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The Development of Peridynamics Through Bond-Associated Nonlocal Deformation
Gradient

by

Xuan Hu

A dissertation submitted in partial satisfaction of the
requirements for the degree of

Doctor of Philosophy

in

Civil and Environmental Engineering

in the

Graduate Division

of the

University of California, Berkeley

Committee in charge:

Professor Shaofan Li, Chair
Assistant Professor Ziqi Wang
Associate Professor Aditya Guntuboyina

Spring 2026

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Abstract

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Professor Shaofan Li, Chair

Peridynamics is a nonlocal reformulation of continuum mechanics aiming at modeling fracture and damage in solids. Unlike the finite element method which relies on a predefined mesh, peridynamics is established upon interactions among discrete material points within a given domain. There are two types of peridynamic formulations: bond-based and state-based. Bond-based peridynamics follows a “bottom-up” philosophy, where the bond-level mechanical interactions are determined first and their aggregated results emerge as the material behavior in macro-scale. In contrast, state-based peridynamics adopts a “top-down” approach where the macroscopic material response is first defined and subsequently distributed to bond-level interactions. This dissertation advances both formulations through new theoretical developments and practical engineering applications.

The foundation of this work is the establishment of a unified bond-associated nonlocal deformation gradient. Based on this, a nonlocal-deformation-field-driven bond-based peridynamics framework is introduced. Compared to conventional bond-based formulation, this novel formulation offers (1) consistent kinematic relations in meso- and macro-scales, (2) a more versatile family of pairwise bond potentials that account for both bond stretch and shear, and (3) clear and consistent connections between meso-scale bond behaviors and macro-scale material responses.

Furthermore, a unified framework of bond-associated state-based peridynamics is proposed. This framework employs the bond-associated nonlocal deformation gradient to construct nonlocal strain measure, which can be directly integrated into any constitutive models developed in continuum mechanics to obtain stress measures and hence force density state. Compared with conventional state-based formulation, the newly proposed approach eliminates the common issues of material instability or zero-energy mode systematically, while achieving the same accuracy in continuum mechanics problems as finite element method.

Both newly-developed formulations are rigorously examined for linear and angular momentum balance, as well as material frame-indifference (stress objectivity). A comprehensive set of numerical examples, from elasticity and nonlinear cohesive fracture to dynamic failure, demonstrates the effectiveness of the methods.

Overall, this work provides unified and robust frameworks for advanced bond-based and state-based peridynamic formulations, and it is intended to serve as a valuable reference for further development and application of peridynamics formulations in engineering problems.

Peridynamics; bond-associated formulation; nonlocal continuum mechanics; zero-energy mode; cohesive zone model.

DEDICATION

To my family, whose unwavering love and support made this journey possible.

Contents

Contents	ii
List of Figures	iv
List of Tables	vi
1 Introduction	1
1.1 Bond-based peridynamics	2
1.2 State-based peridynamics	3
1.3 definitions and notations	4
2 Bond-associated nonlocal deformation gradient	6
2.1 Overview	6
2.2 Conventional model	8
2.3 Sub-horizon-based model	9
2.4 Bond-correction-based model	10
2.5 Lagrange-multiplier-based model	11
2.6 Non-spherical-influence-function-based model	12
2.7 Summary	13
2.8 Validation on bond mapping	14
3 Nonlocal-deformation-field-driven bond-based models	17
3.1 Finite-strain-based bond kinematics	17
3.2 Bond force states, stress measures, and equilibrium	22
3.3 Constitutive Relations: Family of Bond Potentials	33
4 Bond-associated state-based material correspondence models	43
4.1 Bond force states	43
4.2 Momentum balance and objectivity	47
5 Numerical implementation	53
5.1 Formula discretization	53
5.2 Solver configuration	54

6	Numerical examples: bond-based model	57
6.1	Plate with a hole	57
6.2	Gypsum specimen with center flaw	59
6.3	The Kalthoff-Winkler problem	62
6.4	Energy competition mechanism	65
7	Numerical examples: state-based model	70
7.1	Elastic Deformation Prediction	71
7.2	Elastic Wave Propagation Modeling	75
7.3	Finite Elastoplastic Deformation Analysis	80
7.4	Linear elastic fracture analysis	84
8	Conclusions and future work	88
8.1	Conclusions	88
8.2	Future work	89
	Bibliography	91
A	Solutions of Four Integrals	99
A.1	Integrals in Two-Dimensional Case	99
A.2	Integrals in Three-Dimensional Case	102

List of Figures

1.1	The material point horizon, neighbor and bonds in Peridynamics.	4
2.1	The sub-horizon proposed in the literature for PD.	9
2.2	The particles' position before and after the applied deformation field.	15
3.1	Deformation of material fiber/material bond connecting two points in three formulations.	18
3.2	Schematic illustrations of shear deformation in continuum mechanics	19
3.3	relation between bond deformation and bond force density	24
3.4	Schematic diagram of the Xu-Needleman (XN) Model	39
3.5	Schematic diagram of Peierls-Rice-Beltz Model	41
6.1	Diagram of plate with a hole specimen	58
6.2	Stress distribution on the plate with a hole specimen	58
6.3	Convergence analysis on SVK1 model	59
6.4	Geometric configuration and mesh of a gypsum specimen with a center flaw	60
6.5	Crack pattern obtained from different models	61
6.6	Crack evolution on the gypsum specimen with center flaw	62
6.7	Stress fields on the gypsum specimen (a) stress component σ_{12} (b) stress component σ_{22}	63
6.8	Geometric configuration and mesh of a double notched steel plate	64
6.9	Crack propagation patterns caused by different energy release rates (unit: N/mm)	65
6.10	configuration of edge crack problem (a) Size of specimen and boundary conditions (b) BCC lattice structure in [001] plane (c) FCC lattice structure in [111] plane	66
6.11	Crack pattern and σ_{11} stress distribution in BCC lattice structure with (a) $\alpha_t/\alpha_n = 2$, $\gamma_s/\gamma_{us} = 197.39$ (b) $\alpha_t/\alpha_n = 1$, $\gamma_s/\gamma_{us} = 49.35$ (c) $\alpha_t/\alpha_n = 1/2$, $\gamma_s/\gamma_{us} = 12.34$ (d) $\alpha_t/\alpha_n = 1/3$, $\gamma_s/\gamma_{us} = 5.48$	67
6.12	Crack pattern and the von-Mises stress distribution in an FCC crystal with (a) $\alpha_t/\alpha_n = 1$, $\gamma_s/\gamma_{us} = 49.35$ (b) $\alpha_t/\alpha_n = 1/2$, $\gamma_s/\gamma_{us} = 12.34$ (c) $\alpha_t/\alpha_n = 1/4$, $\gamma_s/\gamma_{us} = 3.08$ (d) $\alpha_t/\alpha_n = 1/5$, $\gamma_s/\gamma_{us} = 1.97$	68
6.13	relation between materials' ductility and the ratio of γ_s/γ_{us}	69
7.1	Schematic diagram of elastic square plate with centered hole.	71

7.2	Comparison of prediction error and runtime among different formulations. . . .	72
7.3	Comparison of absolute error in predicted x -displacement for different models: (a) BHPD with $m' = 3$, (b) BCPD, (c) HPPD with $np = 4$, (d) LMPD with $\lambda = 1000$, (e) NSPD with $n_1 = n_2 = 10$, and (f) CPD.	73
7.4	Comparison of absolute error in predicted y -displacement for different models: (a) BHPD with $m' = 3$, (b) BCPD, (c) HPPD with $np = 4$, (d) LMPD with $\lambda = 1000$, (e) NSPD with $n_1 = n_2 = 10$, and (f) CPD.	74
7.5	Schematic diagram of elastic bar subjected to z-direction displacement load. . .	75
7.6	Time history of displacement u_z at the center point for various bond-associated models.	76
7.7	Summary and comparison of wave propagation predictions using various bond- associated models.	77
7.8	Time history of displacement u_z at the center point for various bond-associated models with unit influence function.	78
7.9	Summary and comparison of wave propagation predictions using various bond- associated models with unit influence function.	79
7.10	Schematic explanation for phase shift in sub-horizon-based models using variable spherical influence function.	80
7.11	Dog-bone shaped thin plate under uni-axial displacement loading and the finite element discretization using 33,340 Q4 elements.	81
7.12	Comparison of PD and FE results: displacement u_x , strain ϵ_{zz} and effective plastic strain $\bar{\epsilon}_p$ (top row: PD; bottom row: FE).	82
7.13	Comparison of PD and FE results: stresses σ_{xx} , σ_{xy} and σ_{yy} (top row: PD; bottom row: FE).	83
7.14	Comparison of PD and FE results: force-displacement curves of the bottom edge.	84
7.15	A single-edge-notch elastic plate under tension and uniform discretization using 10,174 material points.	85
7.16	Crack initiation and propagation for the single-edge-notch-tension problem. The length of crack is $l = 0.06, 0.26, 0.88$ and 1.40 respectively from left to right. . .	85
7.17	Stress distribution during the crack propagation process. The length of crack is $l = 0.06, 0.26, 0.88$ and 1.40 respectively from left to right.	87
7.18	Distribution of σ_{xx} , σ_{xy} and σ_{yy} on a circle around crack tip with various crack length l	87
A.1	geometric relation of material points within two-dimensional horizon	100
A.2	geometric relation of material points within three-dimensional horizon	103

List of Tables

2.1	Average relative errors of nonlocal deformation gradients in mapping bonds under given deformation. (np - number of uniform partitions, starting with the x -axis in counter-clockwise manner; The sign '-' indicates no error measure was calculated for such case.)	16
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Chapter 1

Introduction

Peridynamics is a nonlocal continuum mechanics theory designed to overcome key limitations of classical local theory, particularly in modeling spatial discontinuities and capturing material behavior across different dimensions [75, 72, 4, 5, 13, 9]. The development of peridynamics began with the seminal work by Silling [75], who reformulated elastic mechanics to incorporate discontinuities through pairwise bond-based interactions among material points within a finite region. This formulation, now referred to as bond-based peridynamics (BB-PD), follows a “bottom-up” philosophy. It begins with the local bond kinematics, primarily bond stretch. Then the force state or force density is derived from meso-scale pairwise potential energy functions. Following this, Noll’s Lemma and “homogenization procedure” is used to obtain the materials’ response at macro-scale. This makes the bond-based formulation a two-scale approach [37].

Subsequent developments led to the introduction of state-based peridynamics (SB-PD) [72], where material point behavior is characterized through generalized “states” rather than simple pairwise interactions. Among various SB-PD formulations, the material correspondence formulation within non-ordinary-state-based peridynamics is widely used. This approach enables directly transplant of constitutive models from classical continuum mechanics to the nonlocal peridynamics framework. In material correspondence formulation, the nonlocal deformation state of the center particle is first evaluated by considering the relative displacements of all particles nearby. Afterwards, the stress state of each particle is derived through the classical stress-strain constitutive models. In the end, the force state at bond-level can be determined. This formulation embodies a “top-down” methodology because it first computes the macro-scale material response and then determine the meso-scale force state at bond level subsequently.

This chapter begins by a detailed presentation of BB-PD and SB-PD, highlighting their respective strengths and limitations. It then provides the shared notations and foundational concepts for both formulations.

1.1 Bond-based peridynamics

In BB-PD, the pairwise potential energy function plays an important role, as it determines the bond interactions and consequently the material mechanical responses. For now, only a few bond potential energy functions have been reported in literature [73, 26, 93]. In 2000, Silling [73] first proposed a prototype micro-brittle (PMB) model. In PMB model, the force state is directly proportional to the axial stretch of the bond, and the bond breaks when the stretch surpasses a critical value. Despite its simplicity, this spring-like bond potential model is able to capture a certain range of linear elastic and fracturing response of both homogeneous and heterogeneous materials [83]. However, there is a gap between the measurement of one-dimensional bond interactions by PMB model and continuum mechanics stress measure. Furthermore, it has notable limitations on characterizing material properties. For instance, the Poisson's ratio in isotropic linear elastic material obtained by PMB model is fixed at $1/3$ for plane stress case, and $1/4$ for plane strain and three-dimensional case. Such drawbacks are due to the fact that the PMB model only considers the deformation of bonds analogues to that of structural trusses, while neglecting other possible bond deformation states, such as shear deformation. From a microscopic perspective, shear deformation arises from the collective interaction among three or more atoms (See [53]). At the macroscopic scale, shear deformation is essential for accurately modeling ductile fracture behavior in materials. To account for the shear deformation at bond level, many attempts have been made under BB-PD framework:

1. The micropolar peridynamics e.g. [28, 19, 21, 96, 82], in which an extra balance of momentum integral equation is needed to solve rotational deformation degree,
2. The so-called extended bond-based peridynamics (XBB-PD) e.g. [85, 98]. In XBB-PD, both stretch and the rotation of bond are considered. As a result, unlike conventional bond-based peridynamics, the force density of XBB-PD comprises two components that correspond to the two deformation states of a bond, respectively. However, the method is mainly formulated for infinitesimal deformation, and it is mainly used for brittle fracture simulations. Besides, the resulting nonlocal continuum mechanics has not been established nor discussed, and
3. The cohesive peridynamics, e.g. [34, 37, 33, 58], which makes use of a series of cohesive continuum models developed in 1980s such as the Xu-Needleman model, the Beltz-Rice model. In the cohesive bond-based peridynamics, the specific bond kinematics assumptions are assumed in order to satisfy the objectivity requirement. However, the correspondence of macro-scale deformation state and the meso-scale deformation state has not been established. Thus the zero-energy mode issue is not completely resolved.

It may be noted that Li et al. [51] proved that the peridynamics stress is the static first Piola-Kirchhoff virial stress. Nevertheless, the nonlocal first Piola-Kirchhoff stress does not immediately lead to material objectivity.

In summary, three primary challenges persist in the current BB-PD research:

1. the lack of a consistent methodology that can seamlessly connect bond-level deformation with continuum strain measure,
2. the existence of zero-energy modes induced by the current nonlocal deformation measures, and
3. the lack of the direct link between bond-level potential and material level strain energy density, as well as the bond force states and nonlocal continuum stress measures.

To address these issues, in this work we developed a generic nonlocal-deformation-field-driven bond-based peridynamics (NDFD BB-PD) formulation that utilizes Green-Lagrange strain. The primary goal of this formulation is to integrate the principles of finite deformation theory from continuum mechanics into bond-based peridynamics, enabling a more comprehensive understanding and modeling of material deformation at the bond level. Different from the conventional bond-based peridynamics, the bond-associated nonlocal deformation field, which has been proved accurate in representing bond deformation [14, 15], is used as the primary deformation measure at bond level, and the bond kinematics, which includes both stretch and shear components, is then determined accordingly. By utilizing the nonlocal strain energy density functions, the formulation simplifies the derivation of stress measures, which is theoretically consistent with the force states obtained from pairwise potentials. This straightforward derivation is crucial as it facilitates the easy establishment of the correspondence model, which links the peridynamics framework with classical continuum mechanics. This integration potentially enhances the predictive capabilities of peridynamics, especially in scenarios involving large deformations and complex material behaviors.

1.2 State-based peridynamics

The SB-PD, specifically the correspondence formulation, has been successfully used in simulating linear elastic, elastoplastic, viscoplastic and fracturing behaviors of materials [76, 65, 2, 46, 45]. However, the material correspondence formulation is not without challenges. One well-known issue of the formulation is the existence of material instability or zero-energy modes manifested in the form of oscillations in the predicted displacement field. These modes arise when certain deformation states do not contribute to the strain energy, leading to non-physical solutions and numerical instabilities. This material instability can be traced back to the non-injective relationship between the nonlocal deformation gradient state and the bond force state. Many stabilization schemes have been proposed to address this issue, including fictitious spring-force based methods and stabilized field state based methods [92, 52, 88, 59, 50]. Among existing strategies proposed in the literature to address this issue, the bond-associated formulations are the most effective and provide more accurate accounting of bond-level quantities such as deformation gradient and stresses. Since the pioneering work done by Chowdhury et al. [18] and Chen et al. [12, 17], numerous theoretical investigations [14, 15, 30, 81], as well as engineering applications [31, 89, 94] have been carried

out using bond-associated formulations. A state-of-the-art review on various stabilization techniques for the material correspondence formulation can be found in Ref. [57].

Although different bond-associated approaches were proposed independently, a detailed examination of these bond-associated formulations finds that a unified framework is shared among them. It is one of the goals of this paper to present a unified framework for bond-associated state-based peridynamics material correspondence models and examine the physical properties of the framework. This framework will not only address the zero-energy modes issue but also enhance the model's capability to accurately represent the deformation state at the bond level, thus paving the way for more robust and flexible peridynamics simulations.

1.3 definitions and notations

In peridynamics, the geometric domain of interest in the reference configuration $\mathcal{B}_0$ is modeled as an assembly of material points with volume. For a material point $\mathbf{X}$, it interacts with its neighboring material points located within a Euclidean distance δ , known as *horizon*, through nonlocal interactions via bonds. The point within the horizon is called *neighbor*, and the collection of all neighbors is referred to as *neighborhood*, denoted as $\mathcal{H}$. The *relative position in reference configuration* $\mathcal{B}_0$ between a material point $\mathbf{X}$ and its neighbor $\mathbf{X}'$ is a bond as $\boldsymbol{\xi} = \mathbf{X}' - \mathbf{X}$. Let $\mathbf{y}(\mathbf{X}, t)$ represents a new position of the material point $\mathbf{X}$ in the current configuration $\mathcal{B}_t$, with time $t \geq 0$, $\mathbf{y} = \mathbf{X} + \mathbf{u}$ where $\mathbf{u}$ is the displacements. The *relative position in current configuration* $\mathcal{B}_t$ between two neighboring points is $\boldsymbol{\zeta} = \mathbf{y}'(\mathbf{X}', t) - \mathbf{y}(\mathbf{X}, t)$. See Fig. 1.1 for reference of material point horizon and neighbor and bonds between material points.

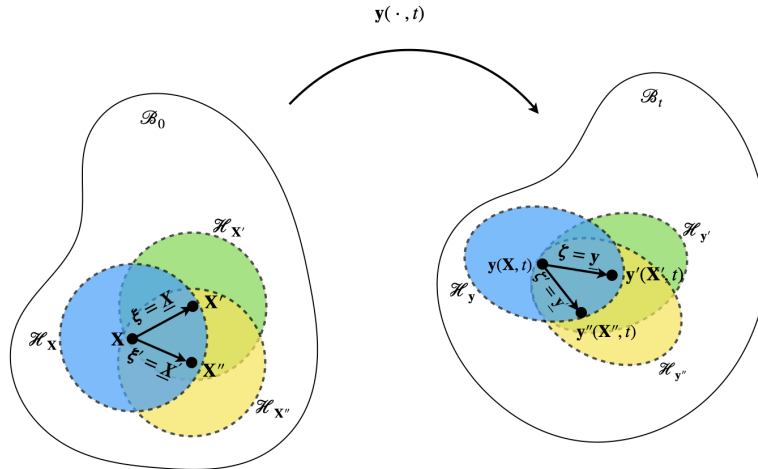


Figure 1.1: The material point horizon, neighbor and bonds in Peridynamics.

The development of the peridynamic formulation employs the concept of state [72]. A

state of order m is a function $\underline{\mathbf{A}}\langle\bullet\rangle : \mathcal{H} \rightarrow \mathcal{L}_m$, which maps a vector in the neighborhood $\mathcal{H}$ to the tensor space $\mathcal{L}_m$ of order m . For instance, if $m = 0$, a bond is mapped to a scalar space $\mathcal{L}_0$, and this is referred to as a scalar state. Scalar states are usually written in lowercase with an underscore, such as $\omega\langle\boldsymbol{\xi}\rangle$. If $m = 1$, a bond is mapped to a vector space $\mathcal{L}_1$, and the state is called vector state. Vector states and other states of order $m \geq 1$ are conventionally written in uppercase boldface with an underscore, such as $\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle$ and $\underline{\mathbf{A}}\langle\boldsymbol{\xi}\rangle$. According to this definition, a state can be readily identified that maps the initial bond vector $\boldsymbol{\xi}$ to the current bond vector $\boldsymbol{\zeta}$. This is termed the *deformed state* and denoted by $\underline{\mathbf{y}}\langle\boldsymbol{\xi}\rangle$. For a bond connecting a material point $\mathbf{X}$ and one of its neighbors at any time t , the deformed state is $\underline{\mathbf{y}}[\mathbf{X}, t]\langle\boldsymbol{\xi}\rangle = \mathbf{y}'(\mathbf{X}', t) - \mathbf{y}(\mathbf{X}, t) = \boldsymbol{\zeta}$. For clarity, square brackets are introduced to indicate the spatial and/or temporal information on which a state depends, e.g., $[\mathbf{X}, t]$, while parentheses are adopted to denote all other quantities that the state depends on, e.g., $(\boldsymbol{\xi}, \boldsymbol{\xi}')$. In addition, the standard convention in the classical continuum mechanics theory is followed in this paper. Variables with uppercase subscripts, such as X_I , refer to the components defined in the reference configuration $\mathcal{B}_0$ while the ones with lowercase subscripts, such as y_j denote the components in the current configuration $\mathcal{B}_t$. Einstein summation notation is also employed here to facilitate the representation of complex tensor operations. Boldface letter indicates a vector or a tensor.

The rest of the dissertation is organized as follows: Chapter 2 provides an introduction to the bond-associated nonlocal deformation gradient, which serves as the foundation for the subsequent developments. Chapter 3 presents the formulation of nonlocal-deformation-field-driven bond-based models, while Chapter 4 introduces the bond-associated state-based material correspondence models. Both Chapter 3 and 4 include detailed derivations of the bond force states, verification of momentum balance, and demonstration of the stress measure objectivity. Chapter 6 and 7 offer the numerical examples corresponding to the bond-based and state-based models, respectively. Finally, the dissertation concludes with a summary of key findings and discussions in the conclusion chapter.

Chapter 2

Bond-associated nonlocal deformation gradient

2.1 Overview

The conventional nonlocal deformation gradient is obtained based on the concept of multi-variable linear regression and least square estimation. For each material point, a loss function is constructed,

$$\mathcal{L}(\mathbf{X}) = \int_{\mathcal{H}} \underline{\omega}(\underline{\xi}') [\mathbf{F}\underline{\xi}' - \underline{\mathbf{y}}']^T \cdot [\mathbf{F}\underline{\xi}' - \underline{\mathbf{y}}'] dV_{\mathbf{X}''} \quad (2.1)$$

where $\underline{\omega}(\underline{\xi}')$ is a influence function. By taking derivative with respect to deformation gradient, the optimum $\mathbf{F}$ that minimizes the loss function given in Eq. (2.1) can be achieved, which is denoted as $\mathbf{F}_{\mathbf{X}}$. The explicit expression of $\mathbf{F}_{\mathbf{X}}$ writes

$$\mathbf{F}_{\mathbf{X}} = \left[\int_{\mathcal{H}} \underline{\omega}(\underline{\xi}') \underline{\mathbf{y}}' \otimes \underline{\xi}' dV_{\mathbf{X}''} \right] \cdot \mathbf{K}^{-1} \quad (2.2)$$

where $\mathbf{K}$ is a second order tensor and can be computed as follows,

$$\mathbf{K} = \int_{\mathcal{H}} \underline{\omega}(\underline{\xi}') \underline{\xi}' \otimes \underline{\xi}' dV_{\mathbf{X}''} . \quad (2.3)$$

It should be noted that the loss function formulated with radial step influence function treats each data point equally important. Therefore, even though the loss or error is minimized, it cannot characterize the deformation on each single bond precisely, provided the deformation map is not uniform or there are some noises within the horizon. Consequently, there might exist two deformation states that produce the same nonlocal deformation gradient $\mathbf{F}_{\mathbf{X}}$, which is the root of the zero-energy mode issue.

Regarding this, The bond-associated deformation gradient was first introduced by Chen and coworkers [12, 17, 11, 10]. In this formulation, a bond-associated deformation gradient

is constructed for each bond within the horizon based on a subset of the horizon. In general, each bond has its own unique subset, and when the subset takes the whole horizon, the conventional nonlocal deformation gradient model is recovered. Chowdhury et al. [18] proposed to partition the horizon into sub-horizons and construction of the nonlocal deformation gradient is limited to each sub-horizon. Within each sub-horizon, the same nonlocal deformation gradient is used for all bonds within that sub-horizon. Although these two formulations differ slightly, the core idea is to use a subset of the horizon that includes the target bond to characterize the bond deformation and compute the bond-associated deformation gradient. The formulation proposed by Chowdhury et al. can be considered as a special case of the formulation proposed by Chen. Breitzman and Dayal [7] proposed a bond-level deformation gradient by firstly removing the contribution due to the uniform deformation assumption within the horizon using deformation mapping and replacing it with the actual bond deformation. Hou and Zhang [36] developed the so-called bond-augmented deformation gradient, where a penalty term related to a given bond and its deformed state is introduced during the minimization of the least squares error to formulate the nonlocal deformation gradient [12]. In these two studies, the nonlocal deformation gradients are still constructed based on the whole horizon, but they are modified to be bond-specific either through replacement [7] or penalization [36]. Bond-associated deformation gradients can also be obtained using non-spherical influence function. Chen et al. [14, 15] proposed a family of non-spherical influence function and developed the corresponding material correspondence model to improve the accuracy of bond-level quantities such as deformation gradient and stress. Unlike the conventional formulation, where the influence function is spherical and depends only on the bond length, the proposed non-spherical influence functions take into account both the bond length and the bond relative angle (with respect to a target bond). All these bond-associated correspondence models have achieved great success in inherently eliminating the material instability in the conventional formulation.

In this chapter, a unified formula for the bond-associated nonlocal deformation gradient is developed based on the multivariable linear regression and conventional formula presented in Eq. (2.2). The realization of this unified formula for each specific case is discussed in details. For a given bond $\boldsymbol{\xi}$, the generalized bond-associated deformation gradient has the following expression as

$$\mathbf{F}_{\boldsymbol{\xi}} = \left[\int_{\mathcal{H}_{\boldsymbol{\xi}}} \underline{\omega}(\boldsymbol{\xi}') \underline{\mathbf{y}}' \otimes \boldsymbol{\xi}' dV_{\mathbf{X}''} \right] \mathbf{K}_{\boldsymbol{\xi}}^{-1} \underline{\mathbf{A}}(\boldsymbol{\xi}) + \underline{\mathbf{B}}(\boldsymbol{\xi}) \quad (2.4)$$

with

$$\mathbf{K}_{\boldsymbol{\xi}} = \int_{\mathcal{H}_{\boldsymbol{\xi}}} \underline{\omega}(\boldsymbol{\xi}') \boldsymbol{\xi}' \otimes \boldsymbol{\xi}' dV_{\mathbf{X}''}, \quad (2.5)$$

where the subscript ξ indicates that the quantities are associated with the bond ξ , ξ' is an arbitrary bond within the horizon of bond ξ , i.e., $\mathcal{H}_\xi$, $\underline{\omega}$ is a state-valued influence function, $\underline{\mathbf{y}}'$ denotes the deformed state of bond ξ' , and $\otimes$ indicates tensor product. This generalized formula can be adapted into various forms proposed in the literature by specifying $\mathcal{H}_\xi$, $\underline{\omega}(\xi')$, $\underline{\mathbf{A}}(\xi)$ and $\underline{\mathbf{B}}(\xi)$.

2.2 Conventional model

In the conventional correspondence model proposed by Silling et al. [72], the nonlocal deformation gradient can be obtained from Eq. (2.4) by choosing material point horizon as the bond horizon, adopting a spherical influence function that depends solely on bond length $|\xi|$, and taking state $\underline{\mathbf{A}}(\xi)$ as the rank-two identity tensor and the state $\underline{\mathbf{B}}(\xi)$ as the null tensor, i.e.,

$$\mathcal{H}_\xi \Rightarrow \mathcal{H}, \quad \underline{\omega}(\xi') \Rightarrow \underline{\omega}^{\text{CPD}}(|\xi'|)\langle \xi' \rangle, \quad \underline{\mathbf{A}}(\xi) \Rightarrow \mathbf{I}, \quad \underline{\mathbf{B}}(\xi) \Rightarrow \mathbf{0}. \quad (2.6)$$

where $\underline{\omega}^{\text{CPD}}(|\xi'|)\langle \xi' \rangle$ is a spherical influence function that depends solely on bond length $|\xi'|$. Two representative spherical influence functions used in peridynamics are given below,

$$\underline{\omega}^{\text{CPD}}(|\xi'|)\langle \xi' \rangle = \frac{\delta_{\mathcal{H}}}{|\xi'|} \quad (2.7)$$

and

$$\underline{\omega}^{\text{CPD}}(|\xi'|)\langle \xi' \rangle = c \quad (2.8)$$

where $\delta_{\mathcal{H}}$ refers to the radius of the neighborhood $\mathcal{H}$ and c stands for constant number.

Therefore, the conventional nonlocal deformation gradient has the following expression

$$\mathbf{F}^{\text{CPD}} = \left[\int_{\mathcal{H}} \underline{\omega}^{\text{CPD}}(|\xi'|)\langle \xi' \rangle \underline{\mathbf{y}}' \otimes \xi' dV_{\mathbf{x}''} \right] (\mathbf{K}^{\text{CPD}})^{-1} \quad (2.9)$$

with $\mathbf{K}^{\text{CPD}}$ being

$$\mathbf{K}^{\text{CPD}} = \int_{\mathcal{H}} \underline{\omega}^{\text{CPD}}(|\xi'|)\langle \xi' \rangle \xi' \otimes \xi' dV_{\mathbf{x}''} \quad (2.10)$$

It should be noted that the nonlocal deformation gradient $\mathbf{F}^{\text{CPD}}$ remains the same for all bonds within the same horizon. As has been pointed out in the literature [12, 18], the mapping between the conventional nonlocal deformation gradients, by extension the bond force density states, and the bond deformation states is non-injective. This implies that a nonlocal deformation gradient computed by Eq. (2.9) can correspond to more than one deformation state within a given horizon. As a result, there exist non-zero bond deformation states that rise zero energy to the system, i.e., existence of zero-energy modes in the solution.

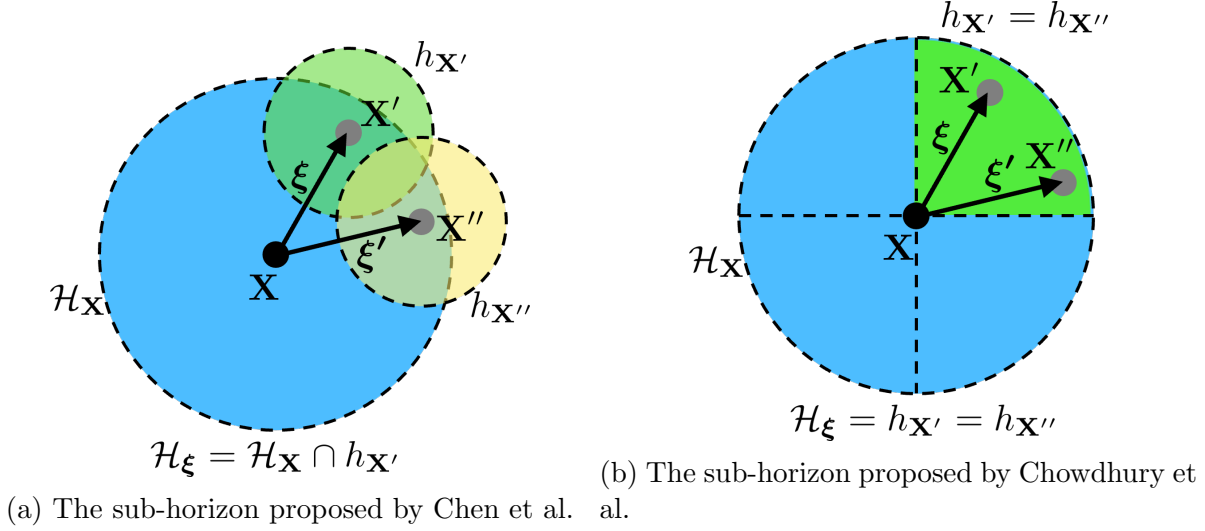


Figure 2.1: The sub-horizon proposed in the literature for PD.

