\xi_2} \left\{ \| T_{AC} \| \frac{\Delta_t + \xi \sin \phi \sin \theta}{\sqrt{\xi^2 \cos^2 \phi + (\xi \sin \theta \sin \phi + \Delta_t)^2 - z^2}} \right\} \xi^2 \sin \phi \, d\xi \, d\phi \, dz \, d\theta. \quad (6.30) \]

where \( \| T_{AC} \| \) is given by (6.26).

### 6.3.1 Case 1 – No bonds have reached critical stretch

Assuming no bonds have reached the critical stretch \( s_c \), from Fig. 6.8, the bounds of integration are

\[ \theta_2 = 2\pi \quad z_2 = \delta \quad \phi_2 = \cos^{-1} (\min(z, \delta)/\delta) \quad \xi_2 = \delta \]
\[ \theta_1 = 0 \quad z_1 = 0 \quad \phi_1 = 0 \quad \xi_1 = \min(\delta, z/cos\phi). \quad (6.31) \]

The integration of (6.31) was performed analytically and the resulting non-linear cohesive traction-separation law is plotted in Fig. 6.10 as the solid line. As was done in Section 6.2, an analysis of the traction-separation law for a cubic particle arrangement, using the same parameters, was performed (Fig. 6.10), showing convergence as the number of particles is refined. The area under the curve for \( 0 \leq \Delta_t/\delta s_c \leq 25 \) can be used as a measure of the relative error with respect to the analytical solution and is summarized in Table 6.3.
Figure 6.10: Tangential traction-separation law obtained analytically (6.30) and by using a series of refined cubic lattices in the absence of bond breakup. A very good agreement is observed for \( dq/\delta \leq 0.125 \).

<table>
<thead>
<tr>
<th>( dq/\delta )</th>
<th>Degrees of freedom</th>
<th>Relative error</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5</td>
<td>39</td>
<td>16.4%</td>
</tr>
<tr>
<td>0.25</td>
<td>633</td>
<td>8.9%</td>
</tr>
<tr>
<td>0.125</td>
<td>2895</td>
<td>3.2%</td>
</tr>
<tr>
<td>0.0625</td>
<td>24471</td>
<td>1.7%</td>
</tr>
</tbody>
</table>

Table 6.3: The relative error of the area under the curve for \( 0 \leq \Delta_t/\delta s_c \leq 25 \) (Fig. 6.10) as a function of the cubic lattice grid spacing, \( dq \), for shear opening \( \Delta_t \) and assuming no bonds have broken.
6.3.2 Case 2 – Bonds have exceeded the critical stretch

Due to the added complexity associated with the $\theta$ dependence of the solution, extracting of the closed-form expression of the integration bounds in 6.30 in the presence of bond breakage has eluded our efforts. However, the mode II cohesive failure law can be extracted numerically using the same cubic lattice model adopted earlier in the normal opening case (Section 6.2). As mentioned earlier, the failure process is substantially more complex in the shear case since some of the bonds experience compression while the ‘upper dome’ of the horizon (i.e., the set of points located above the failure surface) is subjected to shear failure. Various scenarios can then be considered, depending on whether and at what level compressive failure of the bonds is allowed. These scenarios can be characterized by the parameter $\eta$ defined as the (absolute value of the) ratio of critical stretch in compression to that in tension.

Fig. 6.11 presents the cohesive failure law in shear for the case $\eta = \infty$, i.e., when bonds are not allowed to break in compression. Curves corresponding to four grid spacing values \((dq/\delta) = 0.5, 0.25, 0.125\) and 0.0625\) are presented. As apparent in that figure, the absence of failure in compression leads to a substantial reversal of the shear cohesive traction after most of the bonds under tension have failed. This fact is illustrated by the two insets, which depict the evolution of the region (shaded in gray) corresponding to the unbroken bonds. For larger shear displacement jump values (such as $\Delta_t/\delta s_c = 10$), most of the bonds under tension have failed, and those still under compression create a shear cohesive traction in a direction opposite the applied displacement jump $\Delta_t$. Fig. 6.11 also illustrates a grid convergence of the cohesive law similar to that obtained in the tensile case: the traction-separation law converges for $dq/\delta \leq 0.125$. This convergence is quantified in Table 6.4 in terms of the relative error on the area under the traction-separation curve, i.e, the mode II fracture toughness. The relative error is with respect to the fracture toughness presented in Section 5.1, eq. (5.5), which remains valid also under a mode II loading.