2.3 Sub-horizon-based model

To address the issue of zero-energy modes in the conventional model, Chen et al. [12, 17, 11, 10] and Chowdhury et al. [18] proposed the sub-horizon-based stabilization approach. Despite the slight difference, the key idea behind their models is the same and to use a subset of horizon that includes the bond ξ to characterize its deformation and compute the bond-associated deformation gradient. In comparison with the conventional model, the influence function, state $\underline{\mathbf{A}}\langle\xi\rangle$ and state $\underline{\mathbf{B}}\langle\xi\rangle$ remain unchanged. The only modification is that the integration domain of the nonlocal deformation gradient is changed from the full horizon $\mathcal{H}$ to a sub-horizon $\mathcal{H}_\xi$. The two sub-horizons proposed by Chen et al. and Chowdhury et al. are shown in Fig. 2.1. In the model proposed by Chen et al. (BHPD), a bond-associated horizon $h_{\mathbf{X}'}$ was introduced for neighbor $\mathbf{X}'$ and the sub-horizon for bond ξ is the intersection between $\mathcal{H}_{\mathbf{X}}$ and $h_{\mathbf{X}'}$, see Fig. 2.1(a). In Chen et al.'s model, each material point is associated with certain sub-horizon and there is no constraint on the shape or form of the bond-associated horizons. One general sub-horizon division scheme is presented in Fig. 2.1(a). While in the model proposed by Chowdhury et al. (HPPD), the sub-horizons are obtained by partitioning the material point horizon, see Fig. 2.1(b) for the case of even partition of material point horizon $\mathcal{H}_{\mathbf{X}}$ into four sub-horizons $\mathcal{H}_\xi$. If we allow certain material points to share the same sub-horizon, as shown for $\mathbf{X}'$ and $\mathbf{X}''$ in Fig. 2.1(b), then the formulation proposed by Chowdhury et al. can be considered as a special case of the formulation proposed by Chen et al..

For sub-horizon-based models, we have the following values for the influence function

$\underline{\omega}(\xi')$, the states $\underline{\mathbf{A}}(\xi')$ and $\underline{\mathbf{B}}(\xi')$:

$$\underline{\omega}(\xi') \Rightarrow \underline{\omega}(|\xi'|)\langle \xi' \rangle, \quad \underline{\mathbf{A}}(\xi) \Rightarrow \mathbf{I}, \quad \underline{\mathbf{B}}(\xi) \Rightarrow \mathbf{0} \quad (2.11)$$

Therefore, the bond-associated deformation gradient for the sub-horizon-based models has the following expression.

$$\mathbf{F}_\xi = \left[\int_{\mathcal{H}_\xi} \underline{\omega}(|\xi'|)\langle \xi' \rangle \underline{\mathbf{y}}' \otimes \xi' dV_{\mathbf{x}''} \right] \mathbf{K}_\xi^{-1} \quad (2.12)$$

with

$$\mathbf{K}_\xi = \int_{\mathcal{H}_\xi} \underline{\omega}(|\xi'|)\langle \xi' \rangle \xi' \otimes \xi' dV_{\mathbf{x}''}. \quad (2.13)$$

and $\mathcal{H}_\xi$ takes a different form for the BHPD model and the HPPD model, as illustrated in Fig. 2.1.

The above deformation gradient can be reformulated by changing the sub-horizon dependency from the integration domain to the influence function. To do so, the influence function for each sub-horizon is written as:

$$\underline{\omega}^{\text{SHPD}}(|\xi'|)\langle \xi' \rangle = \begin{cases} \underline{\omega}^{\text{CPD}}(|\xi'|)\langle \xi' \rangle, & \mathbf{x}'' \in \mathcal{H}_\xi \\ 0, & \text{otherwise.} \end{cases} \quad (2.14)$$

As a result, the bond-associated deformation gradient for the sub-horizon-based models has the following expression, with $\mathcal{H}_\xi \Rightarrow \mathcal{H}$ and $\underline{\omega}(|\xi'|)\langle \xi' \rangle \Rightarrow \underline{\omega}^{\text{SHPD}}(|\xi'|)\langle \xi' \rangle$,

$$\mathbf{F}_\xi^{\text{SHPD}} = \left[\int_{\mathcal{H}} \underline{\omega}^{\text{SHPD}}(|\xi'|)\langle \xi' \rangle \underline{\mathbf{y}}' \otimes \xi' dV_{\mathbf{x}''} \right] (\mathbf{K}_\xi^{\text{SHPD}})^{-1} \quad (2.15)$$

and

$$\mathbf{K}_\xi^{\text{SHPD}} = \int_{\mathcal{H}} \underline{\omega}^{\text{SHPD}}(|\xi'|)\langle \xi' \rangle \xi' \otimes \xi' dV_{\mathbf{x}''}. \quad (2.16)$$

2.4 Bond-correction-based model

Breitzman and Dayal [7] proposed a bond-level deformation gradient by correcting the average deformation gradient for the entire horizon. The correction process is performed by first removing the contribution due to the assumption of uniform deformation on a bond ξ through the use of a removal tensor and then replacing it with the actual deformation. In this approach, the influence function remains a spherical state-valued function, while the state

$\underline{\mathbf{A}}(\boldsymbol{\xi})$ and state $\underline{\mathbf{B}}(\boldsymbol{\xi})$ take the value of the removal tensor and actual deformation tensor, respectively, i.e.,

$$\mathcal{H}_{\boldsymbol{\xi}} \Rightarrow \mathcal{H}, \quad \underline{\omega}(\boldsymbol{\xi}') \Rightarrow \underline{\omega}^{\text{CPD}}(|\boldsymbol{\xi}'|)\langle \boldsymbol{\xi}' \rangle, \quad \underline{\mathbf{A}}(\boldsymbol{\xi}) \Rightarrow \mathbf{I} - \frac{\boldsymbol{\xi} \otimes \boldsymbol{\xi}}{|\boldsymbol{\xi}|^2}, \quad \underline{\mathbf{B}}(\boldsymbol{\xi}) \Rightarrow \frac{\underline{\mathbf{y}} \otimes \boldsymbol{\xi}}{|\boldsymbol{\xi}|^2}. \quad (2.17)$$

Hence, the expression for this bond-associated deformation gradient is

$$\mathbf{F}_{\boldsymbol{\xi}}^{\text{BCPD}} = \left[\int_{\mathcal{H}} \underline{\omega}^{\text{CPD}}(|\boldsymbol{\xi}'|)\langle \boldsymbol{\xi}' \rangle \underline{\mathbf{y}}' \otimes \boldsymbol{\xi}' dV_{\mathbf{x}''} \right] (\mathbf{K}_{\boldsymbol{\xi}}^{\text{CPD}})^{-1} \left(\mathbf{I} - \frac{\boldsymbol{\xi} \otimes \boldsymbol{\xi}}{|\boldsymbol{\xi}|^2} \right) + \frac{\underline{\mathbf{y}} \otimes \boldsymbol{\xi}}{|\boldsymbol{\xi}|^2} \quad (2.18)$$

with $\mathbf{K}_{\boldsymbol{\xi}}^{\text{CPD}}$ given in Eq. (2.10) and integrated over the entire material point horizon $\mathcal{H}$.

This model not only eliminates non-physical deformations such as interpenetration and material instability issues, but also accurately represents both the average deformation within one neighborhood and the stretch of specific bond [7].

2.5 Lagrange-multiplier-based model

Hou and Zhang [36] constructed a so-called bond-augmented deformation gradient to stabilize the conventional material correspondence model. Similarly to the Lagrange multiplier method, a penalty term related to bond $\boldsymbol{\xi}$ and its deformed state $\underline{\mathbf{y}}(\boldsymbol{\xi})$ is introduced during the minimization of the least squares error. In this approach, the state $\underline{\mathbf{A}}(\boldsymbol{\xi})$ and $\underline{\mathbf{B}}(\boldsymbol{\xi})$, as well as the bond horizon $\mathcal{H}_{\boldsymbol{\xi}}$, becomes

$$\begin{aligned} \mathcal{H}_{\boldsymbol{\xi}} &\Rightarrow \mathcal{H} \setminus \boldsymbol{\xi}, \quad \underline{\omega}(\boldsymbol{\xi}') \Rightarrow \underline{\omega}^{\text{CPD}}(|\boldsymbol{\xi}'|)\langle \boldsymbol{\xi}' \rangle, \quad \underline{\mathbf{A}}(\boldsymbol{\xi}) \Rightarrow \mathbf{I}, \\ \underline{\mathbf{B}}(\boldsymbol{\xi}) &\Rightarrow \lambda \int_{\mathcal{H}} (\hat{\delta}[\boldsymbol{\xi}' - \boldsymbol{\xi}] \underline{\omega}^{\text{CPD}}(|\boldsymbol{\xi}'|)\langle \boldsymbol{\xi}' \rangle \underline{\mathbf{y}}' \otimes \boldsymbol{\xi}') \cdot \mathbf{K}_{\boldsymbol{\xi}}^{-1} dV_{\mathbf{x}''}, \end{aligned} \quad (2.19)$$

where operator $\setminus$ indicates exclusion, λ is a penalty factor, and $\hat{\delta}[\cdot]$ is the Dirac delta function that $\hat{\delta} = 1$ when $\boldsymbol{\xi}' = \boldsymbol{\xi}$ and $\hat{\delta} = 0$ otherwise. As a result, the bond-associated deformation gradient $\mathbf{F}_{\boldsymbol{\xi}}$ and the shape tensor $\mathbf{K}_{\boldsymbol{\xi}}$ are transformed into the following expressions for the LMPD model.

$$\begin{aligned} \mathbf{F}_{\boldsymbol{\xi}}^{\text{LMPD}} &= \left[\int_{\mathcal{H} \setminus \boldsymbol{\xi}} \underline{\omega}^{\text{CPD}}(|\boldsymbol{\xi}'|)\langle \boldsymbol{\xi}' \rangle \underline{\mathbf{y}}' \otimes \boldsymbol{\xi}' dV_{\mathbf{x}''} \right] (\mathbf{K}_{\boldsymbol{\xi}}^{\text{LMPD}})^{-1} + \\ &\quad \lambda \int_{\mathcal{H}} (\hat{\delta}[\boldsymbol{\xi}' - \boldsymbol{\xi}] \underline{\omega}^{\text{CPD}}(|\boldsymbol{\xi}'|)\langle \boldsymbol{\xi}' \rangle \underline{\mathbf{y}}' \otimes \boldsymbol{\xi}') \cdot (\mathbf{K}_{\boldsymbol{\xi}}^{\text{LMPD}})^{-1} dV_{\mathbf{x}''} \end{aligned} \quad (2.20)$$

and

$$\begin{aligned} \mathbf{K}_{\boldsymbol{\xi}}^{\text{LMPD}} &= \int_{\mathcal{H} \setminus \boldsymbol{\xi}} \underline{\omega}^{\text{CPD}}(|\boldsymbol{\xi}'|)\langle \boldsymbol{\xi}' \rangle \boldsymbol{\xi}' \otimes \boldsymbol{\xi}' dV_{\mathbf{x}''} + \\ &\quad \lambda \int_{\mathcal{H}} \hat{\delta}[\boldsymbol{\xi}' - \boldsymbol{\xi}] \underline{\omega}^{\text{CPD}}(|\boldsymbol{\xi}'|)\langle \boldsymbol{\xi}' \rangle \boldsymbol{\xi}' \otimes \boldsymbol{\xi}' dV_{\mathbf{x}''}. \end{aligned} \quad (2.21)$$

It is evident that the difference between the mapped bond, as product of $\mathbf{F}_\xi^{\text{LMPD}}$ and ξ , and the bond in the deformed configuration $\underline{\mathbf{y}}\langle\xi\rangle$ decreases as the penalty factor λ increases. However, an extremely large λ may result in a singular shape tensor leading to numerical error. Therefore, in practice, a reasonably large penalty factor should be chosen. Hou and Zhang [36] recommended a value of 10,000.

In the model proposed by Hou and Zhang [36], the penalty term together with the penalty factor is explicitly expressed in Eqs. (2.20) and (2.21) using the Dirac delta function. However, it is more convenient to incorporate the penalty term into the influence function and reformulate the expression given above for the deformation gradient and the shape tensor. To this end, after absorbing the penalty factor, the influence function can be written as

$$\underline{\omega}^{\text{LMPD}}(|\xi'|)\langle\xi'\rangle = \begin{cases} \lambda \underline{\omega}^{\text{CPD}}(|\xi'|)\langle\xi'\rangle, & \xi' = \xi \\ \underline{\omega}^{\text{CPD}}(|\xi'|)\langle\xi'\rangle, & \xi' \neq \xi \end{cases}. \quad (2.22)$$

Therefore, the nonlocal deformation gradient in the LMPD model can be alternatively expressed as

$$\mathbf{F}_\xi^{\text{LMPD}} = \left[\int_{\mathcal{H}} \underline{\omega}^{\text{LMPD}}(|\xi'|)\langle\xi'\rangle \underline{\mathbf{y}}' \otimes \xi' dV_{\mathbf{x}''} \right] (\mathbf{K}_\xi^{\text{LMPD}})^{-1} \quad (2.23)$$

with

$$\mathbf{K}_\xi^{\text{LMPD}} = \int_{\mathcal{H}} \underline{\omega}^{\text{LMPD}}(|\xi'|)\langle\xi'\rangle \xi' \otimes \xi' dV_{\mathbf{x}''}. \quad (2.24)$$

2.6 Non-spherical-influence-function-based model

Chen et al. [14, 15] proposed a bond-associated deformation gradient by using non-spherical influence function. In contrast to the spherical influence function that depends only on the bond length, the non-spherical influence function depends on both the bond length and the relative angle between the bond of interest ξ and any other bonds ξ' within the horizon. This type of bond-associated model can be obtained from Eq. (2.4) by using non-spherical influence functions and setting $\underline{\mathbf{A}}\langle\xi\rangle$ and $\underline{\mathbf{B}}\langle\xi\rangle$ as $\mathbf{I}$ and $\mathbf{0}$ respectively, i.e.,

$$\mathcal{H}_\xi \Rightarrow \mathcal{H}, \quad \underline{\omega}\langle\xi'\rangle \Rightarrow \underline{\omega}^{\text{NSPD}}(\xi, \xi')\langle\xi'\rangle, \quad \underline{\mathbf{A}}\langle\xi\rangle \Rightarrow \mathbf{I}, \quad \underline{\mathbf{B}}\langle\xi\rangle \Rightarrow \mathbf{0}. \quad (2.25)$$

The non-spherical influence function proposed by Chen et al. [14, 15] has the following form as

$$\underline{\omega}^{\text{NSPD}}(\xi, \xi')\langle\xi'\rangle = \exp\left(-n_1 \frac{\|\xi\| - \|\xi'\|}{\delta_{\mathcal{H}}}\right) \left(\frac{1}{2} + \frac{1}{2} \cos(\widehat{\xi\xi'})\right)^{n_2}, \quad (2.26)$$

where $\exp(\cdot)$ is the exponential function, $n_1 > 0$ and $n_2 > 0$ are control parameters that can be used to control the weights of different bonds within the same horizon on the current bond,

and the operator $\widehat{\cdot}$ indicates the angle between two bonds. Chen et al. [15] recommended a value of 8 for both control parameters.

In addition, Hu and Li [38] proposed an alternative form of the non-spherical influence function in their study, which is given as

$$\underline{\omega}^{\text{NSPD}}(\boldsymbol{\xi}, \boldsymbol{\xi}') \langle \boldsymbol{\xi}' \rangle = \exp \left(-n_1 \frac{|\boldsymbol{\xi} - \boldsymbol{\xi}'|^2}{\delta_{\mathcal{H}}^2} \right). \quad (2.27)$$

In contrast to the function proposed by Chen et al. [14, 15] (Eq. (2.26)), which separately considers the influence of bond length and angle, the function proposed by Hu and Li [38] (Eq. (2.27)) combines such information through a single term $\boldsymbol{\xi} - \boldsymbol{\xi}'$. Nevertheless, both functions consider both bond length and angle, and hence lead to the same effect. In the numerical study of this work, only the function in Eq. (2.26) will be used.

The bond-associated deformation gradient using the non-spherical influence function shares the same expressions as the Lagrange-multiplier-based model, i.e., Eqs. (2.23) and (2.24), but with the influence function given in Eq. (2.26). Even though the Lagrange-multiplier-based model and the non-spherical-influence-function-based model originate from different perspectives, they share one common feature: the influence function assigns varying weights to different bonds within the horizon when computing bond-level deformation gradient for one specific bond. In the Lagrange-multiplier-based model, a higher weight for the bond of interest is explicitly provided by the singular penalty factor whereas in the non-spherical-influence-function-based model, this is achieved through a smooth continuous function.

2.7 Summary

In summary, the specific expressions of the above discussed nonlocal deformation gradients are listed as follows:

$$\begin{aligned}
 \text{CPD} : \mathbf{F}^{\text{CPD}} &= \left[\int_{\mathcal{H}} \underline{\omega}^{\text{CPD}} \underline{\mathbf{y}}' \otimes \underline{\boldsymbol{\xi}}' dV_{\mathbf{x}''} \right] (\mathbf{K}^{\text{CPD}})^{-1}, \mathbf{K}^{\text{CPD}} = \int_{\mathcal{H}} \underline{\omega}^{\text{CPD}} \underline{\boldsymbol{\xi}}' \otimes \underline{\boldsymbol{\xi}}' dV_{\mathbf{x}''} \\
 \text{SHPD} : \mathbf{F}_{\boldsymbol{\xi}}^{\text{SHPD}} &= \left[\int_{\mathcal{H}} \underline{\omega}^{\text{SHPD}} \underline{\mathbf{y}}' \otimes \underline{\boldsymbol{\xi}}' dV_{\mathbf{x}''} \right] (\mathbf{K}_{\boldsymbol{\xi}}^{\text{SHPD}})^{-1}, \mathbf{K}_{\boldsymbol{\xi}}^{\text{SHPD}} = \int_{\mathcal{H}} \underline{\omega}^{\text{SHPD}} \underline{\boldsymbol{\xi}}' \otimes \underline{\boldsymbol{\xi}}' dV_{\mathbf{x}''} \\
 \text{BCPD} : \mathbf{F}_{\boldsymbol{\xi}}^{\text{BCPD}} &= \left[\int_{\mathcal{H}} \underline{\omega}^{\text{CPD}} \underline{\mathbf{y}}' \otimes \underline{\boldsymbol{\xi}}' dV_{\mathbf{x}''} \right] (\mathbf{K}^{\text{CPD}})^{-1} \left(\mathbf{I} - \frac{\underline{\boldsymbol{\xi}} \otimes \underline{\boldsymbol{\xi}}}{|\underline{\boldsymbol{\xi}}|^2} \right) + \frac{\underline{\mathbf{y}} \otimes \underline{\boldsymbol{\xi}}}{|\underline{\boldsymbol{\xi}}|^2} \\
 \text{LMPD} : \mathbf{F}_{\boldsymbol{\xi}}^{\text{LMPD}} &= \left[\int_{\mathcal{H}} \underline{\omega}^{\text{LMPD}} \underline{\mathbf{y}}' \otimes \underline{\boldsymbol{\xi}}' dV_{\mathbf{x}''} \right] (\mathbf{K}_{\boldsymbol{\xi}}^{\text{LMPD}})^{-1}, \mathbf{K}_{\boldsymbol{\xi}}^{\text{LMPD}} = \int_{\mathcal{H}} \underline{\omega}^{\text{LMPD}} \underline{\boldsymbol{\xi}}' \otimes \underline{\boldsymbol{\xi}}' dV_{\mathbf{x}''} \\
 \text{NSPD} : \mathbf{F}_{\boldsymbol{\xi}}^{\text{NSPD}} &= \left[\int_{\mathcal{H}} \underline{\omega}^{\text{NSPD}} \underline{\mathbf{y}}' \otimes \underline{\boldsymbol{\xi}}' dV_{\mathbf{x}''} \right] (\mathbf{K}_{\boldsymbol{\xi}}^{\text{NSPD}})^{-1}, \mathbf{K}_{\boldsymbol{\xi}}^{\text{NSPD}} = \int_{\mathcal{H}} \underline{\omega}^{\text{NSPD}} \underline{\boldsymbol{\xi}}' \otimes \underline{\boldsymbol{\xi}}' dV_{\mathbf{x}''}.
 \end{aligned} \tag{2.28}$$

2.8 Validation on bond mapping

First, the accuracy of the nonlocal deformation gradients used in different bond-associated models in mapping bonds between two different configurations is studied and compared in this section. Similar study on the nonlocal deformation gradients for the CPD, the BHPD and the NSPD models has been conducted by Chen and Hu [14] using quadratic and cubic deformation fields. In this study, the following predefined nonlinear oscillating deformation field is applied to a two-dimensional simulation domain to investigate the bond mapping accuracy of all bond-associated deformation gradients.

$$\begin{cases} u_x = 0.5 \cos(X) \\ u_y = 0.5 \cos(Y) \end{cases} \tag{2.29}$$

Without loss of generality, regular discretization is used in this study. And the mesh spacing is $\Delta X = \Delta Y = 1.0$. Three different horizon sizes are studied, namely $\delta_{\mathcal{H}} = 2, 3, 4$. The particles' position before and after this given deformation field is shown in Fig. 2.2 for the case of $\delta_{\mathcal{H}} = 4$, with the arrows indicating the material point correspondence.

To measure the precision of the bond-associated deformation gradients in mapping bonds, the same error metric as used in Ref. [14] is adopted here. The relative error in mapping a single bond is defined as

$$\mathcal{E}_b = \frac{|\text{Proj}_{\boldsymbol{\zeta}_{ref}} \boldsymbol{\zeta}_{con} - |\boldsymbol{\zeta}_{ref}||}{|\boldsymbol{\zeta}_{ref}|} \tag{2.30}$$

where $\text{Proj}_{\boldsymbol{\zeta}_{ref}} \boldsymbol{\zeta}_{con}$ is the vector projection of bond $\boldsymbol{\zeta}_{con}$ that determined using constructed nonlocal deformation gradient onto reference bond $\boldsymbol{\zeta}_{ref}$. The bonds based on the applied deformation field are taken as the reference bonds.

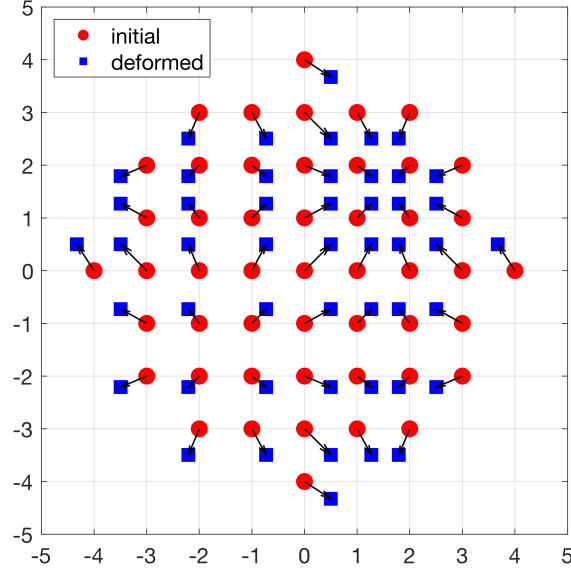


Figure 2.2: The particles' position before and after the applied deformation field.

Using this error metric, the total error of all bonds associated with a material point is calculated. Since a bond connects two material points, the total error of the same set of bonds is calculated using both deformation gradients based on the horizon of the material point $\mathbf{X}$ and those of all its neighbors $\mathbf{X}'$. The results for a material point located at $(X, Y) = (0, 0)$ are tabulated in Table 2.1. Four different values are chosen for the relevant model parameters to investigate their effects on the accuracy of mapping bonds using the corresponding deformation gradient.

As can be seen from the results presented in Table 2.1 for all the models investigated, the BCPD model predicts the exact bond mapping, as the measured error is zero. This can be explained by performing the mapping analytically as follows. Using index notation, the bond mapping operation using the nonlocal deformation gradient of the BCPD model can be performed as

$$\begin{aligned}
 F_{\xi, ij}^{\text{BCPD}} \xi_j &= F_{ik}^{\text{CPD}} (I_{kj} \xi_j - \xi_k \xi_j \xi_j / |\xi|^2) + \underline{y}_i \xi_j \xi_j / |\xi|^2 \\
 &= F_{ik}^{\text{CPD}} (\xi_k - \xi_k) + \underline{y}_i \\
 &= \underline{y}_i.
 \end{aligned} \tag{2.31}$$

Therefore, the BCPD model predicts exact bond mapping. However, as can be seen from Eq. (2.31), the average deformation gradient $\mathbf{F}^{\text{CPD}}$ does not play a role in the bond mapping, as it is canceled out after the first term on the right hand side of the BCPD deformation gradient multiplies bond ξ . The NSPD and LMPD models predict very accurate bond mapping, and the error decreases with increasing values of the relevant parameters for the influence functions. For HPPD, the prediction accuracy improves with increasing the number of partitions np . However, the number of allowed partitions is limited by the number of sufficient

Table 2.1: Average relative errors of nonlocal deformation gradients in mapping bonds under given deformation. (np - number of uniform partitions, starting with the x -axis in counter-clockwise manner; The sign '-' indicates no error measure was calculated for such case.)

Model \ Horizon $\delta_{\mathcal{H}}$		X			X'		
		2	3	4	2	3	4
CPD		2.44E-1	2.76E-1	2.71E-1	4.43E-1	1.25E-1	2.25E-1
BCPD		0	0	0	0	0	0
BHPD (δ_h)	2/3/4	4.76E-2	3.61E-2	6.26E-2	5.70E-2	5.01E-2	8.00E-2
	3/4/5	1.57E-1	1.23E-1	1.38E-1	3.55E-2	3.49E-2	9.85E-2
	-/5/6	-	2.34E-1	2.06E-1	-	8.53E-2	1.66E-1
	-/-/7	-	-	2.55E-1	-	-	2.14E-1
HPPD (np)	2	1.44E-1	1.35E-1	1.32E-1	6.21E-2	9.38E-2	1.46E-1
	3	5.75E-2	5.06E-2	5.25E-2	7.53E-2	7.04E-2	1.02E-1
	4	-	3.47E-2	4.01E-2	-	7.76E-2	9.35E-2
	6	-	3.67E-2	3.92E-2	-	7.59E-2	9.21E-2
LMPD (λ)	10	9.64E-2	1.67E-1	1.98E-1	1.81E-2	7.20E-2	1.62E-2
	100	1.41E-2	3.57E-2	5.68E-2	2.70E-3	1.42E-2	4.43E-2
	1,000	1.48E-3	4.08E-3	7.17E-3	2.84E-3	1.58E-3	5.48E-3
	10,000	1.49E-4	4.14E-4	7.74E-4	2.86E-5	1.60E-4	5.62E-4
NSPD (n_1)	1	3.45E-2	5.24E-2	5.87E-2	6.27E-2	8.17E-2	1.17E-1
	8	4.63E-3	1.34E-2	1.92E-2	7.91E-3	2.58E-2	3.84E-2
	10	1.87E-3	8.47E-3	1.35E-2	3.19E-3	1.57E-2	2.49E-2
	15	1.76E-4	3.19E-3	6.21E-3	2.99E-4	5.49E-3	1.08E-2

bonds within each sub-horizon such that its shape tensor is invertible. For BHPD, there is no monotonic trend in the prediction accuracy change observed using different bond-associated horizon sizes. By selecting the bond-associated horizon size, the prediction improves compared to CPD. The size of bond-associated horizon is restricted by the same requirement on the invertibility of the shape tensor within the sub-horizon. This observation is consistent for all the three different horizon sizes. However, in order to achieve similar bond mapping accuracy among different horizon sizes, different control parameters will need to be used. In summary, based on the results presented in Table 2.1, the BCPD predicts exact bond mapping, the NSPD and LMPD predicts very accurate bond mapping and the larger the control parameters of the influence function the more accurate the prediction. The HPPD and BHPD predict improved bond mapping compared to the CPD.

Chapter 3

Nonlocal-deformation-field-driven bond-based models

3.1 Finite-strain-based bond kinematics

To introduce the nonlocal-deformation-field-driven bond-based peridynamics (NDFD BB-PD), we begin by examining the kinematics of the bond. For a given bond ξ and its corresponding deformed state $\underline{\mathbf{y}} = \zeta$, the relative displacement between the two points can be expressed as

$$\boldsymbol{\eta} := \mathbf{u}(\mathbf{X}', t) - \mathbf{u}(\mathbf{X}, t) = \zeta - \xi, \quad (3.1)$$

where $\mathbf{u}(\mathbf{X}, t)$, $\mathbf{u}(\mathbf{X}', t)$ refer to the displacements of particle $\mathbf{X}$ and $\mathbf{X}'$ respectively.

As depicted in Fig. 3.1, let S_0 be a material curve passing through the initial bond ξ and S_t be its time evolution. In classical continuum mechanics, the motion of fiber is described by deformation gradient $\mathbf{F}$; the continuous curve S_t can never break up, which implies that the continuity of displacement field is always held. On the other hand, the motion of fiber in bond-based peridynamics is determined by relative displacement $\boldsymbol{\eta}$; therefore the continuity is not required and thus not guaranteed [22], this may raise zero energy mode issues even though the numerical oscillation is not observed. In proposed nonlocal-deformation-field-driven bond-based peridynamics, the motion of fiber is guided by the nonlocal Green-Lagrange strain $\mathbf{E}$; thus not only the continuity is preserved (which is indicated by the continuous curve S_t in Fig. 3.1(c)), but also the finite deformation of bond can be considered.

In continuum mechanics, the bond vector ζ can be related to the initial one ξ by the Cauchy-Born rule, i.e.

$$\zeta = \mathbf{F}\xi, \quad (3.2)$$

where $\mathbf{F}$ represents the deformation gradient on the bond. According to the definition of relative displacement given in Eq. (3.1), $\boldsymbol{\eta}$ can be linked to $\mathbf{F}$ as

$$\boldsymbol{\eta} = \mathbf{F}\xi - \xi = (\mathbf{F} - \mathbb{I}^{(2)})\xi, \quad (3.3)$$

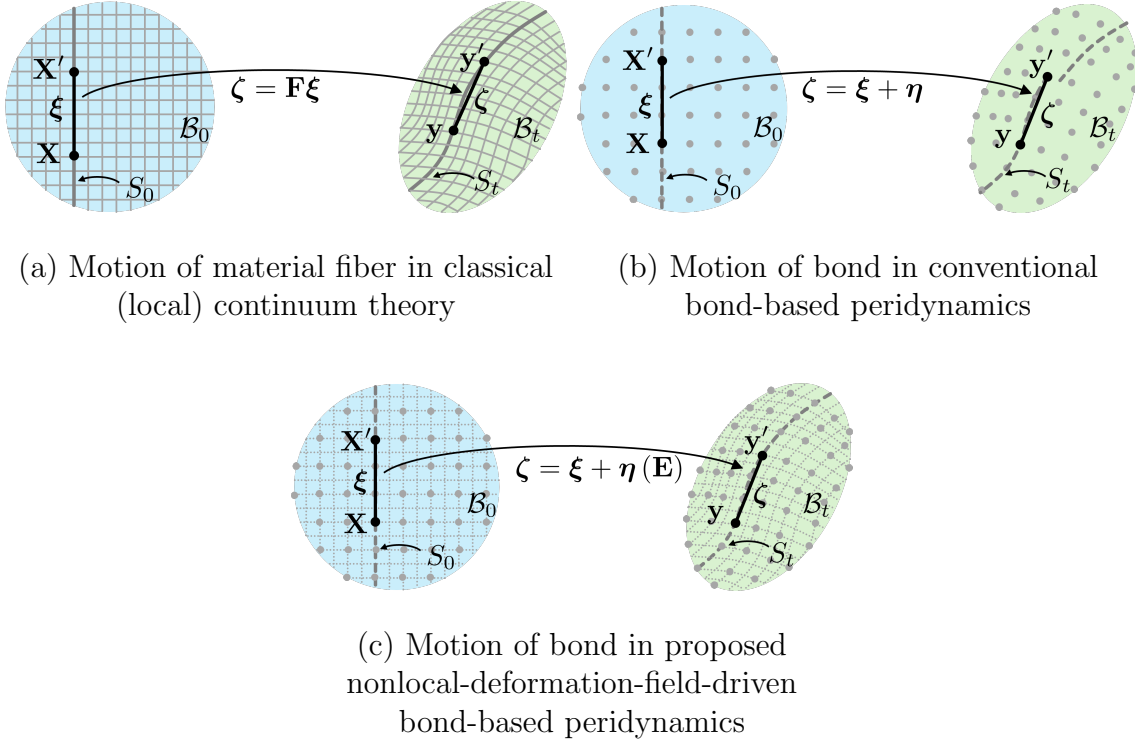


Figure 3.1: Deformation of material fiber/material bond connecting two points in three formulations.

where $\mathbb{I}^{(2)}$ is the second order identity tensor. If we introduce the unit vector along the direction of $\boldsymbol{\xi}$ as

$$\mathbf{N} := \frac{\boldsymbol{\xi}}{\xi}, \quad (3.4)$$

where $\xi := |\boldsymbol{\xi}|$ is the norm of vector $\boldsymbol{\xi}$, then we can divide the relative displacement $\boldsymbol{\eta}$ into two components, i.e.

$$\begin{aligned} \boldsymbol{\eta}_N &= (\boldsymbol{\eta} \cdot \mathbf{N})\mathbf{N}, \\ \boldsymbol{\eta}_T &= \boldsymbol{\eta} - (\boldsymbol{\eta} \cdot \mathbf{N})\mathbf{N}. \end{aligned} \quad (3.5)$$

$\boldsymbol{\eta}_N$ is aligned with the bond unit vector $\mathbf{N}$ while $\boldsymbol{\eta}_T$ is perpendicular to $\mathbf{N}$. A schematic illustration is provided in Fig. 3.2(b). This decomposition is widely used in bond-based peridynamics, especially extended bond-based peridynamics. However, there is a significant zero-energy mode under rigid body rotation, and many discussions concerning this issue have been conducted, see [20, 34, 37, 61, 85, 98].

The derivative of $\boldsymbol{\eta}$ with respect to deformation gradient $\mathbf{F}$ can be inferred from Eq. (3.3). In indicial notation, it writes,

$$\frac{\partial \eta_i}{\partial F_{aB}} = \frac{\partial F_{iJ}}{\partial F_{aB}} \xi_J = \delta_{ia} \xi_B \quad (3.6)$$

that can account for both infinitesimal and large strains in materials [77]. Furthermore, it is frame indifferent. the explicit formula of the Green-Lagrange strain tensor writes

$$\mathbf{E} := \frac{1}{2} [\mathbf{F}^T \mathbf{F} - \mathbb{I}^{(2)}] . \quad (3.10)$$

Based on the Green-Lagrange strain, the relative deformation of the bond may be reformulated as follows:

$$\mathbf{E}_\mathbf{N} = \mathbf{E} \mathbf{N} = \frac{1}{2} [\mathbf{F}^T \mathbf{F} - \mathbb{I}^{(2)}] \mathbf{N} . \quad (3.11)$$

In this sense, the stretch of the bond would be

$$E_{NN} \mathbf{N} \quad \text{with} \quad E_{NN} := \mathbf{E}_\mathbf{N} \cdot \mathbf{N} . \quad (3.12)$$

In terms of shear deformation, this study proposes and adopts a conjugated bond shear deformation. This method assumes that every real bond $\boldsymbol{\xi}$ has a fictitious bond $\boldsymbol{\xi}^c$ and that the shear deformation of the original real bond shall be equally distributed between the two bonds. This will allow the angular momentum balance to be readily achieved, as discussed further in Section 3.2. Based on this method, the shear deformation on each real bond at $\mathbf{N}$ direction should be:

$$\frac{1}{2} E_{NT} \mathbf{T} \quad \text{with} \quad \mathbf{T} := \frac{\mathbf{E}_\mathbf{N} - E_{NN} \mathbf{N}}{E_{NT}} \quad \text{and} \quad E_{NT} := |\mathbf{E}_\mathbf{N} - E_{NN} \mathbf{N}| . \quad (3.13)$$

As for the fictitious conjugated bond at $\mathbf{T}$ direction. The bond shear deformation is defined as

$$\frac{1}{2} E_{TN} \mathbf{N} \quad \text{with} \quad E_{TN} := E_{NT} = |\mathbf{E}_\mathbf{N} - E_{NN} \mathbf{N}| . \quad (3.14)$$

Remark 1 (1) It can be proved that $\mathbf{T}$ is orthogonal to $\mathbf{N}$. Here is the proof of orthogonality between $\mathbf{N}$ and $\mathbf{T}$.

$$\begin{aligned} \mathbf{N} \cdot \mathbf{T} &= \mathbf{N} \cdot \frac{\mathbf{E}_\mathbf{N} - (\mathbf{N} \cdot \mathbf{E}_\mathbf{N}) \mathbf{N}}{|\mathbf{E}_\mathbf{N} - (\mathbf{N} \cdot \mathbf{E}_\mathbf{N}) \mathbf{N}|} \\ &= \frac{\mathbf{N} \cdot \mathbf{E}_\mathbf{N} - (\mathbf{N} \cdot \mathbf{E}_\mathbf{N}) \mathbf{N} \cdot \mathbf{N}}{|\mathbf{E}_\mathbf{N} - (\mathbf{N} \cdot \mathbf{E}_\mathbf{N}) \mathbf{N}|} \\ &= \frac{\mathbf{N} \cdot \mathbf{E}_\mathbf{N} - \mathbf{N} \cdot \mathbf{E}_\mathbf{N}}{|\mathbf{E}_\mathbf{N} - (\mathbf{N} \cdot \mathbf{E}_\mathbf{N}) \mathbf{N}|} = 0 . \end{aligned}$$

(2) The definitions of $\mathbf{E}_\mathbf{N}$, E_{NN} , E_{NT} , $\mathbf{N}$ and $\mathbf{T}$ are consistent. In fact, one can find that

$$\begin{aligned} E_{NN} \mathbf{N} + E_{NT} \mathbf{T} &= (\mathbf{N} \cdot \mathbf{E}_\mathbf{N}) \mathbf{N} + |\mathbf{E}_\mathbf{N} - (\mathbf{N} \cdot \mathbf{E}_\mathbf{N}) \mathbf{N}| \cdot \frac{\mathbf{E}_\mathbf{N} - (\mathbf{N} \cdot \mathbf{E}_\mathbf{N}) \mathbf{N}}{|\mathbf{E}_\mathbf{N} - (\mathbf{N} \cdot \mathbf{E}_\mathbf{N}) \mathbf{N}|} \\ &= (\mathbf{N} \cdot \mathbf{E}_\mathbf{N}) \mathbf{N} + \mathbf{E}_\mathbf{N} - (\mathbf{N} \cdot \mathbf{E}_\mathbf{N}) \mathbf{N} \\ &= \mathbf{E}_\mathbf{N} \end{aligned}$$

(3) E_{NT} is equivalent to $\mathbf{T} \cdot \mathbf{E}_N$ or $\mathbf{N} \cdot \mathbf{ET}$. In fact,

$$\begin{aligned}
 E_{NT} &= \frac{(\mathbf{E}_N - E_{NN}\mathbf{N}) \cdot (\mathbf{E}_N - E_{NN}\mathbf{N})}{|\mathbf{E}_N - E_{NN}\mathbf{N}|} \\
 &= \frac{\mathbf{E}_N (\mathbb{I}^{(2)} - \mathbf{N} \otimes \mathbf{N}) (\mathbf{E}_N - E_{NN}\mathbf{N})}{|\mathbf{E}_N - E_{NN}\mathbf{N}|} \\
 &= \frac{\mathbf{E}_N (\mathbf{E}_N - E_{NN}\mathbf{N} - E_{NN}\mathbf{N} + E_{NN}\mathbf{N})}{|\mathbf{E}_N - E_{NN}\mathbf{N}|} \\
 &= \mathbf{E}_N \cdot \frac{\mathbf{E}_N - E_{NN}\mathbf{N}}{|\mathbf{E}_N - E_{NN}\mathbf{N}|} \\
 &= \mathbf{E}_N \cdot \mathbf{T} \\
 &= \mathbf{ET} \cdot \mathbf{N}
 \end{aligned}$$

From the definition of E_{NN} and E_{NT} given in Eq. (3.12) and (3.13), it is possible to determine their derivatives with respect to $\mathbf{E}_N$ and $\mathbf{E}$. They are

$$\frac{\partial E_{NN}}{\partial \mathbf{E}_N} = \frac{\partial \mathbf{N} \cdot \mathbf{E}_N}{\partial \mathbf{E}_N} = \mathbf{N} \quad (3.15)$$

$$\frac{\partial E_{NN}}{\partial \mathbf{E}} = \frac{\partial \mathbf{N} \cdot \mathbf{EN}}{\partial \mathbf{E}} = \frac{\partial \mathbf{E} : (\mathbf{N} \otimes \mathbf{N})}{\partial \mathbf{E}} = \mathbf{N} \otimes \mathbf{N} \quad (3.16)$$

and

$$\frac{\partial E_{NT}}{\partial \mathbf{E}_N} = \frac{\partial |\mathbf{E}_N - E_{NN}\mathbf{N}|}{\partial \mathbf{E}_N - \mathbf{E}_{NN}\mathbf{N}} \cdot \frac{\partial \mathbf{E}_N - E_{NN}\mathbf{N}}{\partial \mathbf{E}_N} = \mathbf{T} \cdot (\mathbb{I}^{(2)} - \mathbf{N} \otimes \mathbf{N}) = \mathbf{T} \quad (3.17)$$

$$\frac{\partial E_{NT}}{\partial \mathbf{E}} = \frac{\partial |\mathbf{E}_N - E_{NN}\mathbf{N}|}{\partial \mathbf{E}_N - \mathbf{E}_{NN}\mathbf{N}} \cdot \frac{\partial \mathbf{E}_N - E_{NN}\mathbf{N}}{\partial \mathbf{E}} = \frac{1}{2} (\mathbf{N} \otimes \mathbf{T} + \mathbf{T} \otimes \mathbf{N}) . \quad (3.18)$$

In above derivation, ' $\otimes$ ' stands for the tensor product and $\mathbf{N} \cdot \mathbf{T} = 0$ is utilized.

On the other hand, the derivative of $\mathbf{E}_N$ with respect to the relative displacement of the real bond $\boldsymbol{\eta}$ can be obtained based on Eq. (3.8) and (3.9). In indicial notation, it writes

$$\begin{aligned}
 \frac{\partial E_{N,I}}{\partial \eta_j} &= \frac{\partial E_{IK} N_K}{\partial \eta_j} \\
 &= \frac{1}{\xi} \frac{\partial}{\partial \eta_j} \left[\frac{1}{2} (F_{II} F_{IK} - \delta_{IK}) \xi_K \right] \\
 &= \frac{1}{\xi} \frac{1}{2} \frac{\partial F_{II}}{\partial \eta_j} F_{IK} \xi_K + \frac{1}{2} F_{II} \frac{\partial F_{IK}}{\partial \eta_j} \xi_K \\
 &= \frac{1}{2\xi} \delta_{Ij} \delta_{IK} F_{IK} + \frac{1}{2\xi} F_{II} \delta_{Ij} \\
 &= \frac{1}{\xi} F_{jI} . \quad (3.19)
 \end{aligned}$$

In matrix form, it writes

$$\frac{\partial \mathbf{E}_N}{\partial \boldsymbol{\eta}} = \frac{1}{\xi} \mathbf{F}^T. \quad (3.20)$$

Combining Eq. (3.15), (3.17) with Eq. (3.20), we can get the derivative relations between E_{NN} , E_{NT} and $\boldsymbol{\eta}$, they are

$$\frac{\partial E_{NN}}{\partial \boldsymbol{\eta}} = \frac{\partial E_{NN}}{\partial \mathbf{E}_N} \cdot \frac{\partial \mathbf{E}_N}{\partial \boldsymbol{\eta}} = \frac{1}{\xi} \mathbf{F} \mathbf{N}, \quad (3.21)$$

$$\frac{\partial E_{NT}}{\partial \boldsymbol{\eta}} = \frac{\partial E_{NT}}{\partial \mathbf{E}_N} \cdot \frac{\partial \mathbf{E}_N}{\partial \boldsymbol{\eta}} = \frac{1}{\xi} \mathbf{F} \mathbf{T}. \quad (3.22)$$

Supposing the relative displacement $\boldsymbol{\eta}^c$ on the conjugated fictitious bond $\boldsymbol{\xi}^c$ follows the same deformation gradient $\mathbf{F}$, i.e.

$$\boldsymbol{\eta}^c = (\mathbf{F} - \mathbb{I}^{(2)}) \boldsymbol{\xi}^c \quad \text{with} \quad \mathbf{T} = \frac{\boldsymbol{\xi}^c}{|\boldsymbol{\xi}^c|}. \quad (3.23)$$

We can also establish the derivative relation between E_{NT} and η^c . Following the same procedure as stated above, the relation should be.

$$\frac{\partial E_{NT}}{\partial \eta^c} = \frac{\partial \mathbf{N} \cdot \mathbf{E} \mathbf{T}}{\partial \mathbf{E}_T} \cdot \frac{\partial \mathbf{E}_T}{\partial \eta^c} = \frac{1}{\xi^c} \mathbf{F} \mathbf{N}. \quad (3.24)$$

Remark 2 (1) In BB-PD, the stretch of bond is typically defined as $s = (|\boldsymbol{\zeta}| - |\boldsymbol{\xi}|) / |\boldsymbol{\xi}|$ [73, 70, 71], which corresponds to $\sqrt{\boldsymbol{\xi} \cdot (\mathbf{F}^T \mathbf{F}) \boldsymbol{\xi}} / |\boldsymbol{\xi}| - 1$. On the other hand, in XBB-PD, the stretch of bonds in XBB-PD is usually defined as $s = (\boldsymbol{\zeta} \cdot \boldsymbol{\xi} - |\boldsymbol{\xi}|^2) / |\boldsymbol{\xi}|^2$ [98, 34, 37], which is equivalent to $(\boldsymbol{\xi} \cdot \mathbf{F} \boldsymbol{\xi}) / |\boldsymbol{\xi}|^2 - 1$. These definitions do not agree with each other. Previous studies also adopted one-, two-, and three-neighbor kinematic measures [39, 40, 23]. Although they are consistent with continuum kinematics without explicit notion of strain, it requires repetitive computation among the material points within the horizon, thus leads to high computation costs. In this paper, we aim to address this difficulty by presenting a comprehensive definition of bond stretch and shear deformation using Green-Lagrange strain, which is suitable for infinitesimal and finite deformation problems.

(2) If there is a real bond in the $\mathbf{T}$ direction and the deformation gradient within the horizon is uniform, the relative displacement should be consistent with the result given in Eq. (3.23). However, this ideal condition may not be achieved in actual numerical implementation. Therefore, this paper introduces the concept of fictitious conjugate bond to make the bond-level shear deformation consistent with classical continuum mechanics theory.

3.2 Bond force states, stress measures, and equilibrium

In this work, we derive the force states directly from the bond potential energy based on the definition. It is assumed that the bond potential energy function is not only continuous but

also differentiable with respect to E_{NN} and E_{NT} , i.e.

$$\phi := \phi(\boldsymbol{\xi}, E_{NN}, E_{NT}) \quad (3.25)$$

$$f_N := \frac{\partial \phi}{\partial E_{NN}} \quad (3.26)$$

$$f_T := \frac{\partial \phi}{\partial E_{NT}} \quad (3.27)$$

where ϕ is the bond potential energy function, f_N and f_T are the derived micro-forces corresponding to E_{NN} and E_{NT} respectively. Similar to the definition of force density in BB-PD, the force density in NDFD BB-PD can also be achieved by taking derivative to relative displacement $\boldsymbol{\eta}$ and $\boldsymbol{\eta}^c$. Combining Eq. (3.26), (3.27), (3.15), (3.17) and (3.20) and using the chain rule, the formula for force density can be established.

$$\begin{aligned} \mathbf{f} &:= \mathbf{f}(\boldsymbol{\xi}, E_{NN}, E_{NT}) \\ &= \frac{\partial \phi}{\partial E_{NN}} \cdot \frac{\partial E_{NN}}{\partial \boldsymbol{\eta}} + \frac{1}{2} \cdot \frac{\partial \phi}{\partial E_{NT}} \cdot \frac{\partial E_{NT}}{\partial \boldsymbol{\eta}} + \frac{1}{2} \cdot \frac{\partial \phi}{\partial E_{NT}} \cdot \frac{\partial E_{NT}}{\partial \boldsymbol{\eta}^c} \\ &= \frac{1}{\xi} f_N \mathbf{F} \mathbf{N} + \frac{1}{2\xi} f_T \mathbf{F} \mathbf{T} + \frac{1}{2\xi^c} f_T \mathbf{F} \mathbf{N} \\ &= \frac{1}{\xi} f_N \mathbf{n} + \frac{1}{2\xi} f_T \mathbf{t} + \frac{1}{2\xi^c} f_T \mathbf{n} \end{aligned} \quad (3.28)$$

where new definitions $\mathbf{n} := \mathbf{F} \mathbf{N}$ and $\mathbf{t} := \mathbf{F} \mathbf{T}$ are introduced for the sake of simple statement. The derivative relation between bond potential energy function and Green-Lagrange strain can also be established by using Eq. (3.16) and (3.18), it writes

$$\begin{aligned} \frac{\partial \phi}{\partial \mathbf{E}} &= \frac{\partial \phi}{\partial E_{NN}} \cdot \frac{\partial E_{NN}}{\partial \mathbf{E}} + \frac{\partial \phi}{\partial E_{NT}} \cdot \frac{\partial E_{NT}}{\partial \mathbf{E}} \\ &= f_N \mathbf{N} \otimes \mathbf{N} + \frac{f_T}{2} (\mathbf{N} \otimes \mathbf{T} + \mathbf{T} \otimes \mathbf{N}) . \end{aligned} \quad (3.29)$$

In summary,

$$\mathbf{f} := \mathbf{f}(\boldsymbol{\xi}, E_{NN}, E_{NT}) = \frac{1}{\xi} f_N \mathbf{n} + \frac{1}{2\xi} f_T \mathbf{t} + \frac{1}{2\xi^c} f_T \mathbf{n} = \mathbf{f}^0 + \mathbf{f}^c \quad (3.30)$$

$$\mathbf{f}^0 := \frac{1}{\xi} f_N \mathbf{n} + \frac{1}{2\xi} f_T \mathbf{t}, \quad \mathbf{f}^c := \frac{1}{2\xi^c} f_T \mathbf{n} \quad (3.31)$$

$$\frac{\partial \phi}{\partial \mathbf{E}} := f_N \mathbf{N} \otimes \mathbf{N} + \frac{f_T}{2} (\mathbf{N} \otimes \mathbf{T} + \mathbf{T} \otimes \mathbf{N}) \quad (3.32)$$

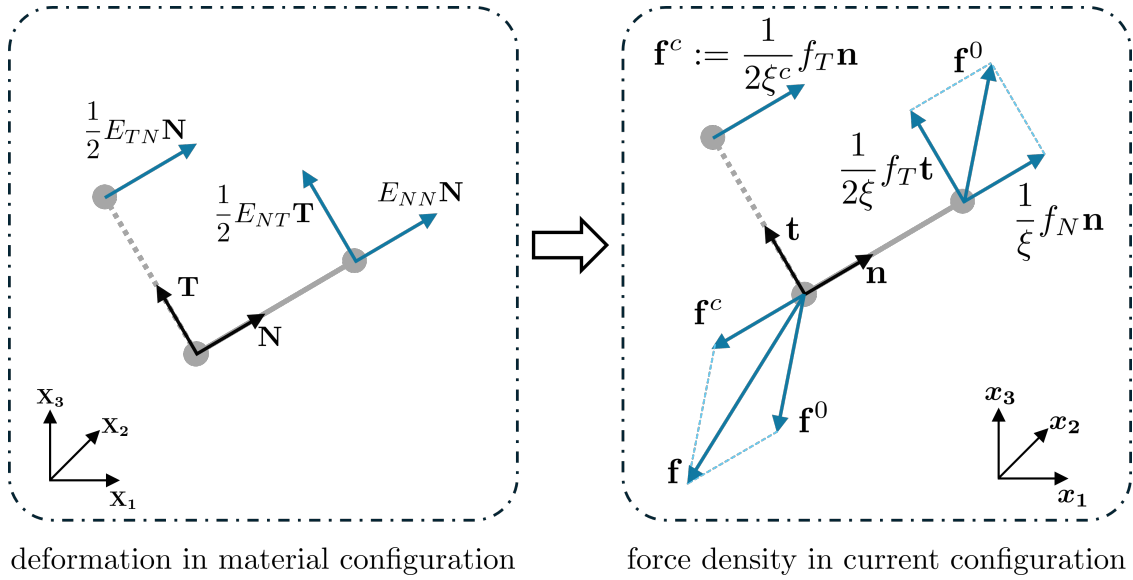


Figure 3.3: relation between bond deformation and bond force density

where $\mathbf{f}^0$ is the force density acting on the original real bond while $\mathbf{f}^c$ refers to the corresponding one on the fictitious conjugate bond. The correspondence relation between the bond deformation states and the force states is depicted in Fig. 3.3.

Nonlocal equation of motion and linear momentum balance

Since the existence of bond potential energy, the nonlocal strain energy density $\mathcal{W}$ at a given material point $\mathbf{X}$ can be expressed as the weighted integration of the bond energy within its horizon $\mathcal{H}_{\mathbf{X}}$, i.e.

$$\begin{aligned}\mathcal{W}(\mathbf{X}) &= \int_{\mathcal{H}_{\mathbf{X}}} \int_{\mathcal{H}_{\mathbf{X}}} \underline{w}(\mathbf{X}', \mathbf{X}'') \frac{1}{2} \phi(\mathbf{X}', \mathbf{X}'') dV_{\mathbf{X}''} dV_{\mathbf{X}'} \\ &= \frac{1}{2} \int_{\mathcal{H}_{\mathbf{X}}} \int_{\mathcal{H}_{\mathbf{X}}} \underline{w}(\mathbf{X}', \mathbf{X}'') \phi(\mathbf{X}', \mathbf{X}'') dV_{\mathbf{X}''} dV_{\mathbf{X}'}\end{aligned}\quad (3.33)$$

where $\mathbf{X}'$ and $\mathbf{X}''$ are two material points within the horizon of center point $\mathbf{X}$; $\phi(\mathbf{X}, \mathbf{X}'') = \phi(\mathbf{X}'' - \mathbf{X}, E_{NN}, E_{NT})$ is the bond potential energy function defined between point $\mathbf{X}'$ and point $\mathbf{X}''$; and $\underline{w}(\mathbf{X}', \mathbf{X}'')$ is a regularized weight function that satisfies

$$\int_{\mathcal{H}_{\mathbf{X}}} \int_{\mathcal{H}_{\mathbf{X}}} \underline{w}(\mathbf{X}', \mathbf{X}'') dV_{\mathbf{X}''} dV_{\mathbf{X}'} = 1$$

For the sake of a simple statement, We will neglect the argument $\mathbf{X}$ for the quantities of interest that belong to point $\mathbf{X}$; for instance, $\mathcal{W}$ stands for $\mathcal{W}(\mathbf{X})$ and $\mathbf{u}$ stands for $\mathbf{u}(\mathbf{X})$.

Therefore, the total external work U , total kinetic energy K , total strain energy Φ , and total energy L of the system writes

$$U = \int_{\mathcal{B}_0} \mathbf{b}\mathbf{u} \, dV_{\mathbf{X}} \quad (3.34)$$

$$K = \int_{\mathcal{B}_0} \frac{1}{2} \rho \dot{\mathbf{u}} \cdot \dot{\mathbf{u}} \, dV_{\mathbf{X}} \quad (3.35)$$

$$\Phi = \int_{\mathcal{B}_0} \mathcal{W} \, dV_{\mathbf{X}} \quad (3.36)$$

$$\begin{aligned} L &= K - (\Phi - U) \\ &= \int_{\mathcal{B}_0} \left[\frac{1}{2} \rho \dot{\mathbf{u}} \cdot \dot{\mathbf{u}} - (\Psi - \mathbf{b}\mathbf{u}) \right] dV_{\mathbf{X}} \end{aligned} \quad (3.37)$$

where $\dot{\mathbf{u}} := \dot{\mathbf{u}}(\mathbf{X})$ is the time derivative of displacement $\mathbf{u} := \mathbf{u}(\mathbf{X})$. Therefore, the Euler-Lagrange Equation of this system can be formulated.

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{\mathbf{u}}} \right) - \frac{\partial L}{\partial \mathbf{u}} = 0 \quad (3.38)$$

The first term of Eq. (3.38) can be expanded as

$$\begin{aligned} \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{\mathbf{u}}} \right) &= \frac{d}{dt} (\rho \dot{\mathbf{u}}) \\ &= \rho \ddot{\mathbf{u}} \end{aligned} \quad (3.39)$$

The second term of Eq. (3.38) can be expanded as

$$\begin{aligned}
 \frac{\partial L}{\partial \mathbf{u}} &= - \frac{\partial}{\partial \mathbf{u}} \int_{\mathcal{B}_0} [\mathcal{W} - \mathbf{b}\mathbf{u}] \, dV_{\mathbf{X}} \\
 &= - \frac{1}{2} \frac{\partial}{\partial \mathbf{u}} \int_{\mathcal{H}_{\mathbf{X}}} \int_{\mathcal{H}_{\mathbf{X}}} \int_{\mathcal{H}_{\mathbf{X}}} \underline{\mathbf{w}}(\mathbf{X}', \mathbf{X}'') \phi(\mathbf{X}', \mathbf{X}'') \, dV_{\mathbf{X}''} \, dV_{\mathbf{X}'} \, dV_{\mathbf{X}'''} + \mathbf{b}(\mathbf{X}) \\
 &= - \frac{1}{2} \int_{\mathcal{H}_{\mathbf{X}}} \int_{\mathcal{H}_{\mathbf{X}}} \underline{\mathbf{w}}(\mathbf{X}, \mathbf{X}'') \frac{\partial \phi(\mathbf{X}, \mathbf{X}'')}{\partial \mathbf{u}} \, dV_{\mathbf{X}''} \, dV_{\mathbf{X}'''} + \\
 &\quad - \frac{1}{2} \int_{\mathcal{H}_{\mathbf{X}}} \int_{\mathcal{H}_{\mathbf{X}}} \underline{\mathbf{w}}(\mathbf{X}', \mathbf{X}) \frac{\partial \phi(\mathbf{X}', \mathbf{X})}{\partial \mathbf{u}} \, dV_{\mathbf{X}'} \, dV_{\mathbf{X}'''} + \mathbf{b} \\
 &= - \frac{1}{2} \int_{\mathcal{H}_{\mathbf{X}}} \left(\underline{\mathbf{w}}(\mathbf{X}, \mathbf{X}') \frac{\partial \phi(\mathbf{X}, \mathbf{X}')}{\partial \mathbf{u}} + \underline{\mathbf{w}}(\mathbf{X}', \mathbf{X}) \frac{\partial \phi(\mathbf{X}', \mathbf{X})}{\partial \mathbf{u}} \right) V_{\mathcal{H}_{\mathbf{X}}} \, dV_{\mathbf{X}'} + \mathbf{b} \\
 &= - \frac{1}{2} \int_{\mathcal{H}_{\mathbf{X}}} \left(\underline{\mathbf{w}}(\mathbf{X}, \mathbf{X}') \mathbf{f}(\mathbf{X}, \mathbf{X}') \cdot (-\mathbb{I}^{(2)}) + \underline{\mathbf{w}}(\mathbf{X}', \mathbf{X}) \mathbf{f}(\mathbf{X}', \mathbf{X}) \cdot \mathbb{I}^{(2)} \right) V_{\mathcal{H}_{\mathbf{X}}} \, dV_{\mathbf{X}'} + \mathbf{b} \\
 &= \frac{1}{2} \int_{\mathcal{H}_{\mathbf{X}}} \underline{\mathbf{w}}(\mathbf{X}, \mathbf{X}') V_{\mathcal{H}_{\mathbf{X}}} [\mathbf{f}(\mathbf{X}, \mathbf{X}') - \mathbf{f}(\mathbf{X}', \mathbf{X})] \, dV_{\mathbf{X}'} + \mathbf{b} \\
 &= \int_{\mathcal{H}_{\mathbf{X}}} \underline{\mathbf{w}}(\mathbf{X}, \mathbf{X}') V_{\mathcal{H}_{\mathbf{X}}} \mathbf{f}(\mathbf{X}, \mathbf{X}') \, dV_{\mathbf{X}'} + \mathbf{b}(\mathbf{X})
 \end{aligned} \tag{3.40}$$

where $\mathbf{f}(\mathbf{X}, \mathbf{X}') = \mathbf{f}(\mathbf{X}' - \mathbf{X}, E_{NN}, E_{NT})$ is the micro-force vector defined in Eq. (3.30).

Remark 3 (1) It should be noted that the ϕ and $\mathbf{f}$ are zero if $\mathbf{X}' = \mathbf{X}''$. This implies they are the same point, thus the bond strain energy and force density should be null.

(2) Given that $\boldsymbol{\eta}(\mathbf{X}, \mathbf{X}') = \mathbf{u}(\mathbf{X}') - \mathbf{u}(\mathbf{X}) = -\boldsymbol{\eta}(\mathbf{X}', \mathbf{X})$ and $\boldsymbol{\eta}^c(\mathbf{X}, \mathbf{X}') = (\mathbf{F} - \mathbb{I}^{(2)})(\mathbf{X}' - \mathbf{X}) = -(\mathbf{F} - \mathbb{I}^{(2)})(\mathbf{X} - \mathbf{X}') = -\boldsymbol{\eta}^c(\mathbf{X}', \mathbf{X})$, the force density $\mathbf{f}(\mathbf{X}, \mathbf{X}')$ derived from Eq. (3.30) has the same magnitude as $\mathbf{f}(\mathbf{X}', \mathbf{X})$ but in the opposite direction, i.e. $\mathbf{f}(\mathbf{X}, \mathbf{X}') = -\mathbf{f}(\mathbf{X}', \mathbf{X})$. To meet the symmetry requirement, we assume the weight function should satisfy the condition $\underline{\mathbf{w}}(\mathbf{X}, \mathbf{X}') = \underline{\mathbf{w}}(\mathbf{X}', \mathbf{X})$.

(3) The derivative of $\phi(\mathbf{X}, \mathbf{X}')$ with respect to $\mathbf{u}(\mathbf{X})$ can be calculated by combining Eq.

(3.30) with the fact $\boldsymbol{\eta}(\mathbf{X}, \mathbf{X}') = \mathbf{u}(\mathbf{X}') - \mathbf{u}(\mathbf{X})$ and $\boldsymbol{\eta}^c(\mathbf{X}, \mathbf{X}'^c) = \mathbf{u}(\mathbf{X}'^c) - \mathbf{u}(\mathbf{X})$, i.e.

$$\begin{aligned}
 \frac{\partial \phi(\mathbf{X}, \mathbf{X}')}{\partial \mathbf{u}(\mathbf{X})} &= \frac{\partial \phi}{\partial \boldsymbol{\eta}} \cdot \frac{\partial \boldsymbol{\eta}(\mathbf{X}, \mathbf{X}')}{\partial \mathbf{u}(\mathbf{X})} + \frac{\partial \phi}{\partial \boldsymbol{\eta}^c} \cdot \frac{\partial \boldsymbol{\eta}^c(\mathbf{X}, \mathbf{X}'^c)}{\partial \mathbf{u}(\mathbf{X})} \\
 &= \frac{\partial \phi}{\partial \boldsymbol{\eta}} \left(-\frac{\partial \mathbf{u}(\mathbf{X})}{\partial \mathbf{u}(\mathbf{X})} \right) + \frac{\partial \phi}{\partial \boldsymbol{\eta}^c} \left(-\frac{\partial \mathbf{u}(\mathbf{X})}{\partial \mathbf{u}(\mathbf{X})} \right) \\
 &= \mathbf{f}(\mathbf{X}, \mathbf{X}') \cdot \left(-\frac{\partial \mathbf{u}(\mathbf{X})}{\partial \mathbf{u}(\mathbf{X})} \right) \\
 &= \mathbf{f}(\mathbf{X}, \mathbf{X}') \cdot (-\mathbb{I}^{(2)}) \\
 &= -\mathbf{f}(\mathbf{X}, \mathbf{X}')
 \end{aligned}$$

The derivative of $\phi(\mathbf{X}', \mathbf{X})$ with respect to $\mathbf{u}(\mathbf{X}')$ can be achieved similarly.