If we allow for failure under compression, we obtain the mode II cohesive laws shown in Fig. 6.12, which correspond to a lattice spacing $dq/\delta = 0.0625$. Nine values of $\eta$ are considered, ranging from 0.25 to $\infty$. As apparent in that figure, no negative shear traction is observed for $\eta \lesssim 2$. As expected, as $\eta$ decreases, i.e., as more bonds fail under compression, the failure process is ‘steeper’. As shown in Fig. 6.13, which present the dependence of the fracture toughness on $\eta$, the mode II fracture toughness when the critical
stretch values in tension and compression are equal \((\eta = 1)\) is equal to that obtained in the absence of compressive failure of the bonds \((\eta = \infty)\), i.e. \(G_c(\eta = 1) \simeq G_c(\eta = \infty)\).

### 6.4 PD-based mixed-mode cohesive law

In this final section, we obtain the cohesive envelopes predicted by the PD modeling of cohesive failure, i.e., the dependence of the normal and tangential cohesive traction on the combined normal and shear displacement jumps. The results corresponding to \(\eta = \infty\) and \(dq/\delta = 0.0625\) are presented in Fig. 6.14. Since the failure process is path dependent, these results are obtained by holding \(\Delta_n\) fixed and then varying \(\Delta_t\) in the \(\Delta_n, \Delta_t\) plane. The coupling between normal and shear failure is clearly visible.
<table>
<thead>
<tr>
<th>$dq/\delta$</th>
<th>Degrees of freedom</th>
<th>$G_c$ relative error</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5</td>
<td>39</td>
<td>16.4%</td>
</tr>
<tr>
<td>0.25</td>
<td>633</td>
<td>8.9%</td>
</tr>
<tr>
<td>0.125</td>
<td>2895</td>
<td>3.2%</td>
</tr>
<tr>
<td>0.0625</td>
<td>24471</td>
<td>1.7%</td>
</tr>
</tbody>
</table>

Table 6.4: Relative error of the fracture toughness, with respect to the fracture toughness $G_c$ presented in Section 5.1, eq. (5.5), as a function of the cubic lattice grid spacing, $dq$, for shear opening $\Delta_t$ and assuming no bonds break in compression ($\eta = \infty$).

Figure 6.12: Traction-separation law obtained numerically with $dq/\delta=0.0625$ when bonds are allowed to fail in compression. $\eta$ is the ratio of critical stretch in compression to that in tension.
Figure 6.13: Variation of the fracture toughness $G_c$ with respect to the ratio of critical stretch in compression to critical stretch in tension.
Figure 6.14: Normal $T_n$ and tangential $T_t$ cohesive traction versus the normal \( \Delta_n \) and tangential \( \Delta_t \) displacement jumps for the case \( \eta = \infty \).
7 Conclusion

7.1 Key accomplishments

The overarching goal of this work has been to further advance the fundamental understanding of the NOSB method for simulating fracture. As mentioned in the introduction (Section 1.2), this work was the first to study in-depth the fundamental characteristics of the NOSB method. In Section 2.1.2, the formulation of the small-strain linearly elastic static implicit implementation of the NOSB PD formulation for static and propagating cracks was presented. An efficient parallel implementation for both structured and unstructured grids capable of handling millions of particles was developed and, to the author’s knowledge, used to solve the largest simulations to-date using the NOSB method.