By substituting Eq. (3.39) and Eq. (3.40) into Eq. (3.38), finally we can formulate the governing equation of NDFD BB-PD as follows,

$$\begin{aligned}
 \rho(\mathbf{X})\ddot{\mathbf{u}}(\mathbf{X}) &= \int_{\mathcal{H}_{\mathbf{X}}} \underline{\mathbf{w}}(\mathbf{X}, \mathbf{X}') V_{\mathcal{H}_{\mathbf{X}}} \mathbf{f}(\mathbf{X}, \mathbf{X}') dV_{\mathbf{X}'} + \mathbf{b}(\mathbf{X}) \\
 &= \int_{\mathcal{H}_{\mathbf{X}}} [\underline{\mathbf{T}}[\mathbf{X}, t]\langle \boldsymbol{\xi} \rangle - \underline{\mathbf{T}}[\mathbf{X}', t]\langle -\boldsymbol{\xi} \rangle] dV_{\mathbf{X}'} + \mathbf{b}(\mathbf{X}) , \quad (3.41)
 \end{aligned}$$

with

$$\underline{\mathbf{T}}[\mathbf{X}, t]\langle \boldsymbol{\xi} \rangle = \frac{\underline{\mathbf{w}} V_{\mathcal{H}_{\mathbf{X}}}}{2} \mathbf{f}(\mathbf{X}, \mathbf{X}') = -\frac{\underline{\mathbf{w}} V_{\mathcal{H}_{\mathbf{X}}}}{2} \mathbf{f}(\mathbf{X}', \mathbf{X}) = \underline{\mathbf{T}}[\mathbf{X}', t]\langle -\boldsymbol{\xi} \rangle . \quad (3.42)$$

In Eq. (3.41) and (3.42), the symbol $\underline{\mathbf{T}}$ is introduced to denote the bond force state so as to make the formula consistent with the state-based models.

Nonlocal stress measures

The nonlocal stress state at each point can be acquired from the definition of the nonlocal strain energy density given in Eq. (3.33). Assuming that the nonlocal deformation gradient $\mathbf{F}$ over a given horizon $\mathcal{H}_{\mathbf{X}}$ is uniform, which implies the Green-Lagrange strain $\mathbf{E}$ is also uniform in the horizon, the work-conjugated second Piola-Kirchhoff (PK2) stress $\mathbf{S}$ can be

written as,

$$\begin{aligned}\mathbf{S}(\mathbf{X}) &:= \frac{\partial \mathcal{W}(\mathbf{X})}{\partial \mathbf{E}} \\ &= \frac{1}{2} \int_{\mathcal{H}_{\mathbf{X}}} \int_{\mathcal{H}_{\mathbf{X}}} \omega(\mathbf{X}', \mathbf{X}'') \frac{\partial \phi(\mathbf{X}', \mathbf{X}'')}{\partial \mathbf{E}} dV_{\mathbf{X}''} dV_{\mathbf{X}'}\end{aligned}$$

By incorporating Eq. (3.32) into the above equation, the explicit expression of PK2 stress can be derived as follows,

$$\mathbf{S}(\mathbf{X}) = \frac{1}{2} \int_{\mathcal{H}_{\mathbf{X}}} \int_{\mathcal{H}_{\mathbf{X}}} \underline{\mathbf{w}}(\mathbf{X}', \mathbf{X}'') \left(f_N \mathbf{N} \otimes \mathbf{N} + \frac{f_T}{2} (\mathbf{N} \otimes \mathbf{T} + \mathbf{T} \otimes \mathbf{N}) \right) dV_{\mathbf{X}''} dV_{\mathbf{X}'} \quad (3.43)$$

The first Piola-Kirchhoff (PK1) stress can also be derived by leveraging chain rule. By using indicial notation, we can write

$$\begin{aligned}P_{aB} &= \frac{\partial \mathcal{W}}{\partial E_{CD}} \cdot \frac{\partial E_{CD}}{\partial F_{aB}} \\ &= \frac{\partial \mathcal{W}}{\partial E_{CD}} \cdot \frac{1}{2} \cdot \frac{\partial (F_{mC} F_{mD} - \delta_{CD})}{\partial F_{aB}} \\ &= S_{CD} \cdot \frac{1}{2} (\delta_{am} \delta_{BC} F_{mD} + F_{mC} \delta_{am} \delta_{BD})\end{aligned} \quad (3.44)$$

$$\begin{aligned}&= \frac{1}{2} F_{aD} S_{BD} + \frac{1}{2} F_{aC} S_{CB} \\ &= \frac{1}{2} \int_{\mathcal{H}_{\mathbf{X}}} \int_{\mathcal{H}_{\mathbf{X}}} \underline{\mathbf{w}}(\mathbf{X}', \mathbf{X}'') \left(f_N F_{aC} N_C N_B + \frac{f_T}{2} F_{aC} (N_C T_B + T_C N_B) \right) dV_{\mathbf{X}''} dV_{\mathbf{X}'} \\ &= \frac{1}{2} \int_{\mathcal{H}_{\mathbf{X}}} \int_{\mathcal{H}_{\mathbf{X}}} \underline{\mathbf{w}}(\mathbf{X}', \mathbf{X}'') \left(f_N n_a N_B + \frac{f_T}{2} (n_a T_B + t_a N_B) \right) dV_{\mathbf{X}''} dV_{\mathbf{X}'}.\end{aligned} \quad (3.45)$$

Here for a clear illustration, the indicial notation is adopted, and the relations $\mathbf{n} = \mathbf{F}\mathbf{N}$ and $\mathbf{t} = \mathbf{F}\mathbf{T}$ are utilized in the above derivations. Reformulating it into tensorial notation, it can be written as follows,

$$\mathbf{P}(\mathbf{X}) = \frac{1}{2} \int_{\mathcal{H}_{\mathbf{X}}} \int_{\mathcal{H}_{\mathbf{X}}} \underline{\mathbf{w}}(\mathbf{X}', \mathbf{X}'') \left(f_N \mathbf{n} \otimes \mathbf{N} + \frac{f_T}{2} (\mathbf{n} \otimes \mathbf{T} + \mathbf{t} \otimes \mathbf{N}) \right) dV_{\mathbf{X}''} dV_{\mathbf{X}'} \quad (3.46)$$

Remark 4 By finite deformation theory, the second Piola-Kirchhoff stress can be converted to the first Piola-Kirchhoff stress by

$$\mathbf{P} = \mathbf{F} \mathbf{S}$$

This conversion also holds between Eq. (3.43) and (3.46). The underlining reason is the work conjugate relation of $\dot{\mathcal{W}} = \mathbf{S} \cdot \dot{\mathbf{E}} = \mathbf{P} \cdot \dot{\mathbf{F}}$. The conversion from the above stress measures to other alternative stress measures can be obtained, as long as they are work conjugated with certain strain measures. For instance, the Kirchhoff stress can be expressed as:

$$\begin{aligned} \boldsymbol{\tau}(\mathbf{X}) &:= \mathbf{F} \mathbf{S}(\mathbf{X}) \mathbf{F}^T \\ &= \frac{1}{2} \int_{\mathcal{H}_{\mathbf{X}}} \int_{\mathcal{H}_{\mathbf{X}}} \underline{\mathbf{w}}(\mathbf{X}', \mathbf{X}'') \left(f_N \mathbf{n} \otimes \mathbf{n} + \frac{f_T}{2} (\mathbf{n} \otimes \mathbf{t} + \mathbf{t} \otimes \mathbf{n}) \right) dV_{\mathbf{X}''} dV_{\mathbf{X}'} \end{aligned}$$

and the Cauchy stress can be written as,

$$\begin{aligned} \boldsymbol{\sigma}(\mathbf{X}) &:= J^{-1} \boldsymbol{\tau}(\mathbf{X}) \\ &= \frac{1}{2J} \int_{\mathcal{H}_{\mathbf{X}}} \int_{\mathcal{H}_{\mathbf{X}}} \underline{\mathbf{w}}(\mathbf{X}', \mathbf{X}'') \left(f_N \mathbf{n} \otimes \mathbf{n} + \frac{f_T}{2} (\mathbf{n} \otimes \mathbf{t} + \mathbf{t} \otimes \mathbf{n}) \right) dV_{\mathbf{X}''} dV_{\mathbf{X}'}, \end{aligned} \quad (3.47)$$

where $J := \det(\mathbf{F})$ is the determinant of deformation gradient

The deformation gradient tensor, as well as the Green-Lagrange strain tensor, can be linearized as

$$\mathbf{F} = \mathbb{I}^{(2)} + \nabla \mathbf{u} + \mathcal{O}(\|\nabla \mathbf{u}\|^2) \quad (3.48)$$

$$\mathbf{E} = \frac{1}{2} \left[\mathbb{I}^{(2)} + \nabla \mathbf{u} + (\nabla \mathbf{u})^T + \mathcal{O}(\|\nabla \mathbf{u}\|^2) - \mathbb{I}^{(2)} \right] \quad (3.49)$$

where the $\nabla \mathbf{u}$ is the displacement gradient that can be defined as $\nabla \mathbf{u} := \mathbf{F} - \mathbb{I}^{(2)}$. In infinitesimal deformation, the Green-Lagrange strain can be approximated by the infinitesimal strain, i.e.

$$\mathbf{E} \rightarrow \boldsymbol{\epsilon} := \text{sym}(\nabla \mathbf{u})$$

where $\text{sym}(\cdot)$ refers to the symmetric part of a tensor. Consequently, under infinitesimal deformation, as an approximation of the PK2 stress, the Cauchy stress at material point $\mathbf{X}$ corresponding may be derived as,

$$\begin{aligned} \boldsymbol{\sigma}(\mathbf{X}) &:= \frac{\partial \mathcal{W}(\mathbf{X})}{\partial \boldsymbol{\epsilon}} \\ &= \frac{1}{2} \int_{\mathcal{H}_{\mathbf{X}}} \int_{\mathcal{H}_{\mathbf{X}}} \underline{\mathbf{w}}(\mathbf{X}', \mathbf{X}'') \left(f_N \mathbf{N} \otimes \mathbf{N} + \frac{f_T}{2} (\mathbf{N} \otimes \mathbf{T} + \mathbf{T} \otimes \mathbf{N}) \right) dV_{\mathbf{X}''} dV_{\mathbf{X}'} \end{aligned} \quad (3.50)$$

Remark 5 *The mechanical response of materials under infinitesimal deformation can be utilized to compute the essential properties of materials, such as elastic modulus. Indeed, the elastic modulus can be determined by taking the derivative of Cauchy stress with respect to infinitesimal strain as strain approaches zero, i.e.*

$$\mathbb{C} = \left. \frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{\epsilon}} \right|_{\boldsymbol{\epsilon} \rightarrow \mathbf{0}}$$

Extended Noll's Lemma and angular momentum balance

It has been proved [51] that the peridynamics stress proposed in Lehoucq and Silling [48], and Silling and Lehoucq [74] is equivalent to the nonlocal first Piola-Kirchhoff stress proposed by Noll [49]. According to Noll's Lemma, the force flux within a given horizon can be linked to the peridynamics stress as follows,

$$\int_{\mathcal{H}} \mathbf{f}(\mathbf{X}, \mathbf{Y}) dV_{\mathbf{Y}} = -\frac{1}{2} \nabla_{\mathbf{X}} \cdot \left[\int_{\mathcal{H}} \int_{\alpha=0}^1 \boldsymbol{\xi} \otimes \mathbf{f}(\mathbf{X} + \alpha \boldsymbol{\xi}, \mathbf{X} - (1 - \alpha) \boldsymbol{\xi}) d\alpha dV_{\boldsymbol{\xi}} \right]. \quad (3.51)$$

where $\int_{\mathcal{H}} \mathbf{f}(\mathbf{X}, \mathbf{Y}) dV_{\mathbf{Y}}$ is the nonlocal force flux and $-\frac{1}{2} \int_{\mathcal{H}} \int_{\alpha=0}^1 \mathbf{f}(\mathbf{X} + \alpha \boldsymbol{\xi}, \mathbf{X} - (1 - \alpha) \boldsymbol{\xi}) \otimes \boldsymbol{\xi} d\alpha dV_{\boldsymbol{\xi}}$ is the nonlocal first Piola-Kirchhoff or peridynamics stress. This paper aims to extend Noll's Lemma for more general cases. The nonlocal force flux can be re-written as

$$\int_{\mathcal{H}_{\mathbf{X}}} \mathbf{f}(\mathbf{X}, \mathbf{Y}) dV_{\mathbf{Y}} = \frac{1}{2} \int_{\mathcal{H}_{\mathbf{X}}} \mathbf{f}(\mathbf{X}, \mathbf{X} - \boldsymbol{\xi}) - \mathbf{f}(\mathbf{X} + \boldsymbol{\xi}, \mathbf{X}) dV_{\boldsymbol{\xi}} \quad (3.52)$$

Since the force densities are imposed on two different bonds and the force-acting points are crucial in deriving the extended Noll's Lemma and angular momentum balance, we should consider them separately. For a simple statement, $\mathbf{f}^c$ is used to illustrate the derivation procedure; the same procedure also applies to $\mathbf{f}^0$. It is noted that

$$\mathbf{f}^c(\mathbf{X} + \boldsymbol{\xi}^c, \mathbf{X}) - \mathbf{f}^c(\mathbf{X}, \mathbf{X} - \boldsymbol{\xi}^c) = \int_{\alpha=0}^1 \frac{\partial}{\partial \alpha} (\mathbf{f}^c(\mathbf{X} + \alpha \boldsymbol{\xi}^c, \mathbf{X} - (1 - \alpha) \boldsymbol{\xi}^c)) d\alpha. \quad (3.53)$$

It is also noted that

$$\nabla_{\mathbf{X}} \mathbf{f}^c(\mathbf{X} + \alpha \boldsymbol{\xi}^c, \mathbf{X} - (1 - \alpha) \boldsymbol{\xi}^c) = \nabla_{\mathbf{v}} \mathbf{f}^c + \nabla_{\mathbf{w}} \mathbf{f}^c \quad (3.54)$$

$$\frac{\partial}{\partial \alpha} (\mathbf{f}^c(\mathbf{X} + \alpha \boldsymbol{\xi}^c, \mathbf{X} - (1 - \alpha) \boldsymbol{\xi}^c)) = (\nabla_{\mathbf{v}} \mathbf{f}^c + \nabla_{\mathbf{w}} \mathbf{f}^c) \cdot \boldsymbol{\xi}^c \quad (3.55)$$

where $\mathbf{v} = \mathbf{X} + \alpha \boldsymbol{\xi}^c$ and $\mathbf{w} = \mathbf{X} - (1 - \alpha) \boldsymbol{\xi}^c$. Plugging the above two equations into Eq. (3.53), we can get

$$\mathbf{f}^c(\mathbf{X} + \boldsymbol{\xi}^c, \mathbf{X}) - \mathbf{f}^c(\mathbf{X}, \mathbf{X} - \boldsymbol{\xi}^c) = \nabla_{\mathbf{X}} \cdot \int_{\alpha=0}^1 \boldsymbol{\xi}^c \otimes \mathbf{f}^c(\mathbf{X} + \alpha \boldsymbol{\xi}^c, \mathbf{X} - (1 - \alpha) \boldsymbol{\xi}^c) d\alpha. \quad (3.56)$$

Similarly, we can have

$$\mathbf{f}^0(\mathbf{X} + \boldsymbol{\xi}, \mathbf{X}) - \mathbf{f}^0(\mathbf{X}, \mathbf{X} - \boldsymbol{\xi}) = \nabla_{\mathbf{X}} \cdot \int_{\alpha=0}^1 \boldsymbol{\xi} \otimes \mathbf{f}^0(\mathbf{X} + \alpha\boldsymbol{\xi}, \mathbf{X} - (1-\alpha)\boldsymbol{\xi}) d\alpha . \quad (3.57)$$

Summing the above two equations up, we will end up with

$$\begin{aligned} \int_{\mathcal{H}_{\mathbf{X}}} \mathbf{f}(\mathbf{X}, \mathbf{Y}) dV_{\mathbf{Y}} = & -\frac{1}{2} \nabla_{\mathbf{X}} \cdot \left[\int_{\mathcal{H}_{\mathbf{X}}} \int_{\alpha=0}^1 \boldsymbol{\xi} \otimes \mathbf{f}^0(\mathbf{X} + \alpha\boldsymbol{\xi}, \mathbf{X} - (1-\alpha)\boldsymbol{\xi}) d\alpha dV_{\boldsymbol{\xi}} \right] + \\ & -\frac{1}{2} \nabla_{\mathbf{X}} \cdot \left[\int_{\mathcal{H}_{\mathbf{X}}} \int_{\alpha=0}^1 \boldsymbol{\xi}^c \otimes \mathbf{f}^c(\mathbf{X} + \alpha\boldsymbol{\xi}^c, \mathbf{X} - (1-\alpha)\boldsymbol{\xi}^c) d\alpha dV_{\boldsymbol{\xi}^c} \right] \end{aligned} \quad (3.58)$$

Following the Hardy-Murdoch sampling procedure stated in [35, 62, 51], we can obtain two explicit formulas that are more friendly for numerical implementation:

$$\begin{aligned} & -\frac{1}{2} \int_{\mathcal{H}_{\mathbf{X}}} \int_{\alpha=0}^1 \boldsymbol{\xi} \otimes \mathbf{f}^0(\mathbf{X} + \alpha\boldsymbol{\xi}, \mathbf{X} - (1-\alpha)\boldsymbol{\xi}) d\alpha dV_{\boldsymbol{\xi}} \\ & \approx \frac{1}{2} \sum_{J \in \mathcal{H}^I} \sum_{K \in \mathcal{H}^I} \underline{\mathbf{w}}^{JK} \mathbf{f}^0(\mathbf{X}^J, \mathbf{X}^K) \otimes \boldsymbol{\xi}^{JK} V^J V^K , \end{aligned} \quad (3.59)$$

$$\begin{aligned} & -\frac{1}{2} \int_{\mathcal{H}_{\mathbf{X}}} \int_{\alpha=0}^1 \boldsymbol{\xi} \otimes \mathbf{f}^c(\mathbf{X} + \alpha\boldsymbol{\xi}^c, \mathbf{X} - (1-\alpha)\boldsymbol{\xi}^c) d\alpha dV_{\boldsymbol{\xi}^c} \\ & \approx \frac{1}{2} \sum_{J \in \mathcal{H}^I} \sum_{K \in \mathcal{H}^I} \underline{\mathbf{w}}^{JK} \mathbf{f}^c(\mathbf{X}^J, \mathbf{X}^{K,c}) \otimes \boldsymbol{\xi}^{JK,c} V^J V^K . \end{aligned} \quad (3.60)$$

where the superscript I refers to the center point of the horizon $\mathcal{H}^I$ while J, K means two arbitrary points within the horizon $\mathcal{H}^I$. Substituting Eq. (3.53), (3.59) and (3.60) into Eq. (3.58) and considering the facts that $\boldsymbol{\xi} = |\boldsymbol{\xi}| \mathbf{N}$, $\boldsymbol{\xi}^c = |\boldsymbol{\xi}^c| \mathbf{T}$, the force flux can be approximated by

$$\int_{\mathcal{H}_{\mathbf{X}}} \mathbf{f}(\mathbf{X}, \mathbf{Y}) dV_{\mathbf{Y}} \approx \frac{1}{2} \nabla_{\mathbf{X}} \cdot \sum_{J \in \mathcal{H}^I} \sum_{K \in \mathcal{H}^I} \underline{\mathbf{w}}^{JK} \left(f_N \mathbf{n} \otimes \mathbf{N} + \frac{f_T}{2} \mathbf{t} \otimes \mathbf{N} + \frac{f_T}{2} \mathbf{n} \otimes \mathbf{T} \right) V^J V^K \quad (3.61)$$

This format is consistent with the PK1 stress we have derived in Eq. (3.46).

Since the derived Cauchy stress in Eq. (3.47) is symmetric, i.e.

$$\boldsymbol{\sigma}(\mathbf{X}) = (\boldsymbol{\sigma}(\mathbf{X}))^T , \quad (3.62)$$

the angular momentum balance should be satisfied. This conclusion can be verified through another approach. Supposing the nonlocal force flux is zero, the nonlocal angular momentum can be computed in current configuration by

$$\begin{aligned}
 & \int_{\mathcal{H}_{\mathbf{x}}} \underline{\mathbf{w}}(\mathbf{X}, \mathbf{X}') V_{\mathcal{H}_{\mathbf{x}}}(\mathbf{y} - \mathbf{x}) \times \mathbf{f}(\mathbf{X}, \mathbf{X}') dv_{\mathbf{x}'} \\
 &= \int_{\mathcal{H}_{\mathbf{x}}} \underline{\mathbf{w}}(\mathbf{X}, \mathbf{X}') V_{\mathcal{H}_{\mathbf{x}}}(\mathbf{y} - \mathbf{x}) \times [\mathbf{f}(\mathbf{X}, \mathbf{X}') + \mathbf{f}^c(\mathbf{X}, \mathbf{X}'^c)] dv_{\mathbf{x}'} \\
 &= \int_{\mathcal{H}_{\mathbf{x}}} \underline{\mathbf{w}} V_{\mathcal{H}_{\mathbf{x}}} [((\mathbf{y} - \mathbf{x}) - (\mathbf{x}' - \mathbf{x})) \times \mathbf{f}^0 + ((\mathbf{y} - \mathbf{x}) - (\mathbf{x}'^c - \mathbf{x})) \times \mathbf{f}^c] dv_{\mathbf{x}'} \\
 &= - \int_{\mathcal{H}_{\mathbf{x}}} \underline{\mathbf{w}} V_{\mathcal{H}_{\mathbf{x}}} [(\mathbf{x}' - \mathbf{x}) \times \mathbf{f}^0 + (\mathbf{x}'^c - \mathbf{x}) \times \mathbf{f}^c] dv_{\mathbf{x}'} \\
 &= - \int_{\mathcal{H}_{\mathbf{x}}} \underline{\mathbf{w}} V_{\mathcal{H}_{\mathbf{x}}} \left[\frac{\mathbf{n}}{|\mathbf{n}|} \times \left(\frac{f_N}{\xi} \mathbf{n} \right) + \frac{\mathbf{n}}{|\mathbf{n}|} \times \left(\frac{f_T}{2\xi} \mathbf{t} \right) + \frac{\mathbf{t}}{|\mathbf{t}|} \times \frac{f_T}{2\xi} \mathbf{n} \right] dv_{\mathbf{x}'} \\
 &= - \int_{\mathcal{H}_{\mathbf{x}}} \underline{\mathbf{w}} V_{\mathcal{H}_{\mathbf{x}}} \left[\frac{f_N}{|\mathbf{n}|\xi} \mathbf{n} \times \mathbf{n} + \frac{f_T}{2\xi|\mathbf{n}|} (\mathbf{n} \times \mathbf{t} + \mathbf{t} \times \mathbf{n}) \right] dv_{\mathbf{x}'} \\
 &= 0
 \end{aligned} \tag{3.63}$$

Thus, the nonlocal angular momentum balance is satisfied.

Objectivity of stress measures

The Cauchy stress is adopted to illustrate the objectivity of the stress measures derived above. Let $\mathbf{Q}(t)$ be a proper orthogonal transformation depending on time t . After a certain time, the deformation gradient becomes $\mathbf{F}^+(t)$ that satisfies

$$\mathbf{F}^+(t) = \mathbf{Q}(t)\mathbf{F}$$

Consequently,

$$\mathbf{n}^+(t) = \mathbf{Q}(t)\mathbf{F}\mathbf{N} = \mathbf{Q}(t)\mathbf{n} \quad \text{and} \quad \mathbf{t}^+(t) = \mathbf{Q}(t)\mathbf{F}\mathbf{N} = \mathbf{Q}(t)\mathbf{t}$$

can be derived. To simplify the following illustration, we ignore the time t . It should also be noted that the following relation

$$J^+ = \det(\mathbf{F}^+) = \det(\mathbf{Q}\mathbf{F}) = \det(\mathbf{Q})\det(\mathbf{F}) = J$$

is held. Thus, the Cauchy stress measured in the current configuration after rigid body rotation can be expressed as

$$\begin{aligned}
 \boldsymbol{\sigma}^+(\mathbf{X}) &= \frac{1}{2J^+} \int_{\mathcal{H}_{\mathbf{x}}} \int_{\mathcal{H}_{\mathbf{x}}} \underline{\mathbf{w}}(\mathbf{X}', \mathbf{X}'') \left(f_N \mathbf{n}^+ \otimes \mathbf{n}^+ + \frac{f_T}{2} (\mathbf{n}^+ \otimes \mathbf{t}^+ + \mathbf{t}^+ \otimes \mathbf{n}^+) \right) dV_{\mathbf{X}''} dV_{\mathbf{X}'} \\
 &= \frac{1}{2J} \int_{\mathcal{H}_{\mathbf{x}}} \int_{\mathcal{H}_{\mathbf{x}}} \underline{\mathbf{w}}(\mathbf{X}', \mathbf{X}'') \left(f_N \mathbf{Q}\mathbf{n} \otimes \mathbf{n}\mathbf{Q}^T + \frac{f_T}{2} (\mathbf{Q}\mathbf{n} \otimes \mathbf{t}\mathbf{Q}^T + \mathbf{Q}\mathbf{t} \otimes \mathbf{n}\mathbf{Q}^T) \right) dV_{\mathbf{X}''} dV_{\mathbf{X}'} \\
 &= \mathbf{Q}\boldsymbol{\sigma}(\mathbf{X})\mathbf{Q}^T
 \end{aligned}$$

Therefore, the objectivity of stress measures is preserved.

3.3 Constitutive Relations: Family of Bond Potentials

• Saint Venant–Kirchhoff - type I model

One of the simplest bond strain energy functions should be the one in quadratic form and only related to the normal deformation of bond E_{NN} , i.e.

$$\phi(E_{NN}, E_{NT}) = \frac{cE_{NN}^2}{2} \mathbf{1}[E_{NN,cr} - E_{NN}] \quad (3.64)$$

where c is the micro-modulus of the bond; $E_{NN,cr}$ represents the critical deformation of bond when breaking; $\mathbf{1}[x]$ is the Heaviside step function that satisfies $\mathbf{1}[x] = 1$ if $x \geq 0$ and $\mathbf{1}[x] = 0$ if $x < 0$. Since we construct this model based on the quadratic form of the Green-Lagrange strain, we name it the Saint Venant-Kirchhoff type I(SVK1) model. By utilizing Eq. (3.26) and (3.30), the corresponding micro-force components and force density can be derived,

$$f_N = cE_{NN} \mathbf{1}[E_{NN,cr} - E_{NN}], \quad f_T = 0 \quad (3.65)$$

$$\mathbf{f} = \frac{1}{\xi} cE_{NN} \mathbf{1}[E_{NN,cr} - E_{NN}] \mathbf{n} \quad (3.66)$$

Combining Eq. (3.65) with Eq. (3.43), taking derivative with respect to $\mathbf{E}$ and assuming $\omega(\mathbf{X}^J, \mathbf{X}^K) = \frac{1}{V_{\mathcal{H}}^2}$. For the sake of simplicity, the fourth-order elastic modulus can be expressed as

$$\mathbb{C} = \frac{c}{2V_{\mathcal{H}}^2} \int_{\mathbf{X}} \int_{\mathbf{X}'} \mathbf{N} \otimes \mathbf{N} \otimes \mathbf{N} \otimes \mathbf{N} dV_{\mathbf{X}'} dV_{\mathbf{X}} \quad (3.67)$$

To illustrate the application of the above formula, we discuss three common cases in the following sections, i.e., two-dimensional plane stress case, two-dimensional plane strain case, and three-dimensional case.

Two dimensional case

In the 2D case, the analytical expression of the Cauchy stress as well as elastic modulus under uniform strain E can be obtained

$$\mathbb{C} = \frac{c}{16} \mathbb{I}^{(2)} \otimes \mathbb{I}^{(2)} + \frac{c}{8} \mathbb{I}^{(4s)} \quad (3.68)$$

For more derivation details, readers are referred to Eq. (A12). Compared with Lamé constants for isotropic material, one can realize that

$$\lambda = \frac{c}{16} \quad \text{and} \quad \mu = \frac{c}{16}.$$

In plane stress case, the Young's modulus as well as the Poisson's ratio can be related to λ and μ by

$$E_{PS} = \frac{4\mu(\lambda + \mu)}{\lambda + 2\mu} = \frac{c}{6} \quad \text{and} \quad \nu_{PS} = \frac{\lambda}{\lambda + 2\mu} = \frac{1}{3} \quad \text{respectively.}$$

As for plane strain, one can derive similar relations, i.e.

$$E_{PE} = \frac{\mu(3\lambda + 2\mu)}{\lambda + \mu} = \frac{5c}{32} \quad \text{and} \quad \nu_{PE} = \frac{\lambda}{2(\lambda + \mu)} = \frac{1}{4}.$$

Three dimensional Case

Similar to the 2D case, the analytic expression of the fourth-order elastic tensor in the 3D case has been obtained in the Appendix. In specific, by leveraging Eq. (A26) we have,

$$\mathbb{C} = \frac{c}{10} \mathbb{I}^{(2)} \otimes \mathbb{I}^{(2)} + \frac{c}{5} \mathbb{I}^{(4s)} \quad (3.69)$$

Following the same procedure, we can obtain the formula between λ, μ and c as

$$\lambda = \frac{c}{10} \quad \text{and} \quad \mu = \frac{c}{10}.$$

Thus, the relation between E, ν and c should be

$$E_{3D} = \frac{\mu(3\lambda + 2\mu)}{\lambda + \mu} = \frac{c}{4} \quad \text{and} \quad \nu_{3D} = \frac{\lambda}{2(\lambda + \mu)} = \frac{1}{4}.$$

We also provide an ad-hoc method to calibrate $E_{N,cr}$ by energy release rate. Assuming that one crack penetrates through the particle $\mathbf{X}$ such that all the bonds between particle $\mathbf{X}$ and its neighbors are cut off. In this scenario, the released energy should be

$$\begin{aligned} \Delta \mathcal{W}(\mathbf{X}) V(\mathbf{X}) &= \frac{1}{2} \int_{\mathcal{H}_{\mathbf{X}}} \int_{\mathcal{H}_{\mathbf{X}}} \frac{1}{V_{\mathcal{H}_{\mathbf{X}}}^2} \frac{c E_{N,cr}^2}{2} dV_{\mathbf{X}''} dV_{\mathbf{X}'} V(\mathbf{X}) \\ &= \frac{1}{4} c E_{N,cr}^2 V(\mathbf{X}) \\ &= 2a B \mathcal{G}_{Ic} \end{aligned} \quad (3.70)$$

where $\mathcal{G}_{Ic}$ is the mode-I energy release rate of material; $2a$ is the length of the assumed crack that exists in the space represented by particle $\mathbf{X}$; and B is the out-of-plane thickness of particle $\mathbf{X}$'s space. In the meantime, the assumption on the weight function $\underline{w}(\mathbf{X}^J, \mathbf{X}^K) = \frac{1}{V_{\mathcal{H}^I}^2}$ is adopted. Let $l_c := V(\mathbf{X})/(2aB)$ be the characteristic length, then

$$\frac{1}{4} c E_{N,cr}^2 l_c = \mathcal{G}_{Ic} \quad (3.71)$$

Finally, the two parameters in the potential energy function c and $E_{N,cr}$ can be calibrated as follows,

$$c = \begin{cases} 6E & \text{Plane Stress} \\ \frac{32}{5}E & \text{Plane Strain} \\ 4E & \text{Three Dimension} \end{cases} \quad (3.72)$$

$$\text{and } E_{N,cr} = \left[\frac{4\mathcal{G}_{Ic}}{c \cdot l_c} \right]^{\frac{1}{2}} \quad (3.73)$$

• **Saint Venant-Kirchhoff - type II model**

If the linear reaction to the bond shear deformation is also considered, the Saint Venant-Kirchhoff type II (SVK2) model may be established. The bond strain energy potential function reads as follows,

$$\phi(E_{NN}, E_{NT}) = \frac{c_n E_{NN}^2}{2} \mathbf{1}_n [E_{NN,cr} - E_{NN}] + \frac{c_t E_{NT}^2}{2} \mathbf{1}_t [E_{NT,cr} - E_{NT}] \quad (3.74)$$

where c_n, c_t are the micro-modulus of the bond in normal and tangential directions, respectively; $E_{NN,cr}, E_{NT,cr}$ represent the critical deformation of the bond when breaking in normal and tangential directions; $\mathbf{1}_n[x]$ and $\mathbf{1}_t[x]$ are both Heaviside functions that satisfy $\mathbf{1}_n[x] = 1$ if $x \geq 0$ otherwise $\mathbf{1}_n[x] = 0$ and $\mathbf{1}_t[x] = 1$ if $x \geq 0$ otherwise $\mathbf{1}_t[x] = 0$ respectively. Similarly, the micro-force and force density can be derived. They are

$$f_N = c_n E_{NN} \mathbf{1}_n [E_{NN,cr} - E_{NN}], \quad f_T = c_t E_{NT} \mathbf{1}_t [E_{NT,cr} - E_{NT}] \quad (3.75)$$

$$\mathbf{f} = \frac{1}{\xi} c_n E_{NN} \mathbf{1}_n \mathbf{n} + \frac{1}{2\xi} c_t E_{NT} \mathbf{1}_t \mathbf{t} + \frac{1}{2\xi} c_t E_{NT} \mathbf{1}_t \mathbf{n} \quad (3.76)$$

respectively. The elastic modulus can be obtained in a more complicated form than the type I model. For clear illustration, it is presented in indicial notation as follows.

$$\begin{aligned} C_{ijkl} &= \left. \frac{\partial S_{ij}}{\partial E_{kl}} \right|_{E_{kl}=0} \\ &= \int_{\mathbf{X}} \int_{\mathbf{X}'} \frac{1}{2V_{\mathcal{H}}^2} \left[c_n N_i N_j N_k N_l \right. \\ &\quad \left. + c_t \frac{1}{4} (N_i \delta_{jk} N_l + N_i \delta_{jl} N_k + \delta_{ik} N_j N_l + \delta_{il} N_j N_k - 4N_i N_j N_k N_l) \right] dV_{\mathbf{X}'} dV_{\mathbf{X}} \quad (3.77) \end{aligned}$$

Two dimensional case

By virtue of Eq. (A12) and Eq. (A13), the analytical expression of the fourth-order elastic

modulus can be obtained. Different from Eq. (3.77), it can be concisely expressed in tensorial form, i.e.

$$\mathbb{C} = \frac{c_n - c_t}{16} \mathbb{I}^{(2)} \otimes \mathbb{I}^{(2)} + \frac{c_n + c_t}{8} \mathbb{I}^{(4s)} \quad (3.78)$$

Compared with Lamé constants for isotropic material, one can find out that

$$\lambda = \frac{c_n - c_t}{16} \quad \text{and} \quad \mu = \frac{c_n + c_t}{16}.$$

Therefore, the Young's modulus and Poisson's ratio in plane stress case are

$$E_{PS} = \frac{4\mu(\lambda + \mu)}{\lambda + 2\mu} = \frac{(c_n + c_t)c_n}{2(3c_n + c_t)} \quad \text{and} \quad \nu_{PS} = \frac{\lambda}{\lambda + 2\mu} = \frac{c_n - c_t}{3c_n + c_t}.$$

As for plane strain case, they are

$$E_{PE} = \frac{\mu(3\lambda + 2\mu)}{\lambda + \mu} = \frac{(c_n + c_t)(5c_n - c_t)}{32c_n} \quad \text{and} \quad \nu_{PE} = \frac{\lambda}{2(\lambda + \mu)} = \frac{c_n - c_t}{4c_n}.$$

It is worth noting that Poisson's ratio for type II model is no more a fixed value due to the introduction of bond-level shear deformation. This feature makes NDFD BB-PD readily applicable in simulating various types of material failures.

Three dimensional case

When it comes to 3D case, the fourth-order elastic tensor can be derived by incorporating Eq. (A26), Eq. (A27) into Eq. (3.77), the analytical expression can then be written in tensorial form as,

$$\mathbb{C} = \frac{c_n - c_t}{10} \mathbb{I}^{(2)} \otimes \mathbb{I}^{(2)} + \frac{2c_n + 3c_t}{10} \mathbb{I}^{(4s)} \quad (3.79)$$

Therefore, the micro-modulus parameters c_n, c_t can be linked with Lamé constants as

$$\lambda = \frac{c_n - c_t}{10} \quad \text{and} \quad \mu = \frac{2c_n + 3c_t}{20}.$$

The corresponding Young's modulus as well as Poisson's ratio can be expressed in terms of c_n and c_t as follows,

$$E_{3D} = \frac{\mu(3\lambda + 2\mu)}{\lambda + \mu} = \frac{(2c_n + 3c_t)c_n}{2(4c_n + c_t)} \quad \text{and} \quad \nu_{3D} = \frac{\lambda}{2(\lambda + \mu)} = \frac{c_n - c_t}{4c_n + c_t}.$$

We keep following the ad-hoc method mentioned above, i.e. linking energy release rate of material in macro-scale with the energy required to break bonds in meso-scale. In Mode I fracture, it reads

$$\begin{aligned} \Delta \mathcal{W}(\mathbf{X}) V(\mathbf{X}) &= \frac{1}{2} \int_{\mathcal{H}_{\mathbf{X}}} \int_{\mathcal{H}_{\mathbf{X}}} \frac{1}{V_{\mathcal{H}_{\mathbf{X}}}^2} \frac{1}{2} c_n E_{NN,cr}^2 dV_{\mathbf{X}''} dV_{\mathbf{X}'} V(\mathbf{X}) \\ &= \frac{1}{4} c_n E_{NN,cr}^2 V(\mathbf{X}) \\ &= 2a_n B \mathcal{G}_{Ic} \end{aligned} \quad (3.80)$$

Similarly, we define a normal characteristic length as $l_{n,c} := V(\mathbf{X})/(2a_n B)$, then

$$\frac{1}{4}c_n E_{NN,cr}^2 l_{n,c} = \mathcal{G}_{Ic} \quad (3.81)$$

Moreover, the meso-scale breakage of peridynamics bonds can also be related to the energy release rate in Mode II, i.e.

$$\begin{aligned} \Delta \mathcal{W}(\mathbf{X}) V(\mathbf{X}) &= \frac{1}{2} \int_{\mathcal{H}_{\mathbf{X}}} \int_{\mathcal{H}_{\mathbf{X}}} \frac{1}{V_{\mathcal{H}_{\mathbf{X}}}^2} \frac{1}{2} c_t E_{NT,cr}^2 dV_{\mathbf{X}''} dV_{\mathbf{X}'} V(\mathbf{X}) \\ &= \frac{1}{4} c_t E_{NT,cr}^2 V(\mathbf{X}) \\ &= 2a_t B \mathcal{G}_{IIc} \end{aligned} \quad (3.82)$$

and by defining $l_{t,c} := V(\mathbf{X})/(2a_t B)$, we will realize the relation,

$$\frac{1}{4} c_t E_{NT,cr}^2 l_{t,c} = \mathcal{G}_{IIc} \quad (3.83)$$

Combining all the formulations derived above together, the four parameters c_n , c_t , $E_{NN,cr}$ and $E_{NT,cr}$ can be calibrated by the elastic and fracture properties of the material as follows,

$$c_n = \begin{cases} \frac{4E}{1-\nu} & \text{Plane Stress} \\ \frac{4E}{(1+\nu)(1-2\nu)} & \text{Plane Strain} \\ \frac{2E}{1-2\nu} & \text{Three Dimension} \end{cases} \quad (3.84)$$

$$c_t = \begin{cases} \frac{4E(1-3\nu)}{(1+\nu)(1-\nu)} & \text{Plane Stress} \\ \frac{4E(1-4\nu)}{(1+\nu)(1-2\nu)} & \text{Plane Strain} \\ \frac{2E(1-4\nu)}{(1+\nu)(1-2\nu)} & \text{Three Dimension} \end{cases} \quad (3.85)$$

$$E_{NN,cr} = \left[\frac{4\mathcal{G}_{Ic}}{c_n \cdot l_{n,c}} \right]^{\frac{1}{2}} \quad (3.86)$$

$$E_{NT,cr} = \left[\frac{4\mathcal{G}_{IIc}}{c_t \cdot l_{t,c}} \right]^{\frac{1}{2}} \quad (3.87)$$

It should be noted that the micro-modulus parameters c_n and c_t are usually positive, which results in the limit on Poisson's ratio to be $\nu < 1/3$ for plane stress case and $\nu < 1/4$ for plane strain and 3D case.

• **Xu-Needleman model**

Type I and Type II models can be considered linear elastic fracture models in the 1D case. This section will present one cohesive model adapted from the original Xu-Needleman model [63, 91, 90]. For the sake of a simple statement, we still name this cohesive model as the Xu-Needleman (XN) model. The potential energy function in this model writes

$$\phi(E_{NN}, E_{NT}) = \phi_n + \phi_n \exp(-\alpha_n E_{NN}) (1 + \alpha_n E_{NN}) [q - 1 - q \cdot \exp(-\alpha_t^2 E_{NT}^2)] \quad (3.88)$$

where ϕ_n refers to the energy required to break a bond in normal direction; $\phi_n q$ is the energy required to break a bond in tangential direction, thus q is the ratio between these two types of energy; α_n, α_t are the dimensionless coefficients. By taking derivative with respect to E_{NN} and E_{NT} respectively, the micro-force writes

$$f_N = \alpha_n \phi_n \cdot (\alpha_n E_{NN}) \exp(-\alpha_n E_{NN}) [q \cdot \exp(-\alpha_t^2 E_{NT}^2) + 1 - q] \quad (3.89)$$

$$f_T = \alpha_t \cdot 2\phi_n q \cdot (\alpha_t E_{NT}) (1 + \alpha_n E_{NN}) \exp(-\alpha_n E_{NN}) \exp(-\alpha_t^2 E_{NT}^2) \quad (3.90)$$

$$\mathbf{f} = \frac{1}{\xi} f_N \mathbf{n} + \frac{1}{2\xi} f_T \mathbf{t} + \frac{1}{2\xi^c} f_T \mathbf{n} \quad (3.91)$$

A schematic diagram of f_N and f_T is given in Fig. 3.4. As shown in Fig. 3.4, both f_N and f_T are nonlinear. To achieve the elastic tensor for this model, we shall linearize this model at infinitesimal deformation, i.e.

$$\begin{aligned} f_N &\approx \alpha_n^2 \phi_n E_{NN}, & \text{when } E_{NN} \rightarrow 0, \quad E_{NT} = 0, \\ f_T &\approx 2\alpha_t^2 \phi_n q E_{NT}, & \text{when } E_{NN} = 0, \quad E_{NT} \rightarrow 0. \end{aligned}$$

The analytical solution to the elastic tensor can be obtained following the same procedure we have done for the SVK2 model. The procedure will not be repeated here again.

Two hypothetical situations will be discussed when it comes to energy release rate. In the first situation, all the bonds within the horizon exhibit significant stretch and zero shear deformation, indicating the material's mode I fracture. In the second situation, all the bonds demonstrate substantial shear deformation and zero stretch, corresponding to the mode II

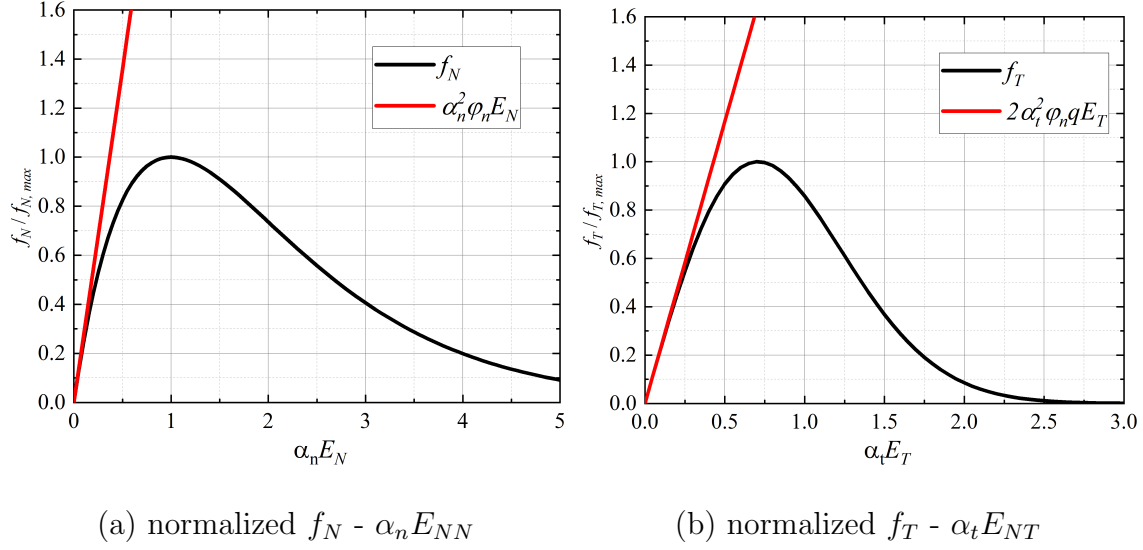


Figure 3.4: Schematic diagram of the Xu-Needleman (XN) Model

fracture. Given that the XN potential energy function is continuous, it can be deduced that

$$\begin{aligned}
 \Delta \mathcal{W}(\mathbf{X}) V(\mathbf{X}) &= \frac{1}{2} \int_{\mathcal{H}_{\mathbf{X}}} \int_{\mathcal{H}_{\mathbf{X}}} \frac{1}{V_{\mathcal{H}_{\mathbf{X}}}^2} \phi_n dV_{\mathbf{X}''} dV_{\mathbf{X}'} V(\mathbf{X}) \\
 &= \frac{1}{2} \phi_n V(\mathbf{X}), \quad \text{when } E_{NN} \rightarrow \infty, E_{NT} = 0
 \end{aligned} \tag{3.92}$$

$$\begin{aligned}
 \Delta \mathcal{W}(\mathbf{X}) V(\mathbf{X}) &= \frac{1}{2} \int_{\mathcal{H}_{\mathbf{X}}} \int_{\mathcal{H}_{\mathbf{X}}} \frac{1}{V_{\mathcal{H}_{\mathbf{X}}}^2} \phi_n q dV_{\mathbf{X}''} dV_{\mathbf{X}'} V(\mathbf{X}) \\
 &= \frac{1}{2} \phi_n q V(\mathbf{X}), \quad \text{when } E_{NT} \rightarrow \infty, E_{NN} = 0
 \end{aligned} \tag{3.93}$$

In summary, the parameters of the XN model can be calibrated by

$$\alpha_n^2 \phi_n = \begin{cases} \frac{4E}{1-\nu} & \text{Plane Stress} \\ \frac{4E}{(1+\nu)(1-2\nu)} & \text{Plane Strain} \\ \frac{2E}{1-2\nu} & \text{Three Dimension} \end{cases} \quad (3.94)$$

$$2\alpha_t^2 \phi_n q = \begin{cases} \frac{4E(1-3\nu)}{(1+\nu)(1-\nu)} & \text{Plane Stress} \\ \frac{4E(1-4\nu)}{(1+\nu)(1-2\nu)} & \text{Plane Strain} \\ \frac{2E(1-4\nu)}{(1+\nu)(1-2\nu)} & \text{Three Dimension} \end{cases} \quad (3.95)$$

$$\phi_n = \frac{2\mathcal{G}_{Ic}}{l_{n,c}} \quad (3.96)$$

$$\phi_t = \phi_n q = \frac{2\mathcal{G}_{IIc}}{l_{t,c}} \quad (3.97)$$

• Peierls-Rice-Beltz model

Another cohesive model was proposed by Rice and Beltz based on the Peierls continuous dislocation model framework, e.g. [66, 68, 67], which was designed for crystalline material. The bond strain energy potential function of this Peierls-Rice-Beltz (PRB) model is constructed as

$$\phi(E_{NN}, E_{NT}) = \phi_n + \phi_n \exp(-\alpha_n E_{NN}) (1 + \alpha_n E_{NN}) [q \cdot \sin^2(\pi \alpha_t E_{NT}) - 1] \quad (3.98)$$

The corresponding micro-forces are

$$f_N = \alpha_n \phi_n \cdot (\alpha_n E_{NN}) \exp(-\alpha_n E_{NN}) [1 - q \cdot \sin^2(\pi \alpha_t E_{NT})] \quad (3.99)$$

$$f_T = \alpha_t \cdot \pi \phi_n q \cdot (1 + \alpha_n E_{NN}) \exp(-\alpha_n E_{NN}) \sin(2\pi \alpha_t E_{NT}) \quad (3.100)$$

$$\mathbf{f} = \frac{1}{\xi} f_N \mathbf{n} + \frac{1}{2\xi} f_T \mathbf{t} + \frac{1}{2\xi^c} f_T \mathbf{n} \quad (3.101)$$

where ϕ_n refers to the energy required to break a bond in normal direction; $\phi_t = \phi_n q$ is the energy required to break a bond in tangential direction, thus q is the ratio between these two types of energy; α_n, α_t are the dimensionless coefficients. As shown in Fig. 3.5, the normal micro-force is similar to the XN mode, while the tangential one is in a sinusoidal form. Notably, this sinusoidal form is intentionally introduced to reflect the force required

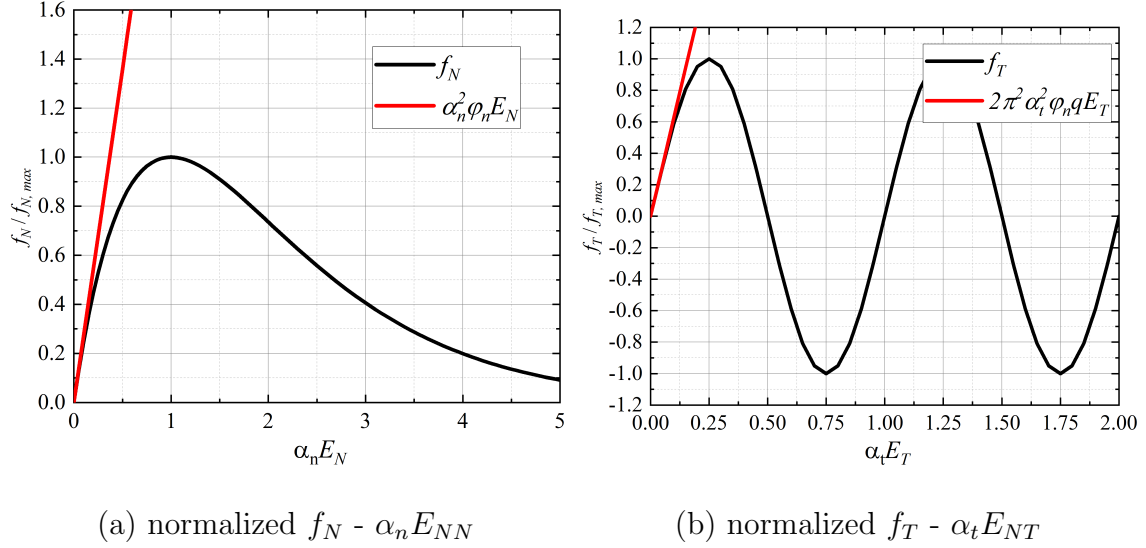


Figure 3.5: Schematic diagram of Peierls-Rice-Beltz Model

to overcome the barrier of dislocations in crystalline material.

When the deformation is infinitesimal, the micro-force can be linearized as follows,

$$\begin{aligned} f_N &\approx \alpha_n^2 \phi_n E_{NN}, & \text{when } E_{NN} \rightarrow 0, \quad E_{NT} = 0, \\ f_T &\approx 2\pi^2 \alpha_t^2 \phi_n q E_{NT}, & \text{when } E_{NN} = 0, \quad E_{NT} \rightarrow 0. \end{aligned}$$

Meanwhile, the change of bond potential energy can be related to the energy release rate of material by

$$\begin{aligned} \Delta \mathcal{W}(\mathbf{X}) V(\mathbf{X}) &= \frac{1}{2} \int_{\mathcal{H}_{\mathbf{X}}} \int_{\mathcal{H}_{\mathbf{X}}} \frac{1}{V_{\mathcal{H}_{\mathbf{X}}}^2} \phi_n dV_{\mathbf{X}''} dV_{\mathbf{X}'} V(\mathbf{X}) \\ &= \frac{1}{2} \phi_n V(\mathbf{X}), & \text{when } E_{NN} \rightarrow \infty, E_{NT} = 0 \end{aligned} \quad (3.102)$$

$$\begin{aligned} \Delta \mathcal{W}(\mathbf{X}) V(\mathbf{X}) &= \frac{1}{2} \int_{\mathcal{H}_{\mathbf{X}}} \int_{\mathcal{H}_{\mathbf{X}}} \frac{1}{V_{\mathcal{H}_{\mathbf{X}}}^2} \phi_n q dV_{\mathbf{X}''} dV_{\mathbf{X}'} V(\mathbf{X}) \\ &= \frac{1}{2} \phi_n q V(\mathbf{X}), & \text{when } E_{NT} = \frac{2k+1}{2\alpha_t}, E_{NN} = 0 \end{aligned} \quad (3.103)$$

where $k = 1, 2, 3, \dots$ represents the integers greater than zero.

The same procedure as that for SVK2 model or XN model is adopted here to calibrate the parameters, and the final results are given below

$$\alpha_n^2 \phi_n = \begin{cases} \frac{4E}{1-\nu} & \text{Plane Stress} \\ \frac{4E}{(1+\nu)(1-2\nu)} & \text{Plane Strain} \\ \frac{2E}{1-2\nu} & \text{Three Dimension} \end{cases} \quad (3.104)$$

$$2\pi^2 \alpha_t^2 \phi_n q = \begin{cases} \frac{4E(1-3\nu)}{(1+\nu)(1-\nu)} & \text{Plane Stress} \\ \frac{4E(1-4\nu)}{(1+\nu)(1-2\nu)} & \text{Plane Strain} \\ \frac{2E(1-4\nu)}{(1+\nu)(1-2\nu)} & \text{Three Dimension} \end{cases} \quad (3.105)$$

$$\phi_n = \frac{2\mathcal{G}_{Ic}}{l_{n,c}} \quad (3.106)$$

$$\phi_t = \phi_n q = \frac{2\gamma_{us}}{l_{t,c}} \quad (3.107)$$

Chapter 4

Bond-associated state-based material correspondence models

4.1 Bond force states

The generalized bond force density state corresponding to the generalized bond-associated deformation gradient in Eq. (2.4) can be derived using the strain energy equivalency approach following the same procedure as outlined by Silling et al. [72]. In the following derivation, the state operating variable $\langle \boldsymbol{\xi} \rangle$ for states $\underline{\mathbf{A}}$ and $\underline{\mathbf{B}}$ is dropped for clarity.

Let's first define the nonlocal strain energy density for bond-associated models as:

$$\mathcal{W} = \int_{\mathcal{H}} \underline{w}(\mathbf{X}') \mathbf{P}_{\boldsymbol{\xi}} : \mathbf{F}_{\boldsymbol{\xi}} dV_{\mathbf{X}'}, \quad (4.1)$$

where $\underline{w}(\mathbf{X}')$ is a scalar weight function that satisfies $\int_{\mathcal{H}} \underline{w}(\mathbf{X}') dV_{\mathbf{X}'} = 1$; $\mathbf{F}_{\boldsymbol{\xi}}$ denotes the deformation gradient associated with bond $\boldsymbol{\xi}$, and $\mathbf{P}_{\boldsymbol{\xi}}$ is the first Piola–Kirchhoff stress (PK1 stress) corresponding to $\mathbf{F}_{\boldsymbol{\xi}}$.

For the bond-associated material correspondence models whose nonlocal deformation gradient is formulated based on the whole horizon, i.e., excluding the sub-horizon-based models, a volume fraction function can be used for the weight function as [15]

$$\underline{w}(\mathbf{X}') = \frac{1}{V_{\mathcal{H}}}, \quad (4.2)$$

where $V_{\mathcal{H}}$ is the volume of the horizon of a material point $\mathbf{X}$.

Assuming $\mathbf{F}_{\boldsymbol{\xi}}$ is differentiable, its Fréchet derivative can be obtained using the following

equation:

$$\begin{aligned}
 \mathbf{F}_\xi(\underline{\mathbf{y}}' + \Delta \underline{\mathbf{y}}') &= \left[\int_{\mathcal{H}_\xi} \underline{\omega}(\xi') \cdot (\underline{\mathbf{y}}' + \Delta \underline{\mathbf{y}}') \otimes \xi' dV_{\mathbf{X}''} \right] \mathbf{K}_\xi^{-1} \underline{\mathbf{A}} + \underline{\mathbf{B}} + \left(\hat{\delta} [\xi' - \xi] \nabla_{\underline{\mathbf{y}}'} \underline{\mathbf{B}} \right) \bullet \Delta \underline{\mathbf{y}}' \\
 &= \left[\int_{\mathcal{H}_\xi} \underline{\omega}(\xi') \cdot \underline{\mathbf{y}}' \otimes \xi' dV_{\mathbf{X}''} \right] \mathbf{K}_\xi^{-1} \underline{\mathbf{A}} + \underline{\mathbf{B}} + \left[\int_{\mathcal{H}_\xi} \underline{\omega}(\xi') \cdot \Delta \underline{\mathbf{y}}' \otimes \xi' dV_{\mathbf{X}''} \right] \mathbf{K}_\xi^{-1} \underline{\mathbf{A}} \\
 &\quad + \left(\hat{\delta} [\xi' - \xi] \nabla_{\underline{\mathbf{y}}'} \underline{\mathbf{B}} \right) \bullet \Delta \underline{\mathbf{y}}',
 \end{aligned} \tag{4.3}$$

where operator $\bullet$ represents the *dot product* of two states. In state-based peridynamics [72], the dot product of two states $\underline{\mathbf{A}}$ and $\underline{\mathbf{B}}$ of the same order is defined as

$$\underline{\mathbf{A}} \bullet \underline{\mathbf{B}} := \int_{\mathcal{H}} \underline{\mathbf{A}} \cdot \underline{\mathbf{B}} dV_{\mathbf{X}'}. \tag{4.4}$$

It should be noted that the above Eq. (4.3) assumes that between states $\underline{\mathbf{A}}$ and $\underline{\mathbf{B}}$ only the state $\underline{\mathbf{B}}$ depends on the deformation state $\underline{\mathbf{y}}'$. This assumption is consistent with all the bond-associated deformation gradients discussed in Chapter 2.

From the Fréchet derivative provided in Eq. (4.3) and letting $\mathbf{F}_\xi(\underline{\mathbf{y}}' + \Delta \underline{\mathbf{y}}') = \mathbf{F}_\xi + \Delta \mathbf{F}_\xi$, the increment of deformation gradient $\Delta F_{\xi,ij}$ can be expressed using index notation as

$$\begin{aligned}
 \Delta F_{\xi,ij} &= \int_{\mathcal{H}} \underline{\omega}(\xi') I_{il} \xi'_Q K_{\xi,QR}^{-1} \underline{A}_{RJ} \Delta y'_l dV_{\mathbf{X}''} + \left(\hat{\delta} [\xi' - \xi] \nabla_{\underline{\mathbf{y}}'_l} \underline{B}_{ij} \right) \bullet \Delta \underline{\mathbf{y}}'_l \\
 &= \left[\underline{\omega}(\xi') I_{il} \xi'_Q K_{\xi,QR}^{-1} \underline{A}_{RJ} + \hat{\delta} [\xi' - \xi] \nabla_{\underline{\mathbf{y}}'_l} \underline{B}_{ij} \right] \bullet \Delta \underline{\mathbf{y}}'_l.
 \end{aligned} \tag{4.5}$$

Therefore, the gradient of deformation gradient with respect to $\underline{\mathbf{y}}'_l$ is

$$\nabla_{\underline{\mathbf{y}}'_l} F_{\xi,ij} = \underline{\omega}(\xi') I_{il} \xi'_Q K_{\xi,QR}^{-1} \underline{A}_{RJ} + \hat{\delta} [\xi' - \xi] \nabla_{\underline{\mathbf{y}}'_l} \underline{B}_{ij}. \tag{4.6}$$

It should be noted that this gradient is defined within the framework of the state dot product. Similarly, the increment of the nonlocal strain energy density $\Delta \mathcal{W}$ due to $\Delta \underline{\mathbf{y}}'$ can

be derived using Fréchet derivative as:

$$\begin{aligned}
 \Delta \mathcal{W} &= \int_{\mathcal{H}} \underline{\mathbf{w}}(\mathbf{X}') \mathbf{P}_{\xi} : \Delta \mathbf{F}_{\xi} dV_{\mathbf{X}'} \\
 &= \int_{\mathcal{H}} \underline{\mathbf{w}}(\mathbf{X}') P_{\xi, iJ} \left[\underline{\omega}(\xi') I_{il} \xi'_Q K_{\xi, QR}^{-1} \underline{\mathbf{A}}_{RJ} + \hat{\delta}[\xi' - \xi] \nabla_{y'_l} \underline{\mathbf{B}}_{iJ} \right] \bullet \Delta y'_l dV_{\mathbf{X}'} \\
 &= \int_{\mathcal{H}} \int_{\mathcal{H}} \underline{\mathbf{w}}(\mathbf{X}') P_{\xi, iJ} \left[\underline{\omega}(\xi') I_{il} \xi'_Q K_{\xi, QR}^{-1} \underline{\mathbf{A}}_{RJ} + \hat{\delta}[\xi' - \xi] \nabla_{y'_l} \underline{\mathbf{B}}_{iJ} \right] \cdot \Delta y'_l dV_{\mathbf{X}''} dV_{\mathbf{X}'} \\
 &= \int_{\mathcal{H}} \left\{ \left[\int_{\mathcal{H}} \underline{\mathbf{w}}(\mathbf{X}') \underline{\omega}(\xi') P_{\xi, lJ} \underline{\mathbf{A}}_{RJ} K_{\xi, QR}^{-1} dV_{\mathbf{X}'} \right] \xi'_Q \right\} \cdot \Delta y'_l dV_{\mathbf{X}''} \\
 &\quad + \int_{\mathcal{H}} \left[\int_{\mathcal{H}} \underline{\mathbf{w}}(\mathbf{X}') \hat{\delta}[\xi' - \xi] P_{\xi, iJ} \nabla_{y'_l} \underline{\mathbf{B}}_{iJ} dV_{\mathbf{X}'} \right] \cdot \Delta y'_l dV_{\mathbf{X}''} \\
 &= \left\{ \left[\int_{\mathcal{H}} \underline{\mathbf{w}}(\mathbf{X}') \underline{\omega}(\xi') \mathbf{P}_{\xi} \underline{\mathbf{A}}^T \mathbf{K}_{\xi}^{-1} dV_{\mathbf{X}'} \right] \xi' + \int_{\mathcal{H}} \underline{\mathbf{w}}(\mathbf{X}') \hat{\delta}[\xi' - \xi] \mathbf{P}_{\xi} : \nabla_{\mathbf{y}'} \underline{\mathbf{B}} dV_{\mathbf{X}'} \right\} \bullet \Delta \mathbf{y}'.
 \end{aligned} \tag{4.7}$$

Therefore, the unified force density state based on the unified bond-associated deformation gradient is obtained based on the work conjugate relation as

$$\begin{aligned}
 \underline{\mathbf{T}}\langle \xi \rangle &= \left[\int_{\mathcal{H}} \underline{\mathbf{w}}(\mathbf{X}'') \underline{\omega}(\xi') \mathbf{P}_{\xi'} \underline{\mathbf{A}}^T \langle \xi' \rangle \mathbf{K}_{\xi'}^{-1} dV_{\mathbf{X}''} \right] \xi \\
 &\quad + \int_{\mathcal{H}} \underline{\mathbf{w}}(\mathbf{X}'') \hat{\delta}[\xi - \xi'] \mathbf{P}_{\xi'} : \nabla_{\mathbf{y}} \underline{\mathbf{B}} \langle \xi' \rangle dV_{\mathbf{X}''}.
 \end{aligned} \tag{4.8}$$

It should be noted that the expression of the force density state in Eq. (4.8) is presented for bond ξ , instead of bond ξ' as directly from Eq. (4.7). The expression is given in a general form in terms of $\underline{\mathbf{A}}$ and $\underline{\mathbf{B}}$ without any assumptions of their specific forms. In the following, the specific expressions corresponding to different bond-associated deformation gradients are presented.