One advantage of the NOSB method is that it removes the bond-based restriction of requiring a Poisson’s ratio of 1/4 for isotropic linear elastic materials. Furthermore, the NOSB formulation represents the forces in the bonds in terms of strain and stress tensors and, consequently, these bonds are able to carry the stresses in any direction. The NOSB formulation, therefore, allows for classical continuum mechanics definitions such as deformation gradient and stress tensor for use in constitutive models. However, this convenience also comes at a price. One of the basic premises of the state-based PD is that the deformation vector state $\mathbf{Y}$ can be nonlinear and, most importantly, discontinuous. However, in the NOSB formulation we take it a step further by accruing the various discontinuous deformation states, $\mathbf{Y}$, into a –best approximation– deformation gradient (2.4). One consequence of this approximation is the zero-energy modes as examined in Section 3.1. It can not be stated strongly enough that despite the efforts and relative success in controlling the zero-energy modes, their effects, while minimized, still pervaded in one way or another throughout all the simulations in this work.

The ability of NOSB PD to capture key local fracture parameters commonly affiliated with non-propagating crack problems was presented in Chapter 4. The method captured the crack-tip near fields very well, including
the stress intensity factor and the stress and strain concentrations around notches. This is an impressive accomplishment as the solution field naturally occurs as a consequence of the fundamental PD equations.

Crack propagation and crack trajectory were investigated in Chapter 5, where it was found that the NOSB method can capture well the propagation of cracks when the grid is aligned in the direction of crack growth. For mixed mode fracture, when the grid is often not aligned with the predicted crack trajectory, the NOSB has some issues with grid dependency as highlighted in the sharp V-notched Brazilian disc experiments (Section 5.5). Lastly, the analytical and numerical study of the link between PD and cohesive zone modeling under Mode I, Mode II and mixed-mode loading was presented in Chapter 6. It was observed that the Mode I, Mode II and mixed-mode PD-based cohesive laws resulted in a profile typically found in some of the polynomial and exponential relationships found in the literature.

7.2 Future work

Since this work is the first in-depth review of the NOSB PD in capturing crack kinematics, it makes a sound basis for future work. Although the methods of zero-energy control worked reasonably well, the need for the user to pick an optimum constant coefficient is not ideal. The need for the zero-energy control to flow from the fundamental equations needs to be further investigated.

Additionally, the issue of grid dependency needs to be addressed and investigated further. An adaptive grid orientation scheme based on the stress state could be an option in mediating the dependency. Also, a classical fracture mechanics criterion can be used as one, not ideal, option of orientating the grid to the predicted crack path. Other types of particle arrangements can also be further investigated to address the dependency. All the crack propagation simulations in this work had an initial crack, so an investigation into crack nucleation is also warranted. Also, by using the cohesive analysis outlined in Section 6, one should be able to derive the bond failure relation that leads to a desired failure law, thereby forming a link between PD CZM and cohesive laws available in the literature.

In terms of enhancements to the NOSB formulation, the list is long. At the top of the list would be the implementation of an adaptive grid scheme. This would allow, for example, refinement around notches and other stress concentrating geometrical features. The computational savings would have been substantial for the penny shaped crack and notched specimen tests.
mentioned in Chapter 4 had this been available. Some work has already begun on this task [60, 68] for the bond-based methods. Also, it would be beneficial to have a robust adaptive load stepping scheme to prevent too many broken bonds per load step, as this usually has a negative effect on the crack-tip singularity. Additionally, the solver routines should take into account the fact that the stiffness matrix remains relatively the same during the bond breaking iteration loop. Thus, only matrix entries affected by broken bonds would be recomputed, saving time in the matrix assembly. And lastly, the standard list of features usually available in local continuum codes would be welcome, such as a finite strain formulation, a contact detection scheme for completely broken bond surfaces and a nonlinear solver for handling nonlinear material models and finite strains.
Discretized shape tensor