• Conventional model (CPD)

Considering the conditions presented in Eq. (2.6), the force density state for CPD has the following form:

$$\underline{\mathbf{T}}^{\text{CPD}}\langle \xi \rangle = \left[\int_{\mathcal{H}} \underline{\mathbf{w}}(\mathbf{X}'') \underline{\omega}^{\text{CPD}} \mathbf{P}_{\xi'} (\mathbf{K}_{\xi'}^{\text{CPD}})^{-1} dV_{\mathbf{X}''} \right] \xi = \underline{\omega}^{\text{CPD}}\langle \xi \rangle \mathbf{P}(\mathbf{K}^{\text{CPD}})^{-1} \xi. \tag{4.9}$$

Since the deformation gradient tensors and the shape tensors are identical for all bonds within the same horizon, the PK1 stress tensors are also identical. In this sense, the weighted average of $\mathbf{P}_{\xi'} (\mathbf{K}_{\xi'}^{\text{CPD}})^{-1}$ is identical to the one associated with each bond. Therefore, it can be simplified as $\mathbf{P}(\mathbf{K}^{\text{CPD}})^{-1}$.

• **Sub-horizon-based models (SHPD)**

For sub-horizon-based models subject to the conditions specified in Eq. (2.11), the evaluation of the force density state is also straightforward.

$$\underline{\mathbf{T}}^{\text{SHPD}} \langle \boldsymbol{\xi} \rangle = \left[\int_{\mathcal{H}} \underline{\mathbf{w}}^{\text{SHPD}}(\mathbf{X}'') [\boldsymbol{\xi}'] \underline{\boldsymbol{\omega}}^{\text{SHPD}} \langle \boldsymbol{\xi} \rangle \mathbf{P}_{\boldsymbol{\xi}'} (\mathbf{K}_{\boldsymbol{\xi}'}^{\text{SHPD}})^{-1} dV_{\mathbf{X}''} \right] \boldsymbol{\xi}. \quad (4.10)$$

It should be noted that in the above expression of the force density state for SHPD, the weight function $\underline{\mathbf{w}}^{\text{SHPD}}(\mathbf{X}'')$ is sub-horizon dependent. In terms of the function given in Eq. (4.2), the sub-horizon dependent weight function for the SHPD model is defined as

$$\underline{\mathbf{w}}^{\text{SHPD}}(\mathbf{X}'') = \begin{cases} 1/V_{\mathcal{H}}, & \mathbf{X}'' \in \mathcal{H}_{\boldsymbol{\xi}} \\ 0, & \text{otherwise.} \end{cases} \quad (4.11)$$

In the work of Chowdhury et al. [18], the whole horizon $\mathcal{H}$ is partitioned into several non-overlapping sub-horizons $\mathcal{H}_{\boldsymbol{\xi}}$. See Fig. 2.1b for the case of even partitioning of a 2D horizon into four sub-horizons. The bond-associated deformation gradient $\mathbf{F}_{\boldsymbol{\xi}}$ and the shape tensor $\mathbf{K}_{\boldsymbol{\xi}}$, therefore the PK1 stress $\mathbf{P}_{\boldsymbol{\xi}}$, are calculated for each sub-horizon and they are assumed to be identical for all bonds within the same sub-horizon. Therefore, for this case, the force density state for a given sub-horizon becomes

$$\underline{\mathbf{T}}^{\text{HPPD}} \langle \boldsymbol{\xi} \rangle = \left[\int_{\mathcal{H}} \underline{\mathbf{w}}^{\text{SHPD}}(\mathbf{X}'') dV_{\mathbf{X}''} \right] \underline{\boldsymbol{\omega}}^{\text{SHPD}} \langle \boldsymbol{\xi} \rangle \mathbf{P}_{\boldsymbol{\xi}} (\mathbf{K}_{\boldsymbol{\xi}}^{\text{SHPD}})^{-1} \boldsymbol{\xi} = \frac{V_{\mathcal{H}_{\boldsymbol{\xi}}}}{V_{\mathcal{H}}} \underline{\boldsymbol{\omega}}^{\text{SHPD}} \langle \boldsymbol{\xi} \rangle \mathbf{P}_{\boldsymbol{\xi}} (\mathbf{K}_{\boldsymbol{\xi}}^{\text{SHPD}})^{-1} \boldsymbol{\xi}, \quad (4.12)$$

where $V_{\mathcal{H}_{\boldsymbol{\xi}}}$ represents the volume of the sub-horizon that includes the bond $\boldsymbol{\xi}$.

In the initial work by Chen et al. [12, 17, 11], each bond has its own sub-horizon, and overlap exists among sub-horizons of bonds within the same material point horizon (see Fig. 2.1a). By distributing the strain energy of each bond by volume fraction within each sub-horizon, Chen et al. derived the same force density state as given in Eq. (4.12). Later, Chen and Chan [10] reformulated the force density state by removing the volume distribution assumption and derived the general form of the bond force density state given in Eq. (4.10).

• **Bond-correction-based model (BCPD)**

As for the conditions stated in Eq. (2.17) for the bond-correction-based model, the expression for the bond force density state involves the gradient of non-zero state $\underline{\mathbf{B}}$. Carrying out the calculation, the bond force density state for the bond-correction-based model can be obtained as

$$\underline{\mathbf{T}}^{\text{BCPD}} \langle \boldsymbol{\xi} \rangle = \left[\underline{\boldsymbol{\omega}}^{\text{CPD}} \langle \boldsymbol{\xi} \rangle \int_{\mathcal{H}} \underline{\mathbf{w}}(\mathbf{X}'') \mathbf{P}_{\boldsymbol{\xi}'} \left(\mathbf{I} - \frac{\boldsymbol{\xi}' \otimes \boldsymbol{\xi}'}{|\boldsymbol{\xi}'|^2} \right) (\mathbf{K}_{\boldsymbol{\xi}'}^{\text{CPD}})^{-1} dV_{\mathbf{X}''} + \frac{\underline{\mathbf{w}}(\mathbf{X}')}{|\boldsymbol{\xi}|^2} \mathbf{P}_{\boldsymbol{\xi}} \right] \boldsymbol{\xi}. \quad (4.13)$$

• **Lagrange-multiplier-based model (LMPD)**

Based on the updated form for the bond-associated deformation gradient given in Eq. (2.23) for the Lagrange-multiplier-based model, the bond force density state can be obtained from the general form as

$$\underline{\mathbf{T}}^{\text{LMPD}}\langle\boldsymbol{\xi}\rangle = \left[\int_{\mathcal{H}} \underline{\mathbf{w}}(\mathbf{X}') \underline{\omega}^{\text{LMPD}}\langle\boldsymbol{\xi}\rangle \mathbf{P}_{\boldsymbol{\xi}'} (\mathbf{K}_{\boldsymbol{\xi}'}^{\text{LMPD}})^{-1} dV_{\mathbf{X}''} \right] \boldsymbol{\xi}. \quad (4.14)$$

When $\lambda = 1$ in Eq. (2.22), this expression will degenerate to the one for the conventional model (Eq. (4.9)).

• **Non-spherical-influence-function-based model (NSPD)**

The bond force density state for the non-spherical-influence-function-based model shares the same form as that of the Lagrange-multiplier-based model, except the influence function $\underline{\omega}\langle\boldsymbol{\xi}\rangle$ for these two models is different. The non-spherical influence function $\underline{\omega}_{\text{NSPD}}(\boldsymbol{\xi}, \boldsymbol{\xi}')\langle\boldsymbol{\xi}'\rangle$ for this model is given in Eq. (2.26).

In summary, the specific expressions of the above discussed bond force density states are listed as follows:

$$\begin{aligned} \text{CPD} : \underline{\mathbf{T}}^{\text{CPD}}\langle\boldsymbol{\xi}\rangle &= \underline{\omega}^{\text{CPD}}\langle\boldsymbol{\xi}\rangle \mathbf{P}(\mathbf{K}^{\text{CPD}})^{-1} \boldsymbol{\xi} \\ \text{SHPD} : \underline{\mathbf{T}}^{\text{SHPD}}\langle\boldsymbol{\xi}\rangle &= \left[\int_{\mathcal{H}} \underline{\mathbf{w}}^{\text{SHPD}}(\mathbf{X}'') \underline{\omega}^{\text{SHPD}}\langle\boldsymbol{\xi}\rangle \mathbf{P}_{\boldsymbol{\xi}'} (\mathbf{K}_{\boldsymbol{\xi}'}^{\text{SHPD}})^{-1} dV_{\mathbf{X}''} \right] \boldsymbol{\xi} \\ \text{BCPD} : \underline{\mathbf{T}}^{\text{BCPD}}\langle\boldsymbol{\xi}\rangle &= \left[\underline{\omega}^{\text{CPD}}\langle\boldsymbol{\xi}\rangle \int_{\mathcal{H}} \underline{\mathbf{w}}(\mathbf{X}'') \mathbf{P}_{\boldsymbol{\xi}'} \left(\mathbf{I} - \frac{\boldsymbol{\xi}' \otimes \boldsymbol{\xi}'}{|\boldsymbol{\xi}'|^2} \right) (\mathbf{K}_{\boldsymbol{\xi}'}^{\text{CPD}})^{-1} dV_{\mathbf{X}''} + \frac{\underline{\mathbf{w}}(\mathbf{X}')}{|\boldsymbol{\xi}|^2} \mathbf{P}_{\boldsymbol{\xi}} \right] \boldsymbol{\xi} \\ \text{LMPD} : \underline{\mathbf{T}}^{\text{LMPD}}\langle\boldsymbol{\xi}\rangle &= \left[\int_{\mathcal{H}} \underline{\mathbf{w}}(\mathbf{X}'') \underline{\omega}^{\text{LMPD}}\langle\boldsymbol{\xi}\rangle \mathbf{P}_{\boldsymbol{\xi}'} (\mathbf{K}_{\boldsymbol{\xi}'}^{\text{LMPD}})^{-1} dV_{\mathbf{X}''} \right] \boldsymbol{\xi} \\ \text{NSPD} : \underline{\mathbf{T}}^{\text{NSPD}}\langle\boldsymbol{\xi}\rangle &= \left[\int_{\mathcal{H}} \underline{\mathbf{w}}(\mathbf{X}'') \underline{\omega}^{\text{NSPD}}\langle\boldsymbol{\xi}\rangle \mathbf{P}_{\boldsymbol{\xi}'} (\mathbf{K}_{\boldsymbol{\xi}'}^{\text{NSPD}})^{-1} dV_{\mathbf{X}''} \right] \boldsymbol{\xi}. \end{aligned} \quad (4.15)$$

4.2 Momentum balance and objectivity

The equation of motion for the unified framework of bond-associated material correspondence models is the same as that for the conventional model proposed by Silling et al. [72], which is written as

$$\rho(\mathbf{X})\ddot{\mathbf{u}}(\mathbf{X}, t) = \int_{\mathcal{H}} \left\{ \underline{\mathbf{T}}[\mathbf{X}, t] \langle \boldsymbol{\xi} \rangle - \underline{\mathbf{T}}[\mathbf{X}', t] \langle -\boldsymbol{\xi} \rangle \right\} dV_{\mathbf{X}'} + \mathbf{b}(\mathbf{X}, t), \quad (4.16)$$

where $\rho(\mathbf{X})$ is the mass density of material point $\mathbf{X}$, $\ddot{\mathbf{u}}(\mathbf{X}, t) := \partial^2 \mathbf{u} / \partial t^2$ represents the second-order derivative of displacements $\mathbf{u}$ with respect to time t , and $\mathbf{b}(\mathbf{X}, t)$ is the body force density of material point $\mathbf{X}$.

The above equation of motion can be derived from the perspective of energy conservation. Given an arbitrary domain $\mathcal{B}_0$, the total kinetic energy $K(t)$, the total external work $U(t)$, and the total strain energy $\Phi(t)$ can be computed by

$$K(t) = \frac{1}{2} \int_{\mathcal{B}_0} \rho \dot{\mathbf{u}} \cdot \dot{\mathbf{u}} dV_{\mathbf{X}}, \quad U(t) = \int_0^t \int_{\mathcal{B}_0} \mathbf{b} \cdot \dot{\mathbf{u}} dV_{\mathbf{X}} dt, \quad \Phi(t) = \int_{\mathcal{B}_0} \mathcal{W} dV_{\mathbf{X}}, \quad (4.17)$$

where $\dot{\mathbf{u}} := \partial \mathbf{u} / \partial t$ is the first order derivative of displacements $\mathbf{u}$ with respect to time t .

As a result of conservation of energy and assuming $K(0) = U(0) = \Phi(0) = 0$ when $t = 0$, the following two equalities must be held:

$$U(t) = \Phi(t) + K(t), \quad \forall t \geq 0 \quad (4.18)$$

$$\dot{U}(t) = \dot{\Phi}(t) + \dot{K}(t), \quad \forall t \geq 0, \quad (4.19)$$

where

$$\dot{U}(t) = \int_{\mathcal{B}_0} \mathbf{b} \cdot \dot{\mathbf{u}} dV_{\mathbf{X}}, \quad (4.20)$$

$$\dot{K}(t) = \frac{1}{2} \int_{\mathcal{B}_0} [\rho \ddot{\mathbf{u}} \cdot \dot{\mathbf{u}} + \rho \dot{\mathbf{u}} \cdot \ddot{\mathbf{u}}] dV_{\mathbf{X}} = \int_{\mathcal{B}_0} \rho \ddot{\mathbf{u}} \cdot \dot{\mathbf{u}} dV_{\mathbf{X}}, \quad (4.21)$$

and

$$\dot{\Phi}(t) = \int_{\mathcal{B}_0} \dot{\mathcal{W}} dV_{\mathbf{X}} \quad (4.22)$$

denote the time derivative of $U(t)$, $K(t)$ and $\Phi(t)$, respectively. The $\dot{\Phi}(t)$ can be further expanded in terms of the bond force density state $\underline{\mathbf{T}}\langle \boldsymbol{\xi} \rangle$ and the bond deformed state $\underline{\mathbf{y}}\langle \boldsymbol{\xi} \rangle$

as

$$\begin{aligned}
 \dot{\Phi}(t) &= \int_{\mathcal{B}_0} \dot{\mathcal{W}} \, dV_{\mathbf{X}} = \int_{\mathcal{B}_0} \underline{\mathbf{T}}\langle \boldsymbol{\xi} \rangle \bullet \dot{\underline{\mathbf{y}}}\langle \boldsymbol{\xi} \rangle \, dV_{\mathbf{X}} = \int_{\mathcal{B}_0} \int_{\mathcal{H}} \underline{\mathbf{T}}\langle \boldsymbol{\xi} \rangle \cdot \dot{\underline{\mathbf{y}}} \, dV_{\mathbf{X}'} \, dV_{\mathbf{X}} \\
 &= \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \underline{\mathbf{T}}\langle \boldsymbol{\xi} \rangle \cdot \dot{\underline{\mathbf{y}}} \, dV_{\mathbf{X}'} \, dV_{\mathbf{X}} = \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \underline{\mathbf{T}}\langle \boldsymbol{\xi} \rangle \cdot (\dot{\mathbf{u}}' - \dot{\mathbf{u}}) \, dV_{\mathbf{X}'} \, dV_{\mathbf{X}} \\
 &= \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \underline{\mathbf{T}}\langle \boldsymbol{\xi} \rangle \cdot \dot{\mathbf{u}}' \, dV_{\mathbf{X}'} \, dV_{\mathbf{X}} - \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \underline{\mathbf{T}}\langle \boldsymbol{\xi} \rangle \cdot \dot{\mathbf{u}} \, dV_{\mathbf{X}'} \, dV_{\mathbf{X}} \\
 &= \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \left[\underline{\mathbf{T}}\langle \boldsymbol{\xi} \rangle - \underline{\mathbf{T}}'\langle -\boldsymbol{\xi} \rangle \right] \cdot \dot{\mathbf{u}} \, dV_{\mathbf{X}'} \, dV_{\mathbf{X}} \\
 &= \int_{\mathcal{B}_0} \left\{ \int_{\mathcal{H}} \left[\underline{\mathbf{T}}\langle \boldsymbol{\xi} \rangle - \underline{\mathbf{T}}'\langle -\boldsymbol{\xi} \rangle \right] \, dV_{\mathbf{X}'} \right\} \cdot \dot{\mathbf{u}} \, dV_{\mathbf{X}}, \tag{4.23}
 \end{aligned}$$

where $\underline{\mathbf{T}}'\langle -\boldsymbol{\xi} \rangle = \underline{\mathbf{T}}[\mathbf{X}', t] \langle -\boldsymbol{\xi} \rangle$.

Substituting Eqs. (4.20), (4.21) and (4.23) back into Eq. (4.19) and applying the localization theorem, the equation of motion shown in Eq. (4.16) is then obtained.

• Balance of linear momentum

For a bounded body $\mathcal{B}_0$ subjected to a body force density field $\mathbf{b}$, the balance of linear momentum is always held [72]. The proof is briefly provided below.

$$\begin{aligned}
 \int_{\mathcal{B}_0} \rho \ddot{\mathbf{u}} - \mathbf{b} \, dV_{\mathbf{X}} &= \int_{\mathcal{B}_0} \int_{\mathcal{H}} \left\{ \underline{\mathbf{T}}\langle \boldsymbol{\xi} \rangle - \underline{\mathbf{T}}'\langle -\boldsymbol{\xi} \rangle \right\} \, dV_{\boldsymbol{\xi}} \, dV_{\mathbf{X}} \\
 &= \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \left\{ \underline{\mathbf{T}}\langle \boldsymbol{\xi} \rangle - \underline{\mathbf{T}}'\langle -\boldsymbol{\xi} \rangle \right\} \, dV_{\mathbf{X}'} \, dV_{\mathbf{X}} \\
 &= \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \underline{\mathbf{T}}\langle \boldsymbol{\xi} \rangle \, dV_{\mathbf{X}'} \, dV_{\mathbf{X}} - \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \underline{\mathbf{T}}'\langle -\boldsymbol{\xi} \rangle \, dV_{\mathbf{X}'} \, dV_{\mathbf{X}} \\
 &= \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \underline{\mathbf{T}}\langle \boldsymbol{\xi} \rangle \, dV_{\mathbf{X}'} \, dV_{\mathbf{X}} - \int_{\mathcal{B}_0} \int_{\mathcal{B}_0} \underline{\mathbf{T}}\langle \boldsymbol{\xi} \rangle \, dV_{\mathbf{X}'} \, dV_{\mathbf{X}} \\
 &= 0 \tag{4.24}
 \end{aligned}$$

Since $\underline{\mathbf{T}}\langle \boldsymbol{\xi} \rangle = \mathbf{0}$ whenever $\boldsymbol{\xi} \notin \mathcal{H}$, the limit of integration on the inner integral may be changed from $\mathcal{H}$ to $\mathcal{B}_0$. In the meantime, the order of integration can be exchanged. Therefore, the linear momentum balance is satisfied.

• Balance of angular momentum

The angular momentum balance is another important law of physics that must be followed. According to Proposition 8.1 in Ref. [72], for a bounded body $\mathcal{B}_0$, the balance of angular momentum is satisfied if

$$\int_{\mathcal{B}_0} \underline{\mathbf{y}}\langle \boldsymbol{\xi} \rangle \times \underline{\mathbf{T}}\langle \boldsymbol{\xi} \rangle \, dV_{\mathbf{X}'} = 0 \tag{4.25}$$

is true for the material correspondence formulation.

Similarly, the force density state $\underline{\mathbf{T}}(\underline{\boldsymbol{\xi}}) = \mathbf{0}$ if the bond $\underline{\boldsymbol{\xi}}$ falls outside the horizon $\mathcal{H}$. Thus, the integration domain can be changed from $\mathcal{B}_0$ to $\mathcal{H}$. After substituting Eq. (4.8) into $\underline{\mathbf{T}}(\underline{\boldsymbol{\xi}})$, the angular momentum yields

$$\begin{aligned}
 \left(\int_{\mathcal{H}} \underline{\mathbf{y}}(\underline{\boldsymbol{\xi}}) \times \underline{\mathbf{T}}(\underline{\boldsymbol{\xi}}) dV_{\mathbf{X}'} \right)_i &= e_{ijl} \int_{\mathcal{H}} \underline{y}_j \left[\int_{\mathcal{H}} \underline{w}(\mathbf{X}'') \underline{\omega}(\underline{\boldsymbol{\xi}}) P_{\xi',lQ} \underline{A}_{QR}^T(\underline{\boldsymbol{\xi}}') K_{\xi',RS}^{-1} dV_{\mathbf{X}''} \xi_S \right] dV_{\mathbf{X}'} \\
 &\quad + e_{ijl} \int_{\mathcal{H}} \underline{y}_j \left[\int_{\mathcal{H}} \underline{w}(\mathbf{X}'') \hat{\delta}[\underline{\boldsymbol{\xi}} - \underline{\boldsymbol{\xi}}'] P_{\xi',mQ} \underline{B}_{mQ,l}(\underline{\boldsymbol{\xi}}') dV_{\mathbf{X}''} \right] dV_{\mathbf{X}'} \\
 &= e_{ijl} \int_{\mathcal{H}} \underline{w}(\mathbf{X}'') \left[\int_{\mathcal{H}} \underline{\omega}(\underline{\boldsymbol{\xi}}) \underline{y}_j \xi_S dV_{\mathbf{X}'} \right] K_{\xi',SR}^{-1} P_{\xi',lQ} \underline{A}_{QR}^T(\underline{\boldsymbol{\xi}}') dV_{\mathbf{X}''} \\
 &\quad + e_{ijl} \int_{\mathcal{H}} \underline{y}_j \left[\int_{\mathcal{H}} \underline{w}(\mathbf{X}'') \hat{\delta}[\underline{\boldsymbol{\xi}} - \underline{\boldsymbol{\xi}}'] P_{\xi',mQ} \underline{B}_{mQ,l}(\underline{\boldsymbol{\xi}}') dV_{\mathbf{X}''} \right] dV_{\mathbf{X}'} \\
 &= e_{ijl} \int_{\mathcal{H}} \underline{w}(\mathbf{X}'') F_{\xi',jR} P_{\xi',lQ} \underline{A}_{QR}^T(\underline{\boldsymbol{\xi}}') dV_{\mathbf{X}''} \\
 &\quad + e_{ijl} \int_{\mathcal{H}} \underline{y}_j \left[\int_{\mathcal{H}} \underline{w}(\mathbf{X}'') \hat{\delta}[\underline{\boldsymbol{\xi}} - \underline{\boldsymbol{\xi}}'] P_{\xi',mQ} \underline{B}_{mQ,l}(\underline{\boldsymbol{\xi}}') dV_{\mathbf{X}''} \right] dV_{\mathbf{X}'} .
 \end{aligned} \tag{4.26}$$

Eq. (4.26) is a generalized expression for the angular momentum based on the unified deformation gradient and bond force density state. This expression will be examined for different cases of the bond-associated models.

$$\circ \quad \underline{\mathbf{A}}(\underline{\boldsymbol{\xi}}) = \mathbf{I} \quad \text{and} \quad \underline{\mathbf{B}}(\underline{\boldsymbol{\xi}}) = \mathbf{0}$$

$\underline{\mathbf{A}}(\underline{\boldsymbol{\xi}}) = \mathbf{I}$ and $\underline{\mathbf{B}}(\underline{\boldsymbol{\xi}}) = \mathbf{0}$ is the most common conditions in the bond-associated correspondence models, including the conventional model (Eq. (2.6)), the sub-horizon-based model (Eq. (2.11)), the Lagrange-multiplier-based model (Eq. (2.19)) and the non-spherical-influence-function-based model (Eq. (2.25)). For these models, Eq. (4.26) can be simplified as

$$\begin{aligned}
 \left(\int_{\mathcal{H}} \underline{\mathbf{y}}(\underline{\boldsymbol{\xi}}) \times \underline{\mathbf{T}}(\underline{\boldsymbol{\xi}}) dV_{\mathbf{X}''} \right)_i &= e_{ijl} \int_{\mathcal{H}} \underline{w}(\mathbf{X}'') F_{\xi',jR} P_{\xi',lQ} I_{QR} dV_{\mathbf{X}''} \\
 &= e_{ijl} \int_{\mathcal{H}} \underline{w}(\mathbf{X}'') F_{\xi',jR} P_{\xi',lR} dV_{\mathbf{X}''} \\
 &= e_{ijl} \int_{\mathcal{H}} \underline{w}(\mathbf{X}'') F_{\xi',jR} S_{\xi',RQ} F_{\xi',Ql}^T dV_{\mathbf{X}''} \\
 &= 0,
 \end{aligned} \tag{4.27}$$

where $\mathbf{S}$ is the second Piola-Kirchhoff stress tensor.

Therefore, the angular momentum balance is obtained for bond-associated models when $\underline{\mathbf{A}}(\underline{\boldsymbol{\xi}}) = \mathbf{I}$ and $\underline{\mathbf{B}}(\underline{\boldsymbol{\xi}}) = \mathbf{0}$.

$$\circ \underline{\mathbf{A}}\langle \boldsymbol{\xi} \rangle \neq \mathbf{I} \quad \text{and} \quad \underline{\mathbf{B}}\langle \boldsymbol{\xi} \rangle \neq \mathbf{0}$$

For bond-associated models that $\underline{\mathbf{A}}\langle \boldsymbol{\xi} \rangle \neq \mathbf{I}$ and $\underline{\mathbf{B}}\langle \boldsymbol{\xi} \rangle \neq \mathbf{0}$ in general, such as the bond-correction-based model (Eq. (2.17)), the angular momentum balance can be derived in a slightly different manner. For the case of bond-correction-based model, plugging the conditions given in Eq. (2.17) into Eq. (4.26), the angular momentum becomes

$$\begin{aligned} \left(\int_{\mathcal{H}} \underline{\mathbf{y}}\langle \boldsymbol{\xi} \rangle \times \underline{\mathbf{T}}\langle \boldsymbol{\xi} \rangle dV_{\mathbf{X}'} \right)_i &= e_{ijl} \int_{\mathcal{H}} \underline{w}(\mathbf{X}'') F_{\xi',jR} P_{\xi',lQ} \left(I_{QR} - \frac{\xi'_Q \xi'_R}{|\boldsymbol{\xi}'|^2} \right) dV_{\mathbf{X}''} \\ &\quad + e_{ijl} \int_{\mathcal{H}} \underline{y}_j \left[\int_{\mathcal{H}} \frac{\underline{w}(\mathbf{X}'')}{|\boldsymbol{\xi}'|^2} \delta[\boldsymbol{\xi} - \boldsymbol{\xi}'] P_{\xi',lQ} \xi'_Q dV_{\mathbf{X}''} \right] dV_{\mathbf{X}'} \\ &= e_{ijl} \int_{\mathcal{H}} \underline{w}(\mathbf{X}'') F_{\xi',jR} P_{\xi',lQ} I_{QR} dV_{\mathbf{X}''} - e_{ijl} \int_{\mathcal{H}} \underline{w}(\mathbf{X}'') F_{\xi',jR} P_{\xi',lQ} \frac{\xi'_Q \xi'_R}{|\boldsymbol{\xi}'|^2} dV_{\mathbf{X}''} \\ &\quad + e_{ijl} \int_{\mathcal{H}} \underline{y}_j \frac{\underline{w}(\mathbf{X}')}{|\boldsymbol{\xi}|^2} P_{\xi,lQ} \xi_Q dV_{\mathbf{X}'} \\ &= e_{ijl} \int_{\mathcal{H}} \underline{w}(\mathbf{X}'') F_{\xi',jR} P_{\xi',lQ} I_{QR} dV_{\mathbf{X}'} - e_{ijl} \int_{\mathcal{H}} \frac{\underline{w}(\mathbf{X}'')}{|\boldsymbol{\xi}'|^2} \underline{y}_j \langle \boldsymbol{\xi}' \rangle P_{\xi',lQ} \xi'_Q dV_{\mathbf{X}''} \\ &\quad + e_{ijl} \int_{\mathcal{H}} \frac{\underline{w}(\mathbf{X}')}{|\boldsymbol{\xi}|^2} \underline{y}_j \langle \boldsymbol{\xi}' \rangle P_{\xi,lQ} \xi_Q dV_{\mathbf{X}'} \\ &= e_{ijl} \int_{\mathcal{H}} \underline{w}(\mathbf{X}'') F_{\xi',jR} P_{\xi',lQ} I_{QR} dV_{\mathbf{X}''} \\ &= 0. \end{aligned} \tag{4.28}$$

Therefore, the angular momentum balance is also obtained for bond-associated models when $\underline{\mathbf{A}}\langle \boldsymbol{\xi} \rangle \neq \mathbf{I}$ and $\underline{\mathbf{B}}\langle \boldsymbol{\xi} \rangle \neq \mathbf{0}$.

• Objectivity

To show the objectivity of the bond-associated correspondence models, let us assume there is a rigid body rotation $\mathbf{Q}$ superposed on the domain $\mathcal{B}_0$. Accordingly, the bond-associated deformation gradient for the body becomes

$$\mathbf{F}_{\xi'}^+ = \mathbf{Q} \mathbf{F}_{\xi'}. \tag{4.29}$$

From the invariance of strain energy density under rigid body motion, it can be deduced that the PK1 stress after imposing rigid body rotation, denoted as $\mathbf{P}_{\xi'}^+$, should be $\mathbf{Q} \mathbf{P}_{\xi'}$, i.e.,

$$\mathcal{W}(\mathbf{F}_{\xi'}) = \mathcal{W}(\mathbf{Q} \mathbf{F}_{\xi'}) \quad \rightarrow \quad \mathbf{P}_{\xi'} : \mathbf{F}_{\xi'} \equiv \mathbf{P}_{\xi'}^+ : \mathbf{F}_{\xi'}^+ \quad \rightarrow \quad \mathbf{P}_{\xi'}^+ = \mathbf{Q} \mathbf{P}_{\xi'}. \tag{4.30}$$

Replacing $\mathbf{P}_{\xi'}$ with $\mathbf{P}_{\xi'}^+$ in the unified force density state shown in Eq. (4.8) yields

$$\begin{aligned}
 \underline{\mathbf{T}}^+ \langle \xi \rangle &= \underline{\omega} \langle \xi \rangle \left[\int_{\mathcal{H}} \underline{\mathbf{w}}(\mathbf{X}'') \mathbf{P}_{\xi'}^+ \underline{\mathbf{A}}^T \langle \xi' \rangle \mathbf{K}_{\xi'}^{-1} dV_{\mathbf{X}''} \right] \xi + \int_{\mathcal{H}} \underline{\mathbf{w}}(\mathbf{X}'') \hat{\delta}[\xi - \xi'] \mathbf{P}_{\xi'}^+ : \nabla_{\mathbf{y}} \underline{\mathbf{B}} \langle \xi' \rangle dV_{\mathbf{X}''} \\
 &= \underline{\omega} \langle \xi \rangle \left[\int_{\mathcal{H}} \underline{\mathbf{w}}(\mathbf{X}'') \mathbf{Q} \mathbf{P}_{\xi'} \underline{\mathbf{A}}^T \langle \xi' \rangle \mathbf{K}_{\xi'}^{-1} dV_{\mathbf{X}''} \right] \xi + \int_{\mathcal{H}} \underline{\mathbf{w}}(\mathbf{X}'') \hat{\delta}[\xi - \xi'] \mathbf{Q} \mathbf{P}_{\xi'} : \nabla_{\mathbf{y}} \underline{\mathbf{B}} \langle \xi' \rangle dV_{\mathbf{X}''} \\
 &= \mathbf{Q} \left\{ \underline{\omega} \langle \xi \rangle \left[\int_{\mathcal{H}} \underline{\mathbf{w}}(\mathbf{X}'') \mathbf{P}_{\xi'} \underline{\mathbf{A}}^T \langle \xi' \rangle \mathbf{K}_{\xi'}^{-1} dV_{\mathbf{X}''} \right] \xi + \int_{\mathcal{H}} \underline{\mathbf{w}}(\mathbf{X}'') \hat{\delta}[\xi - \xi'] \mathbf{P}_{\xi'} : \nabla_{\mathbf{y}} \underline{\mathbf{B}} \langle \xi' \rangle dV_{\mathbf{X}''} \right\} \\
 &= \mathbf{Q} \underline{\mathbf{T}} \langle \xi \rangle.
 \end{aligned} \tag{4.31}$$

Apparently, the transformation from state $\underline{\mathbf{T}} \langle \xi \rangle$ to state $\underline{\mathbf{T}}^+ \langle \xi \rangle$, corresponding to the transformation from $\mathbf{F}_{\xi'}$ to $\mathbf{F}_{\xi'}^+$, follows the standard rules of tensor analysis. Therefore, the bond force density state $\underline{\mathbf{T}} \langle \xi \rangle$ is objective.

Chapter 5

Numerical implementation

5.1 Formula discretization

Both the bond-based and state-based models presented above are written in integration form. To implement them, some equations should be discretized and reformulated in summation form. To begin with, the governing equation in Eq. (3.41) or (4.16) should be re-written as

$$\rho(\mathbf{X}^I) \ddot{\mathbf{u}}(\mathbf{X}^I) = \sum_{J \in \mathcal{H}^I} [\underline{\mathbf{T}}[\mathbf{X}^I, t] \langle \boldsymbol{\xi}^{IJ} \rangle - \underline{\mathbf{T}}[\mathbf{X}^J, t] \langle -\boldsymbol{\xi}^{IJ} \rangle] V_{\mathbf{X}^J} + \mathbf{b}(\mathbf{X}^I) , \quad (5.1)$$

where $\mathbf{X}^I$ is the center particle of the horizon $\mathcal{H}^I$ with a finite volume $V_{\mathbf{X}^I}$; $\mathbf{X}^J$ is an arbitrary particle within the horizon, $\underline{\mathbf{T}}$ denotes the bond force state. For the sake of a simple statement, all the quantities of interest that belong to particle I will be denoted with a superscript I in the following equations. Similarly, all quantities belong to particle J will be denoted with a superscript J . As for the quantities that are shared by I and J , such as $\boldsymbol{\xi}^{IJ}$, they will be denoted with the superscript IJ .

In bond-based peridynamics models, $\underline{\mathbf{w}}^{IJ} = 1/V_{\mathcal{H}^I}^2$ is usually taken for the weight function in actual computation. Therefore, the bond force states write

$$\underline{\mathbf{T}}\langle \boldsymbol{\xi}^{IJ} \rangle = \frac{1}{2V_{\mathcal{H}^I}} \mathbf{f}(\mathbf{X}^I, \mathbf{X}^J) \quad \text{and} \quad \underline{\mathbf{T}}\langle -\boldsymbol{\xi} \rangle = -\frac{1}{2V_{\mathcal{H}^I}} \mathbf{f}(\mathbf{X}^I, \mathbf{X}^J) . \quad (5.2)$$

While in state-based models, the bond force state is discretized as

$$\begin{aligned} \underline{\mathbf{T}}\langle \boldsymbol{\xi}^{IJ} \rangle = & \left[\sum_{K \in \mathcal{H}^I} \underline{\mathbf{w}}(\mathbf{X}^K) \underline{\omega}\langle \boldsymbol{\xi}^{IJ} \rangle \mathbf{P}_{\boldsymbol{\xi}^{IK}} \underline{\mathbf{A}}^T \langle \boldsymbol{\xi}^{IK} \rangle \mathbf{K}_{\boldsymbol{\xi}^{IK}}^{-1} V_{\mathbf{X}^K} \right] \boldsymbol{\xi}^{IJ} + \\ & \underline{\mathbf{w}}(\mathbf{X}^J) \mathbf{P}_{\boldsymbol{\xi}^{IJ}} : \nabla_{\underline{\mathbf{y}}} \underline{\mathbf{B}}\langle \boldsymbol{\xi}^{IJ} \rangle V_{\mathbf{X}^J} , \end{aligned} \quad (5.3)$$

where the states $\underline{\mathbf{A}}\langle \boldsymbol{\xi}^{IK} \rangle$ and $\underline{\mathbf{B}}\langle \boldsymbol{\xi}^{IJ} \rangle$ are determined by the specific bond-associated formulation.

The unified bond-associated nonlocal deformation gradient serves as the cornerstone in establishing various peridynamics formulations. In numerical analysis, it is implemented as

$$\mathbf{F}_{\xi^{IJ}} = \left[\sum_{J \in \mathcal{H}^I} \underline{\omega} \langle \xi^{IJ} \rangle \underline{\mathbf{y}}^{IJ} \otimes \xi^{IJ} V_{\mathbf{x}^J} \right] \mathbf{K}_{\xi^{IJ}}^{-1} \underline{\mathbf{A}} \langle \xi^{IJ} \rangle + \underline{\mathbf{B}} \langle \xi^{IJ} \rangle \quad (5.4)$$

with

$$\mathbf{K}_{\xi^{IJ}} = \sum_{J \in \mathcal{H}^I} \underline{\omega} \langle \xi^{IJ} \rangle \xi^{IJ} \otimes \xi^{IJ} V_{\mathbf{x}^J} \quad (5.5)$$

When it comes to the stress measures, the calculation methods for bond-based and state-based models vary.

- **Bond-based models**

In bond-based models, the nonlocal PK2 and PK1 stress presented in Eq. (3.43) and (3.46) should be numerically computed as follows,

$$\mathbf{S}^I = \frac{1}{2V_{\mathcal{H}^I}^2} \sum_{J \in \mathcal{H}^I} \sum_{K \in \mathcal{H}^I} \left(f_N \mathbf{N}^{JK} \otimes \mathbf{N}^{JK} + \frac{f_T}{2} (\mathbf{N}^{JK} \otimes \mathbf{T}^{JK} + \mathbf{T}^{JK} \otimes \mathbf{N}^{JK}) \right) V^J V^K \quad (5.6)$$

$$\mathbf{P}^I = \frac{1}{2V_{\mathcal{H}^I}^2} \sum_{J \in \mathcal{H}^I} \sum_{K \in \mathcal{H}^I} \left(f_N \mathbf{n}^{JK} \otimes \mathbf{N}^{JK} + \frac{f_T}{2} (\mathbf{n}^{JK} \otimes \mathbf{T}^{JK} + \mathbf{t}^{JK} \otimes \mathbf{N}^{JK}) \right) V^J V^K \quad (5.7)$$

where J, K are two arbitrary particles within horizon $\mathcal{H}^I$.

- **State-based models**

As far as the state-based models are concerned, the nonlocal PK1 stress is obtained simply by taking average of the bond-associated stress, i.e.

$$\mathbf{P}^I = \frac{1}{N} \sum_{J \in \mathcal{H}^I} \mathbf{P}_{\xi^{IJ}} \quad (5.8)$$

where N refers to the number of neighboring material points within the horizon $\mathcal{H}^I$.

5.2 Solver configuration

There are in general two types of solvers for mechanics problem, namely explicit solvers and implicit solvers. Explicit solvers calculate the state of a physical system at a future time step directly from the current state while the implicit solvers calculates from both the current and unknown future states. Previous researchers have incorporated both types with various peridynamics formulation, see [97, 25, 60, 56]. Without loss of generality, this paper

Algorithm 1 Pseudo-code for numerical implementation with the half-step explicit solver

```

1: Initialize arrays for displacement, velocity, new and old half-step velocity, and force:
    $\{\mathbf{U}\}, \{\mathbf{V}\}, \{\mathbf{V}_1^{1/2}\}, \{\mathbf{V}_0^{1/2}\}, \{\mathbf{F}\}$ 
2: Apply displacement and force boundary conditions to  $\{\bar{\mathbf{U}}\}$  and  $\{\mathbf{B}\}$  respectively
3: for each time step  $n$  do
4:   Compute damping coefficient  $c$ 
5:   for each particle  $I$  do
6:     if particle  $I$  on the displacement boundaries then
7:       Assign displacement boundary condition:  $\mathbf{U}^I \leftarrow \bar{\mathbf{U}}^I$ 
8:     else if current time step is 1 then
9:       Compute new half-step velocity:  $\mathbf{V}_1^{1/2,I} \leftarrow \mathbf{V}^I + 0.5 (\mathbf{F}^I + \mathbf{B}^I) \cdot dt / \rho$ 
10:      Update velocity:  $\mathbf{V}^I \leftarrow 0.5 (\mathbf{V}_0^{1/2,I} + \mathbf{V}_1^{1/2,I})$ 
11:      Update displacement:  $\mathbf{U}^I \leftarrow \mathbf{U}^I + \mathbf{V}^{1/2,I} \cdot dt$ 
12:      Update old half-step velocity:  $\mathbf{V}_0^{1/2,I} \leftarrow \mathbf{V}_1^{1/2,I}$ 
13:    else
14:      Compute new half-step velocity:
          
$$\mathbf{V}_1^{1/2,I} \leftarrow \left[ (2 - c \cdot dt) \mathbf{V}_0^{1/2,I} + 2 (\mathbf{F}^I + \mathbf{B}^I) \cdot dt / \rho \right] / (2 + c \cdot dt)$$

15:      Update velocity:  $\mathbf{V}^I \leftarrow 0.5 (\mathbf{V}_0^{1/2,I} + \mathbf{V}_1^{1/2,I})$ 
16:      Update displacement:  $\mathbf{U}^I \leftarrow \mathbf{U}^I + \mathbf{V}^{1/2,I} \cdot dt$ 
17:      Update old half-step velocity:  $\mathbf{V}_0^{1/2,I} \leftarrow \mathbf{V}_1^{1/2,I}$ 
18:    end if
19:  end for
20:  for each particle  $I$  do
21:    for each particle  $J$  within  $\mathcal{H}^I$  do
22:      Compute bond-associated deformation gradient  $\mathbf{F}_{\xi^{IJ}}$  by Eq. (5.4)
23:      Compute the force density state  $\underline{\mathbf{T}}\langle \xi^{IJ} \rangle$  by either Eq. (5.2) or (5.3)
24:    end for
25:    Compute the resultant force density  $\mathbf{F}^I \leftarrow \sum [\underline{\mathbf{T}}\langle \xi^{IJ} \rangle - \underline{\mathbf{T}}\langle -\xi^{IJ} \rangle V_{\mathbf{x}^J}]$ 
26:  end for
27:  for each particle  $I$  do
28:    Compute PK1 stress measure by either Eq. (5.7) or (5.8)
29:  end for
30:  Export data for visualization
31: end for

```

adopts half-step explicit solver, a second-order explicit solver, to illustrate the numerical implementation of the proposed peridynamic formulations. The Algorithm is presented in Alg. 1.

In Alg. 1, there are two important parameters, i.e. the time step dt and damping coefficient c . If the time step is set too large, the solution becomes unstable. Consequently, the discretized body "explodes" and the simulation displays nonphysically large deformation. In Gerstle's study [29], it is found that the time step dt should be smaller than the critical time step $(dt)_{cr}$ that is computed by

$$dt \leq (dt)_{cr} = \frac{\Delta x}{\pi \sqrt{\kappa/\rho}} \left(\sqrt{1 + \zeta^2} - \zeta \right) , \quad (5.9)$$

where Δx is the space between material points, κ is the bulk modulus, ρ is the mass density, ζ is damping ratio, and the term $\sqrt{\kappa/\rho}$ denotes the sound speed in linear elastic solid.

The damping effect and damping coefficient c are introduced in a simulation for three main reasons: (1) to represent the actual internal material damping of a solid material; (2) to represent the external damping due to interaction of a solid structure with its surrounding environment; and (3) as a means to artificially force the dynamic simulation to arrive at a static solution as quickly as possible, in what is called the "dynamic relaxation" method.

If the damping effect is introduced into system due to the third reason, damping ratio should satisfy $\zeta \geq 1$. This implies the damping coefficient c should be greater than a critical value c_{cr} . According to the study done by Kilic and Madenci [44], the critical damping coefficient at each time step can be computed by

$$c_{cr} = 2 \sqrt{\frac{\{\mathbf{U}\}^T [\mathbf{K}] \{\mathbf{U}\}}{\{\mathbf{U}\}^T [\mathbf{M}] \{\mathbf{U}\}}} , \quad (5.10)$$

where $[\mathbf{M}]$ and $[\mathbf{K}]$ denote the global mass and stiffness matrices of the system, respectively. Consequently, the damping coefficient is determined by

$$c = \zeta \cdot c_{cr} . \quad (5.11)$$

Chapter 6

Numerical examples: bond-based model

6.1 Plate with a hole

To examine the convergence of the proposed NDFD BB-PD, a comparison study is conducted between the SVK1 model and the finite element method(FEM). This is done through a typical stress analysis problem: a two-dimensional linear elastic plate with a central hole subjected to tension.

Fig. 6.1 shows the dimensions, linear properties, as well as the loading conditions of the specimen. The Young's Modulus and Poisson's ratio of the material are $E = 200$ GPa and $\nu = 1/3$ respectively. A reference solution is obtained by conducting finite element analysis with 45,215 nodes and 89,566 elements in MATLAB. The same geometric dimensions, material properties and loading condition are employed in the PD numerical model. When it comes to the bond parameters, the micro-modulus in SVK1 model can be computed by substituting Young's modulus into Eq. (3.72) while a very large value of $E_{N,cr}$ is adopted to prevent material failure, as the emphasis in this example is not fracture.

Fig. 6.2 illustrates the stress distribution obtained by both the FEM and the proposed PD models. The first row presents the FEM solution for σ_{11} , σ_{12} and σ_{22} while the second row displays the corresponding results from PD. It should be noted that a regular square mesh with a spacing of $\Delta x = 0.5$ mm and a horizon of $H = 1.0$ mm is adopted in PD model. As shown in Fig. 6.2, the proposed SVK1 model can accurately capture the stress concentration at hole's edge. This observation validates that the homogenization method presented in this paper is able to build the correct relation between the bond parameters with material elastic properties.

To quantitatively assess the accuracy and convergence of the proposed SVK1 model, σ_{11} is extracted from both FEM and PD model along the specimen's center line for comparison. In peridynamics, there are two types of convergence analysis, namely δ -convergence and m -convergence, where δ refers to the radius of horizon and $m := \delta/\Delta x$ is the ratio between the

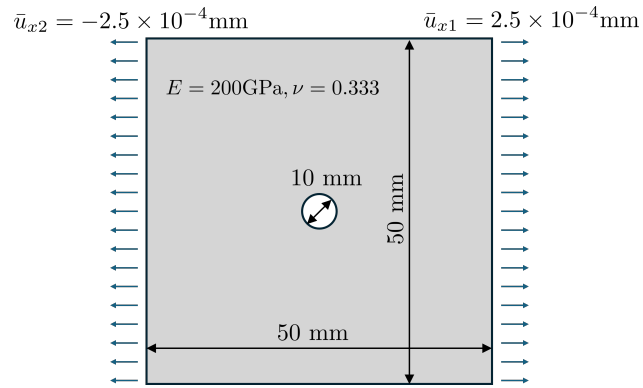


Figure 6.1: Diagram of plate with a hole specimen

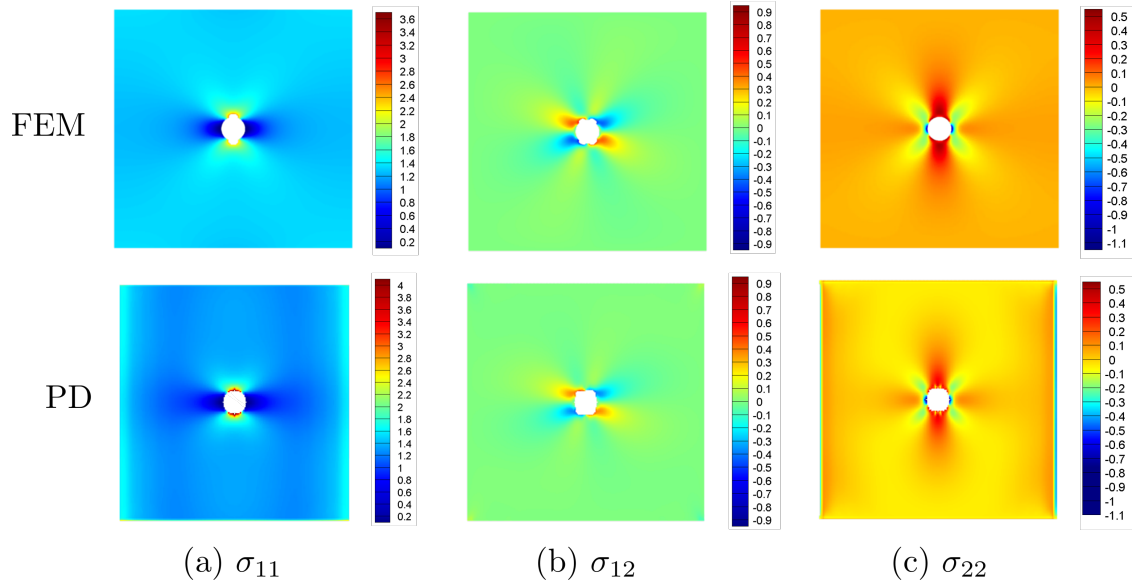


Figure 6.2: Stress distribution on the plate with a hole specimen

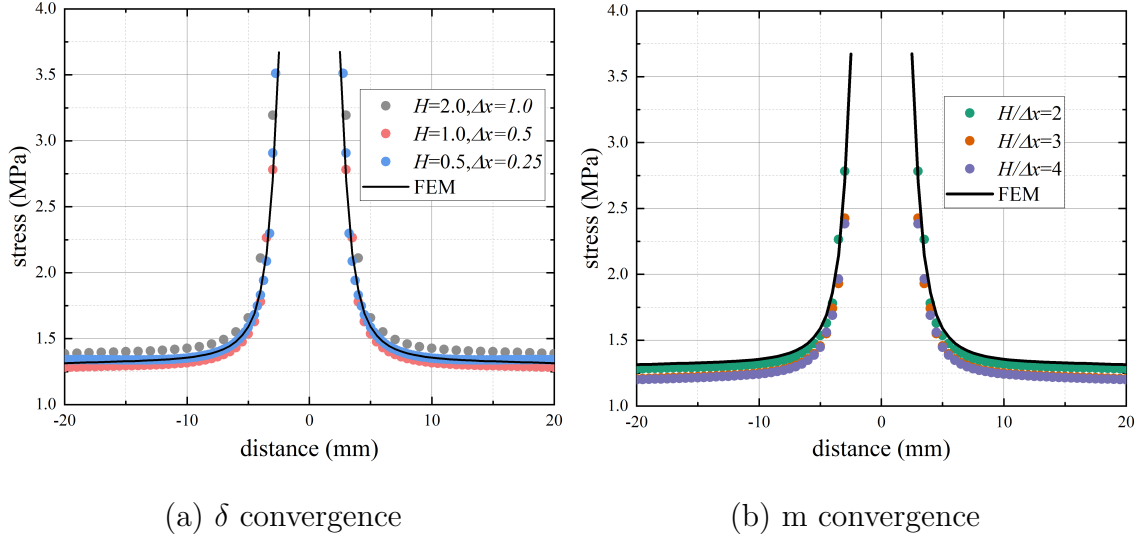


Figure 6.3: Convergence analysis on SVK1 model

radius of horizon and particle space. Fig. 6.3(a) shows the results of δ -convergence analysis. In this analysis, both the horizon size H and the particle spacing Δx vary, while their ratio remains constant. It is evident that as the PD square mesh becomes more refined, σ_{11} from PD converges to the FEM solution. Fig. 6.3(b) corresponds to the m-convergence analysis. From this figure, it can be observed that the stress distribution from PD model converges to that of FEM model as the ratio decreases. The conclusions drawn from both δ -convergence and m-convergence analysis are consistent with authors' previous work [34, 37].

6.2 Gypsum specimen with center flaw

Numerous prior studies, e.g. [6, 87, 86, 95, 27], have conducted experimental or numerical investigations on gypsum specimens with either single or double flaws. In this example, we will analyze crack propagation and coalescence behavior on gypsum plate using SVK1 and SVK2 model respectively. The geometric dimensions of the specimen are depicted in Fig. 6.4(a). Displacement boundary conditions are applied to both top and bottom edges. According to previous research [87], the bulk modulus and shear modulus of gypsum material are $K = 2.84$ GPa and $G = 2.59$ GPa respectively, which suggest that the Young's modulus and Poisson's ratio are $E = 5.96$ GPa and $\nu = 0.15$ respectively. Previous work [6, 27, 85] also reported that the mode-I and mode-II energy release rates of gypsum material are $\mathcal{G}_{Ic} = 0.016$ N/mm and $\mathcal{G}_{IIc} = 0.205$ N/mm respectively. A uniform square mesh with a particle spacing of 0.5 mm is adopted, comprising a total of 46610 particles, as shown in Fig. 6.4(b).

We start with evaluating the applicability of SVK1 model for this problem. Given the

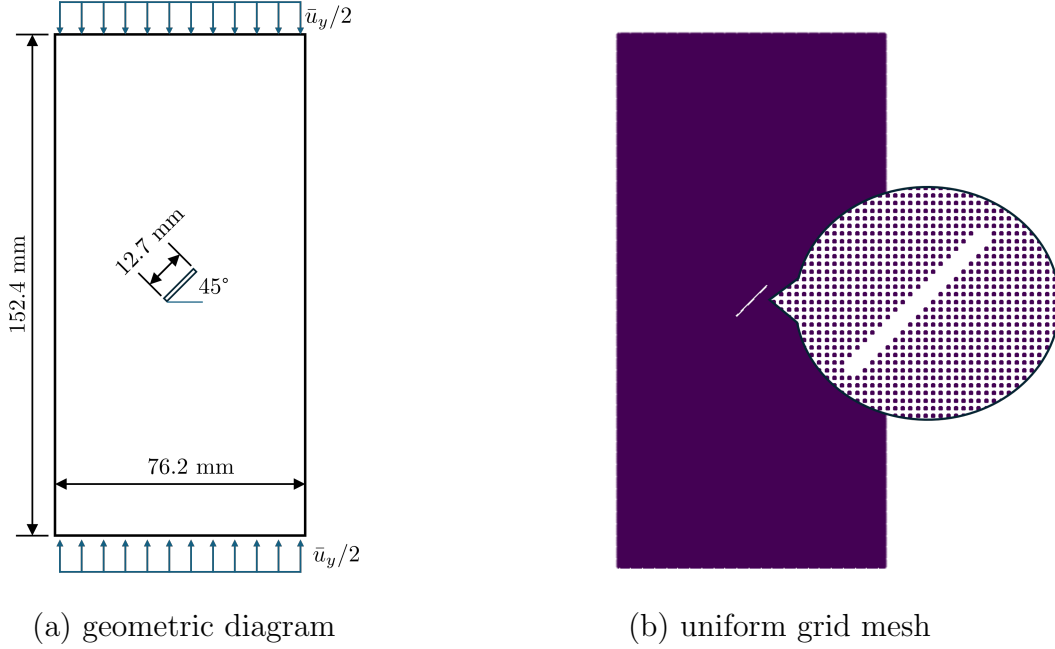


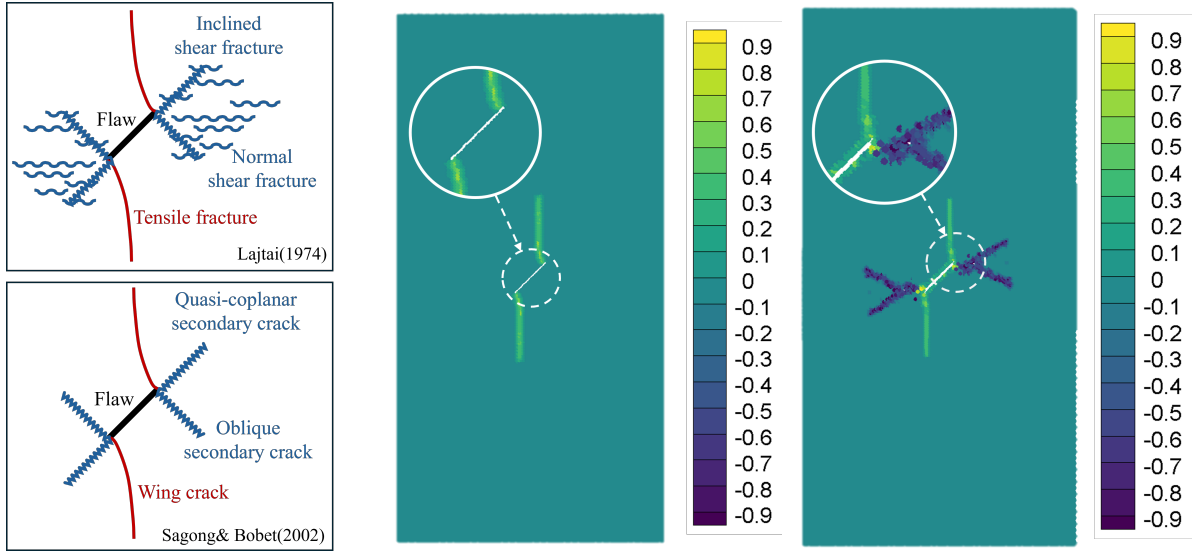
Figure 6.4: Geometric configuration and mesh of a gypsum specimen with a center flaw

Young's modulus $E = 5.96\text{GPa}$ and mode-I energy release rate $\mathcal{G}_{Ic} = 0.016\text{ N/mm}$ and assuming the characteristic length l_c to be half of the particle spacing, i.e. $l_c = 0.25\text{ mm}$, the bond parameters presented in Eq. (3.72) and (3.73) can be calibrated. After running the simulation for 15000 steps with $\bar{u}_y = 2 \times 10^{-4}\text{ mm/step}$, two cracks emerges and propagates from the two ends of the pre-defined flaw. To denote the presence of crack, the damage index is introduced. For each particle I , the damage index is computed by

$$dmg = \frac{N_b}{N_{tot}} \quad (6.1)$$

where N_b refers to the number of broken bonds within horizon $\mathcal{H}^I$ while N_{tot} represents the total number of bonds within the horizon. By utilizing the damage index, the pattern of crack is illustrated in Fig. 6.5(b). Compared with the experimental observations [47, 69] depicted in Fig. 6.5(a), it is evident that the SVK1 model can successfully replicate the propagation of tensile fracture/wing cracks. However, it falls short in accurately representing the shear fracture/secondary cracks. This issue arises from the fact that the SVK1 model solely considers the tensile failure of bond while neglecting the bond failure due to shear.

Regarding this, the SVK2 model is employed. This model, in contrast to SVK1 model, incorporates both normal and shear bond behaviors. By setting $l_{n,c} = l_{n,t} = 0.5\Delta x$ and substituting values of Young's modulus E , Poisson's ratio ν , mode-I and mode-II energy release rates $\mathcal{G}_{Ic}$, $\mathcal{G}_{IIc}$ into Eq. (3.84) through Eq. (3.87), the bond parameters can be determined. Despite the calibration of the critical deformation quantities $E_{N,cr}$ and $E_{T,cr}$,



(a) Experiment results [47, 69]

(b) SVK1 model

(c) SVK2 model

Figure 6.5: Crack pattern obtained from different models

the mix mode fracture criterion has not yet defined. To account for this potential coupling, the bond-breakage criterion proposed in [85] is adopted here. Specifically, the Heaviside step functions $\mathbf{1}_n [E_{N,cr} - E_N]$, $\mathbf{1}_t [E_{T,cr} - E_T]$ are replaced by

$$\mathbf{1}_n [E_{N,cr} - E_N], \mathbf{1}_t [E_{T,cr} - E_T] \rightarrow \mathbf{1}_{nt} = \begin{cases} 0, & E_N > E_{N,cr} \text{ and } \phi_n \geq \lambda\phi \\ 0, & E_T > E_{T,cr} \text{ and } \phi_t \geq (1 - \lambda)\phi \\ 1, & \text{otherwise} \end{cases} \quad (6.2)$$

where $\phi_n := \frac{c_n E_N^2}{2}$ represents the potential energy caused by bond normal deformation, $\phi_t := \frac{c_t E_T^2}{2}$ stands for the energy due to tangential deformation of bond, $\phi := \frac{c_n E_N^2}{2} + \frac{c_t E_T^2}{2}$ denotes the total energy of the bond, λ is a constant and takes value of $\frac{1-2\nu}{2(1-\nu)}$ for plane strain problem.

After running the simulation for 16000 steps with $\bar{u}_y = 6.324 \times 10^{-5}$ mm/step, the results are obtained and depicted in Fig. 6.5(c), Fig. 6.6 and Fig. 6.7. The damage index in SVK2 model is defined as

$$dmg = \begin{cases} \frac{N_{bn}}{N_{tot}}, & \text{if } \frac{N_{bn}}{N_{tot}} > \frac{N_{bt}}{N_{tot}} \\ -\frac{N_{bn}}{N_{tot}}, & \text{if } \frac{N_{bn}}{N_{tot}} < \frac{N_{bt}}{N_{tot}} \end{cases} \quad (6.3)$$

where N_{bn} refers to the number of bonds broken due to normal stretch, N_{bt} is the number of bonds broken due to tangential shear, N_{tot} means the total number of bonds within the

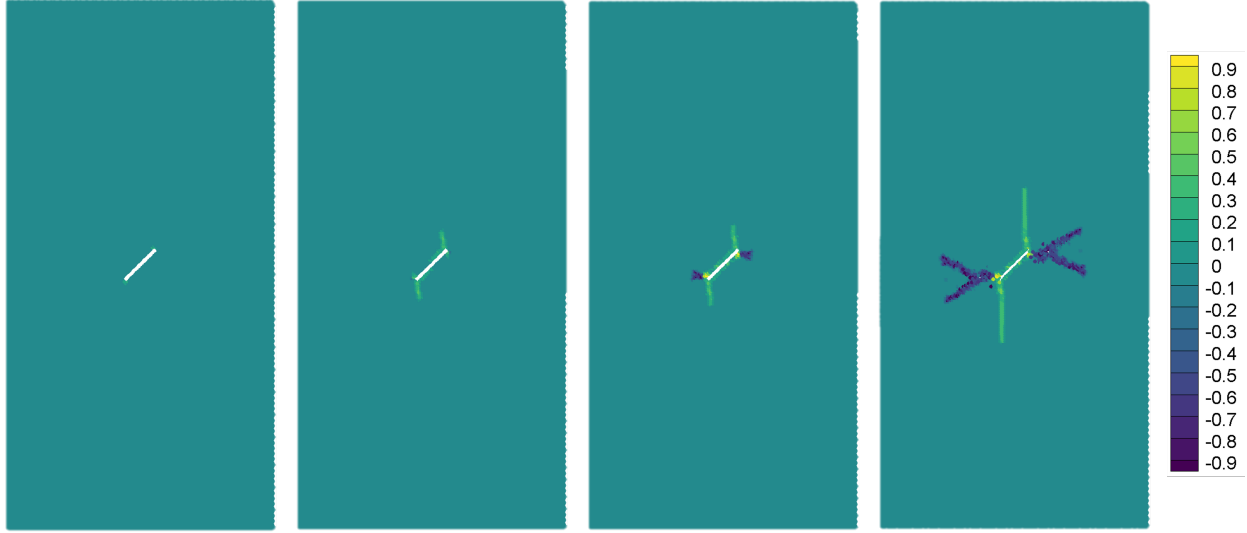


Figure 6.6: Crack evolution on the gypsum specimen with center flaw

horizon. In contrast to SVK1 model, SVK2 model is able to capture both tensile and shear fracture behaviors of the gypsum specimen. In addition, it can be found in Fig. 6.5(c) that the tensile fracture is resulted from the stretch failure of bonds while the shear fracture is caused mainly by the shear failure of bonds.