The components of bond $\xi$ between $x$ and $x'$ in the $x_1$, $x_2$ and $x_3$ directions will be denoted as $\xi_{x,x'}$, $\xi_{y,x'}$ and $\xi_{z,x'}$, respectively. Additionally, $x_j$ is the coordinate location of the point $x$, and the points within $x_j$’s horizon are designated as the $n$th points. For example, if the $j$th node is 2 and the $n$th node is 4 then the components of $\xi$ are $\xi_{x4} = x_n - x_j = x_4 - x_2$, $\xi_{y4} = y_4 - y_2$ and $\xi_{z4} = z_4 - z_2$. The shape tensor evaluated at $x_j$ is given in matrix form as,

$$K(x_j)_{(3\times3)} = \left(\int_{H_x} \omega(|\xi|) (\xi \otimes \xi) dV_\xi\right)^{-1} =$$

$$\begin{bmatrix}
\sum_{n=1}^{m} \omega(|\xi|) \xi_{x_n} \xi_{x_n} V_n & \sum_{n=1}^{m} \omega(|\xi|) \xi_{x_n} \xi_{y_n} V_p & \sum_{n=1}^{m} \omega(|\xi|) \xi_{x_n} \xi_{z_n} V_n \\
\sum_{n=1}^{m} \omega(|\xi|) \xi_{y_n} \xi_{x_n} V_n & \sum_{n=1}^{m} \omega(|\xi|) \xi_{y_n} \xi_{y_n} V_n & \sum_{n=1}^{m} \omega(|\xi|) \xi_{y_n} \xi_{z_n} V_n \\
\sum_{n=1}^{m} \omega(|\xi|) \xi_{z_n} \xi_{x_n} V_n & \sum_{n=1}^{m} \omega(|\xi|) \xi_{z_n} \xi_{y_n} V_p & \sum_{n=1}^{m} \omega(|\xi|) \xi_{z_n} \xi_{z_n} V_n \\
\end{bmatrix}^{-1}$$

(A.1)

Since $K$ is symmetric, positive definite according to Lemma 3.1 [13], the inverse of $K$ is also symmetric and is stored in a $6 \times 9$ matrix

$$K(x_j) = \begin{bmatrix}
K_{11} & 0 & 0 & K_{12} & 0 & 0 & K_{13} & 0 & 0 \\
0 & K_{12} & 0 & 0 & K_{22} & 0 & 0 & K_{23} & 0 \\
0 & 0 & K_{13} & 0 & 0 & K_{23} & 0 & 0 & K_{33} \\
K_{12} & K_{11} & 0 & K_{22} & K_{12} & 0 & K_{23} & K_{13} & 0 \\
K_{13} & 0 & K_{11} & K_{23} & 0 & K_{21} & K_{33} & 0 & K_{13} \\
0 & K_{13} & K_{12} & 0 & K_{23} & K_{22} & 0 & K_{33} & K_{23} \\
\end{bmatrix}. \quad (A.2)$$
Discretized displacement gradient

Using the properties of the outer product,

\[ \mathbf{u} \otimes \mathbf{v} = \mathbf{uv}^T = \begin{bmatrix} u_1 & u_2 & \cdots & u_n \end{bmatrix} \begin{bmatrix} u_1 v_1 & u_1 v_2 & \cdots & u_1 v_n \\ u_2 v_1 & u_2 v_2 & \cdots & u_2 v_n \\ \vdots & \vdots & \ddots & \vdots \\ u_m v_1 & u_m v_2 & \cdots & u_m v_n \end{bmatrix} \]

(B.1)

the tensor products present in (2.9) and (2.13) can be written as

\[
\begin{align*}
(x_n - x_j) \otimes (x_n - x_j) &= \begin{bmatrix} (x_n - x_j)(x_n - x_j) & (x_n - x_j)(y_n - y_j) & (x_n - x_j)(z_n - z_j) \\ (y_n - y_j)(x_n - x_j) & (y_n - y_j)(y_n - y_j) & (y_n - y_j)(z_n - z_j) \\ (z_n - z_j)(x_n - x_j) & (z_n - z_j)(y_n - y_j) & (z_n - z_j)(z_n - z_j) \end{bmatrix}^{-1} \\
&= \begin{bmatrix} 1 & u_1 v_1 & u_1 v_2 & \cdots & u_1 v_n \\ u_2 v_1 & u_2 v_2 & \cdots & u_2 v_n \\ \vdots & \vdots & \ddots & \vdots \\ u_m v_1 & u_m v_2 & \cdots & u_m v_n \end{bmatrix} \\
&= (B.2)
\end{align*}
\]

Similarly,

\[
\begin{align*}
(u_n - u_j) \otimes (x_n - x_j) &= \begin{bmatrix} (u_n - u_j)(x_n - x_j) & (u_n - u_j)(y_n - y_j) & (u_n - u_j)(z_n - z_j) \\ (v_n - v_j)(x_n - x_j) & (v_n - v_j)(y_n - y_j) & (v_n - v_j)(z_n - z_j) \\ (w_n - w_j)(x_n - x_j) & (w_n - w_j)(y_n - y_j) & (w_n - w_j)(z_n - z_j) \end{bmatrix} \\
&= (B.3)
\end{align*}
\]

where \( u, v \) and \( w \) are the displacement components in the \( x, y \) and \( z \) directions, respectively.

Substituting (B.2) and (B.3) into \( \nabla \mathbf{u} \) (2.13),
\[ \nabla u(x_j) = \begin{bmatrix} \sum_{n=1}^{m} \omega(|\xi|) \Delta u \xi_{xn} & \sum_{n=1}^{m} \omega(|\xi|) \Delta u \xi_{yn} & \sum_{n=1}^{m} \omega(|\xi|) \Delta u \xi_{zn} \\ \sum_{n=1}^{m} \omega(|\xi|) \Delta v \xi_{xn} & \sum_{n=1}^{m} \omega(|\xi|) \Delta v \xi_{yn} & \sum_{n=1}^{m} \omega(|\xi|) \Delta v \xi_{zn} \\ \sum_{n=1}^{m} \omega(|\xi|) \Delta w \xi_{xn} & \sum_{n=1}^{m} \omega(|\xi|) \Delta w \xi_{yn} & \sum_{n=1}^{m} \omega(|\xi|) \Delta w \xi_{zn} \end{bmatrix} K(x_j)_{3x3}, \]

where \( \Delta u = u_n - u_j \), \( \Delta v = v_n - v_j \) and \( \Delta w = w_n - w_j \). Using the 6 \( \times \) 9 storage convention for \( K(x_j) \), (A.2), and isolating in (B.4) the displacement components in vector form, (2.16), the resulting in the 9 \( \times \) 3 matrix,

\[ N = \begin{bmatrix} N^{(1)} & 0 & 0 & \cdots & \omega \xi_{xn} V_n & 0 & 0 & \cdots \\ 0 & N^{(1)} & 0 & \cdots & 0 & \omega \xi_{xn} V_n & 0 & \cdots \\ 0 & 0 & N^{(1)} & \cdots & 0 & 0 & \omega \xi_{xn} V_n & \cdots \\ N^{(2)} & 0 & 0 & \cdots & \omega \xi_{yn} V_n & 0 & 0 & \cdots \\ 0 & N^{(2)} & 0 & \cdots & 0 & \omega \xi_{yn} V_n & 0 & \cdots \\ 0 & 0 & N^{(2)} & \cdots & 0 & 0 & \omega \xi_{yn} V_n & \cdots \\ N^{(3)} & 0 & 0 & \cdots & \omega \xi_{zn} V_n & 0 & 0 & \cdots \\ 0 & N^{(3)} & 0 & \cdots & 0 & \omega \xi_{zn} V_n & 0 & \cdots \\ 0 & 0 & N^{(3)} & \cdots & 0 & 0 & \omega \xi_{zn} V_n & \cdots \end{bmatrix} \]

where \( N^{(1)} = - \sum_{n=1}^{m} \omega(|\xi|) \xi_{xn} V_n \), \( N^{(2)} = - \sum_{n=1}^{m} \omega(|\xi|) \xi_{yn} V_n \) and \( N^{(3)} = - \sum_{n=1}^{m} \omega(|\xi|) \xi_{zn} V_n \) for the first three columns and where the remaining triplicate columns correspond to the displacement component vector for point \( x_n \) in the horizon.
C Bibliography


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