The initiation as well as propagation process of cracks is illustrated in Fig. 6.6. The corresponding fields of maximum principal stress and maximum shear stress are depicted in Fig. 6.7. As shown in Fig. 6.6, the wing cracks first appear around the flaw tip and propagate along a curved path as the load increases. In contrast, secondary cracks evolve in two directions, one almost in line with the flaw and the other nearly perpendicular to the flaw. The pattern of crack propagation is consistent with the findings from previous experiments. A notable observation in Fig. 6.6 is that the secondary cracks are significantly wider than the wing cracks. This aligns with previous experimental studies which observed that the secondary cracks could develop into "shear zones" or "bands of micro-cracks" over time. When it comes to stress fields, it can be found from Fig. 6.7(a) that the wing cracks initiate from the point of maximum principal stress concentration while the tips of secondary cracks always corresponds to the point of maximum shear stress concentration.

6.3 The Kalthoff-Winkler problem

In late 1980s, Kalthoff and Winkler conducted a series of experiments [42, 43, 41] involving a double notched steel plate subjected to impact loading. The setup of the tests is illustrated in Fig. 6.8(a). The results of these experiments indicated that the failure mode of the

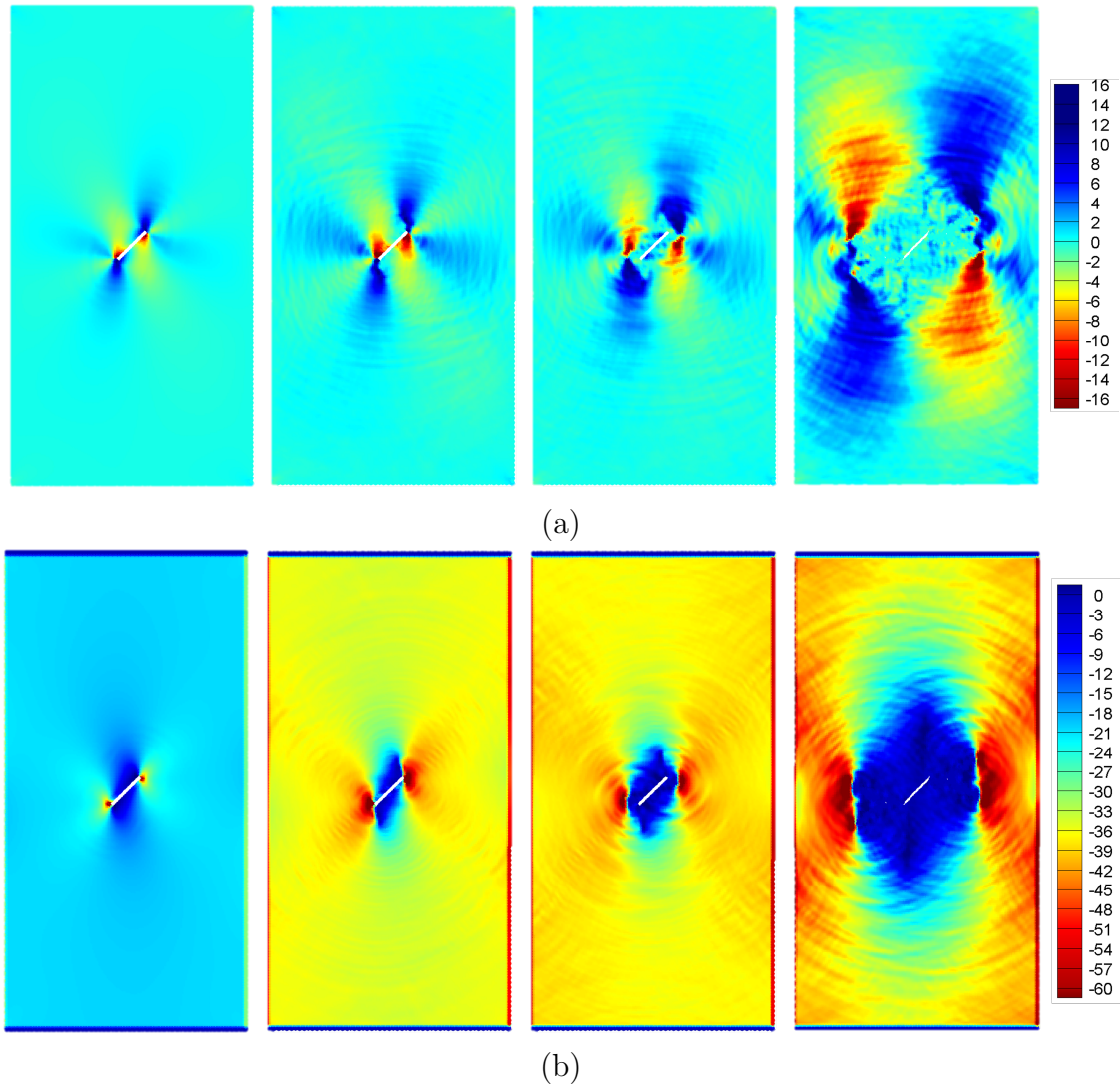


Figure 6.7: Stress fields on the gypsum specimen (a) stress component σ_{12} (b) stress component σ_{22}

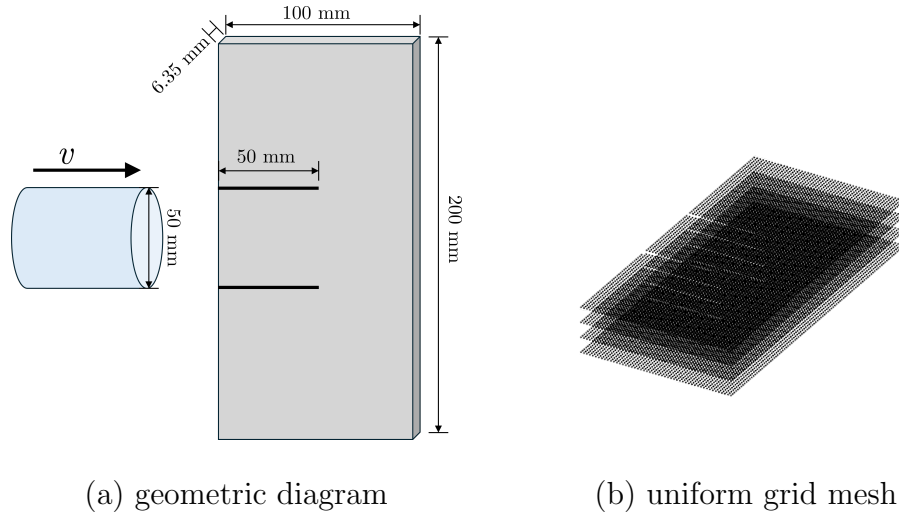


Figure 6.8: Geometric configuration and mesh of a double notched steel plate

metallic plate depends on the impact velocity. At a slower impact velocity, the specimen exhibited failure due to mode I dominated crack propagation in an angle of approximately 70° counterclockwise with respect to the notch axis. On the other hand, at higher impact speeds, a shear band was observed to originate from a point on the lower surface of the notch-tip and propagated at an angle of 10° clockwise from the axis of the notch, i.e., towards the impacted part of the plate [2].

The specimen is discretized into uniform grid mesh with a spacing of 2 mm, resulting in a total of 20,396 particles within the domain. A velocity boundary condition of $v = 32$ m/s is applied to the left edge between two notches to simulate the impact on the specimen while the top and bottom edges are held fixed. According to previous research [32], the Young's modulus and Poisson's ratio are $E = 190$ GPa and $\nu = 0.3$ respectively. The Mode I critical intensity factor is $K_{Ic} = 68 \text{ MPa}\sqrt{\text{m}}$, which suggests the mode I energy release rate is $\mathcal{G}_{Ic} = 22.1 \text{ N/mm}$. However, the mode II energy release rate is not available and will therefore be the subject of investigation in this section. In this example, the Xu-Needleman model is utilized due to its distinct characterization on material's cohesive performance and suitable integration of normal and tangential behaviors.

To begin with, the Mode II energy release rate is assigned the same value as that of mode I, specifically $\mathcal{G}_{IIc} = 22.1 \text{ N/mm}$. By doing so, all parameters in the Xu-Needleman model can be calibrated using Eq. (3.94) through (3.97). Fig. 6.9(a) depicts the initiation and propagation process of cracks under this condition. The tensile cracks first emerge from the notch tips and extend almost horizontally on the specimen, as demonstrated by the bright yellow cracks in the figure. Subsequently, because of shear failure, more bonds along the crack path break, causing the crack directions to change, as indicated by the dark blue cracks in the figure. In the following fracture development process, the cracks are triggered by tensile failure of bonds and widened due to the shear failure. If the crack direction from

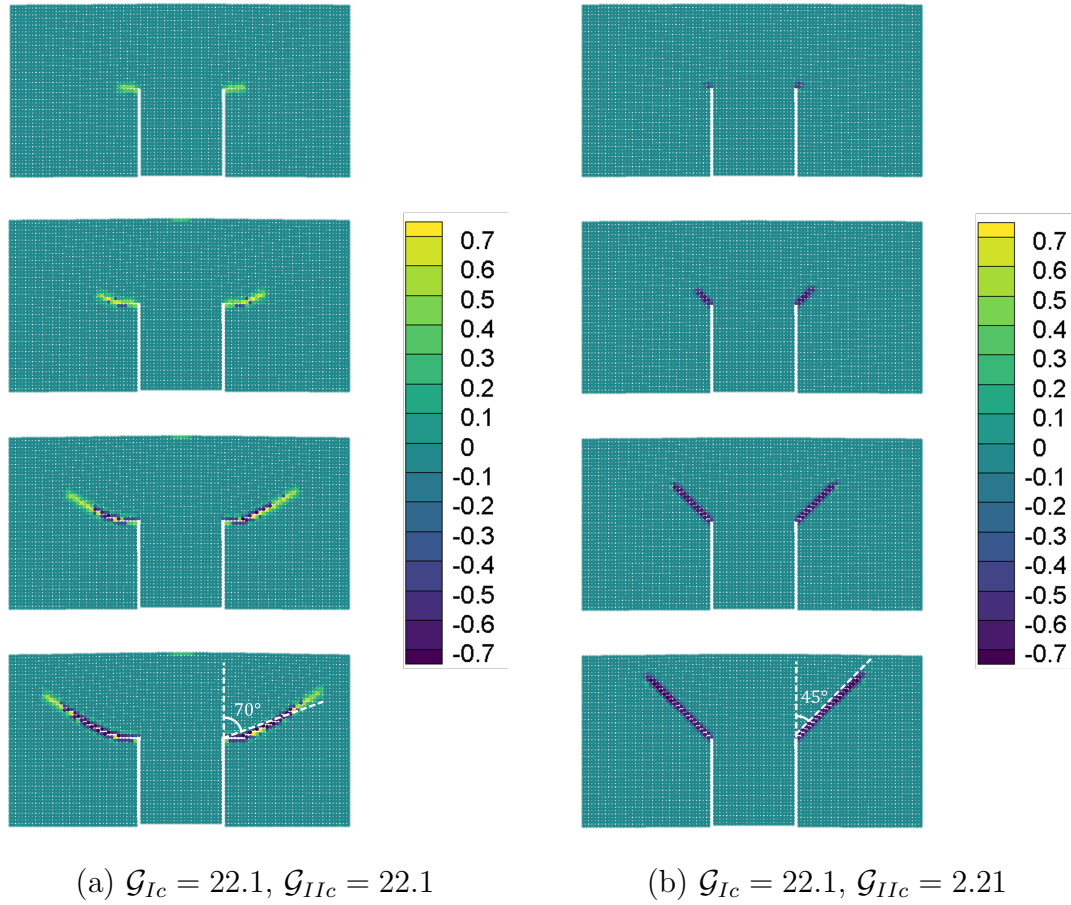


Figure 6.9: Crack propagation patterns caused by different energy release rates (unit: N/mm)

the notch tip is measured by linear regression, the angle would be approximately 70° .

To draw the comparison, we assign the mode II energy release rate a value of $\mathcal{G}_{IIc} = 2.21$ N/mm, which is only 10% of mode I counterpart and run the simulation again. The cracking pattern is depicted in Fig. 6.9(b). Different from the results with $\mathcal{G}_{IIc} = 22.1$ N/mm, the progression of cracks in this case is primarily governed by the shear failure of bonds, as suggested by the dark blue cracks in the figure. In this case, the cracks also start from the notch tips, but propagate as a straight line along 45° directions.

6.4 Energy competition mechanism

In this example, a plane strain edge crack problem is studied to demonstrate the energy competition mechanism. The size of specimen and boundary conditions are presented in Fig. 6.10(a). Two typical structural materials are investigated, namely Grade300 maraging

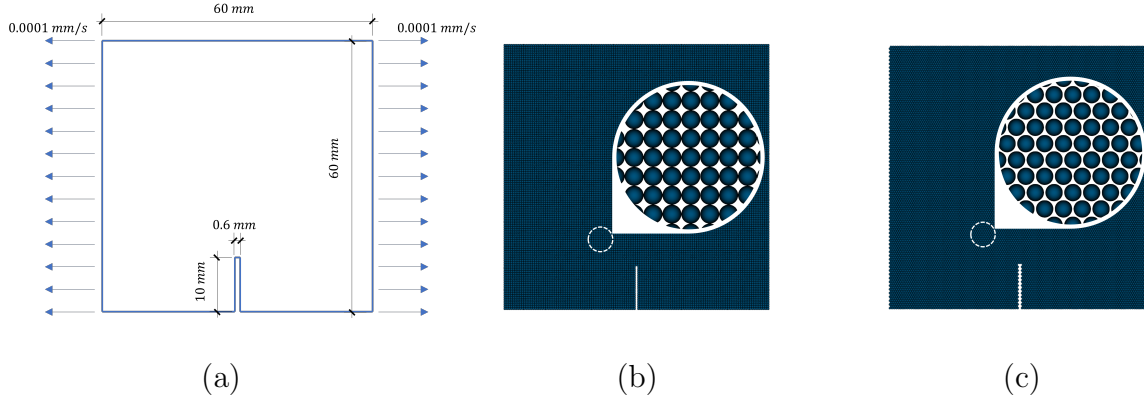


Figure 6.10: configuration of edge crack problem (a) Size of specimen and boundary conditions (b) BCC lattice structure in $[001]$ plane (c) FCC lattice structure in $[111]$ plane

steel and 7079 alloy aluminum. The Young's modulus, Poisson's ratio and plain strain fracture toughness of the former one are $E = 210\text{GPa}$, $\nu = 0.2$ and $K_{Ic} = 93.0\text{MPa}\sqrt{\text{m}}$ while the counterparts for the latter one are $E = 71.7\text{GPa}$, $\nu = 0.2$ and $K_{Ic} = 32.5\text{MPa}\sqrt{\text{m}}$ taken from Broek's book [8]. The energy release rate in plane strain problem, which is also twice of the surface energy, is linked to the fracture toughness by

$$2\gamma_s = \mathcal{G}_{Ic} = \frac{K_{Ic}^2}{E/(1 - \nu^2)} \quad (6.4)$$

Thus the surface energy for these two materials are $19.77\text{MPa} \cdot \text{mm}$ and $6.57\text{MPa} \cdot \text{mm}$ respectively. Since ferrite is a typical body-centered cubic(BCC) metal while aluminum is face-centered cubic(FCC), we use different lattice structures on $[001]$ plane and $[111]$ plane respectively, as shown in Fig. 6.10(b) and (c). One advantage of Peierls-Rice-Beltz model is that the fracture pattern can be controlled by adjusting the ratio of surface energy against unstable stacking fault energy, i.e. γ_s/γ_{us} . In deed, Rice et al. found that the crack tip blunting by dislocation nucleation will occur before conditions for Griffith cleavage decohesion are met. Specifically, when

$$\frac{\gamma_s}{\gamma_{us}} > 4 \frac{1}{(1 + \cos \theta) \sin^2 \theta} \quad (6.5)$$

is satisfied, crack tip will be blunted by the dislocation nucleation, where θ is the inclination angle measured from crack tip to the newly developed crack.

On the other hand, assuming $l_{n,c} = l_{t,c}$ and combining Eq. (3.104), (3.105), (3.106) and (3.107) will yield

$$\frac{\gamma_s}{\gamma_{us}} = \frac{\pi^2}{1 - 4\nu} \left(\frac{\alpha_t}{\alpha_n} \right)^2 \quad (6.6)$$

Eq. (6.6) indicates that the ratio of energy γ_s/γ_{us} is significantly affected by the ratio α_t/α_n . Actually, when α_t/α_n changes from 2 to $1/5$, the ratio of energy will change from 197.39

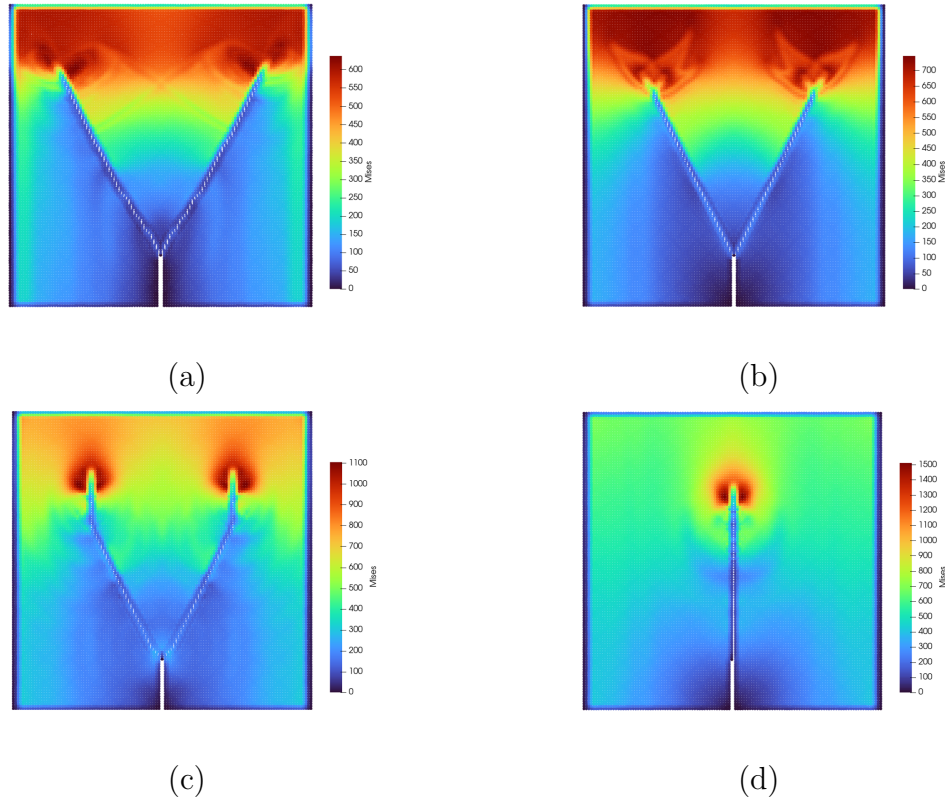


Figure 6.11: Crack pattern and σ_{11} stress distribution in BCC lattice structure with (a) $\alpha_t/\alpha_n = 2$, $\gamma_s/\gamma_{us} = 197.39$ (b) $\alpha_t/\alpha_n = 1$, $\gamma_s/\gamma_{us} = 49.35$ (c) $\alpha_t/\alpha_n = 1/2$, $\gamma_s/\gamma_{us} = 12.34$ (d) $\alpha_t/\alpha_n = 1/3$, $\gamma_s/\gamma_{us} = 5.48$

to 1.97. As a consequence, the cracking pattern will shift from ductile fracture to cleavage fracture.

The numerical results for BCC lattice is given in Fig. 6.11. it can be found in Fig. 6.11 that the cracks in BCC metallic material would develop along the slip plane when α_t/α_n ranges from 2 to 1 (γ_s/γ_{us} from 197.39 to 49.35). This is typical ductile cracking pattern. As the ratio α_t/α_n decreases, cleavage decohesion will gradually take the dominant role in fracture: in Fig. 6.11 (c), the crack tip is blunted at early stage, and later on the cracks will be diverted to the vertical direction. Despite of the cracking pattern transition, the inclination angle measured from the center notch to the crack path doesn't change very much in Fig. 6.11 (a)(b)(c). In fact, the inclination angles in Fig. 6.11 (a)(b)(c) are 31° , 27° and 26° respectively. However, if α_t/α_n keeps decreasing until $\alpha_t/\alpha_n \leq 1/3$ or $\gamma_s/\gamma_{us} \leq 5.48$, cleavage fracture will occur prior to the dislocation, and hence the specimen will subject to pure cleavage fracture.

Similar phenomena can also be observed in FCC lattice structure. When $\alpha_t/\alpha_n \geq 1$ or $\gamma_s/\gamma_{us} \geq 59.22$, ductile fracture can be obtained, as presented in Fig. 6.12 (a) while

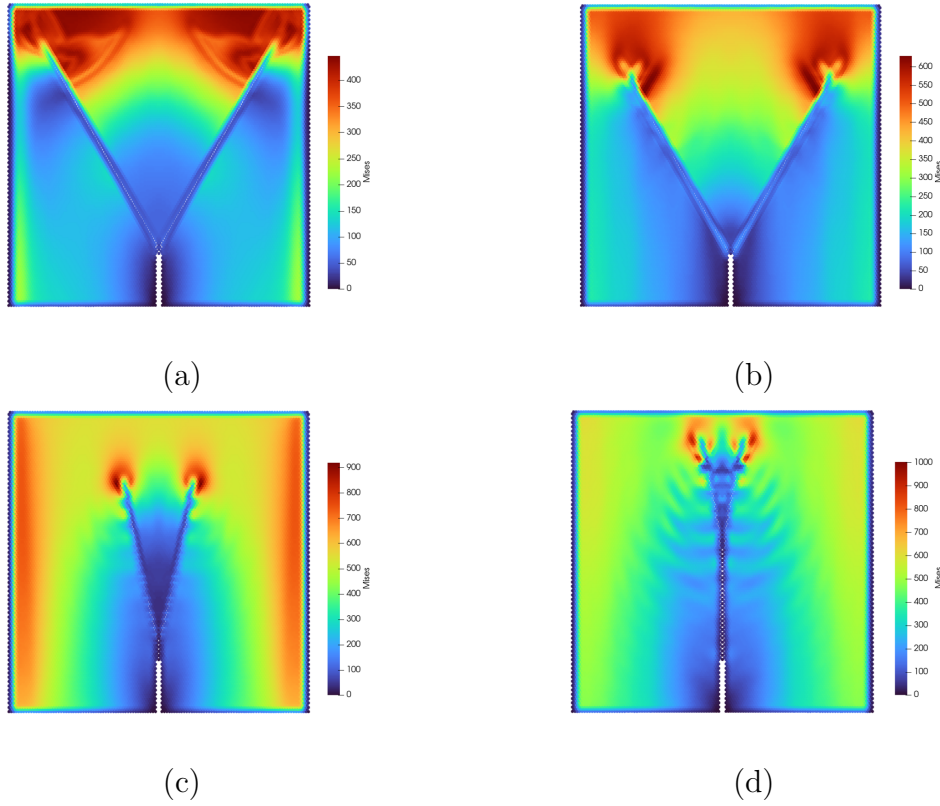


Figure 6.12: Crack pattern and the von-Mises stress distribution in an FCC crystal with (a) $\alpha_t/\alpha_n = 1$, $\gamma_s/\gamma_{us} = 49.35$ (b) $\alpha_t/\alpha_n = 1/2$, $\gamma_s/\gamma_{us} = 12.34$ (c) $\alpha_t/\alpha_n = 1/4$, $\gamma_s/\gamma_{us} = 3.08$ (d) $\alpha_t/\alpha_n = 1/5$, $\gamma_s/\gamma_{us} = 1.97$

when $\alpha_t/\alpha_n \leq 1/5$ or $\gamma_s/\gamma_{us} \leq 1.97$, brittle cracking prevails, as shown in Fig. 6.12 (d). If $1/5 < \alpha_t/\alpha_n < 1$, the cracking pattern will shift gradually from ductile to brittle cleavage fracture. Besides the similarity, there are also some differences. To begin with, the transition between ductility and brittleness in FCC material is more smooth than that of BCC material, which can be reflected by the change of inclination angle. The inclination angle θ in Fig. 6.12 (a) and (b) are both 30° , but that of (c) is 14° . Also, there is no vertical branch of crack in 6.12 (c).

According to Eq. (6.5), one can draw the borderline between ductile and brittle fracture for general materials, as shown in Fig. 6.13. Since the inclination angles have been measured from Fig. 6.11 and 6.12 the energy ratios γ_s/γ_{us} can be computed by Eq. (6.6), each cracking status actually can be represented by a dot on Fig. 6.13. As shown in Fig. 6.13, the cracking patterns presented in Fig. 6.11 (a)(b)(c) as well as those in Fig. 6.12(a)(b) belongs to ductile fracture while the remaining ones belongs to brittle fracture, which confirms that Eq. (6.5) can classify the brittle fracture and ductile fracture reasonably.

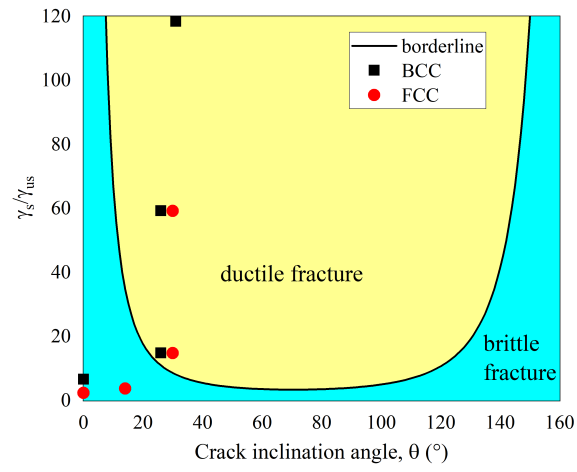


Figure 6.13: relation between materials' ductility and the ratio of γ_s/γ_{us}

Chapter 7

Numerical examples: state-based model

In this section, a comparative study is conducted to evaluate and compare the performance of all the bond-associated material correspondence models presented in Sections 3 and 4. Specifically, these bond-associated models are studied by checking elastic deformation, modeling elastic wave propagation, and modeling brittle fracturing behaviors. The material properties used in this section are dimensionless, with Young's modulus $E = 10^6$ and Poisson's ratio $\nu = 0.3$. Unless otherwise specified, a material point horizon size of $3 \times$ mesh spacing is used. The formulations, together with their notations and specific explanations are provided below to minimize potential confusion for readers.

- CPD: Conventional PeriDynamics, first proposed by Silling et al. [72]. In the CPD formulation, as well as in the subsequent BCPD, BHPD, and LMPD formulations, the spherical influence function given in Eq. (2.7) is used by default unless otherwise specified.
- BCPD: Bond-Correction-based PeriDynamics, which incorporates the bond-level deformation gradient proposed by Breitzman and Dayal [7].
- BHPD: Bond-associated Horizon PeriDynamics, which was first introduced by Chen et al. [12, 17, 11, 10]. BHPD, together with the following HPPD formulation, can also be categorized as Sub-Horizon-based PeriDynamics (SHPD) formulations.
- HPPD: Horizon-Partition PeriDynamics, a sub-horizon-based stabilization approach proposed by Chowdhury et al. [18]. It should be noted that the arbitrary sub-horizon division techniques were demonstrated only for 2D problems in the original work. Since their extension to 3D cases has not been well established and requires further investigation, a commonly used 8-sub-horizon division method is adopted for the 3D examples presented here. In addition, material particles that do not have full horizon, such as those near domain boundaries, are assigned fewer horizon partitions to ensure the invertibility of their shape tensors.

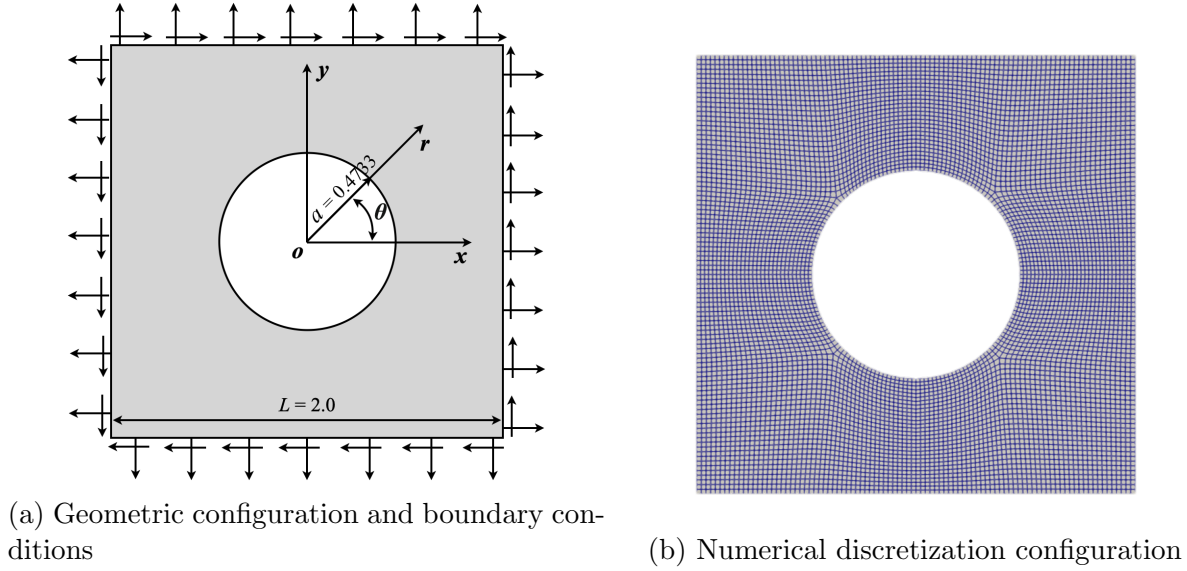


Figure 7.1: Schematic diagram of elastic square plate with centered hole.

- LMPD: Lagrange-Multiplier-based PeriDynamics presented in Hou and Zhang's work [36].
- NSPD: Non-Spherical-influence-function-based PeriDynamics, that initially proposed by Chen et al. [14, 15]. The parameters for the non-spherical influence function given in Eq. (2.26) are set to be equal, namely $n_1 = n_2$.

Several numerical techniques were implemented to reduce computational cost and accelerate the simulations. The bond-associated shape tensor $\mathbf{K}_\xi$ for each bond is precomputed during program initiation and stored for subsequent use. Additionally, OpenMP interface is employed to speed up the evaluation of bond-associated deformation gradients, PK1 stresses, and force density states.

7.1 Elastic Deformation Prediction

In this subsection, the comparison of prediction accuracy for elastic deformation problems among bond-associated models is assessed. A two-dimensional 2×2 square plate with centered hole ($a = 0.4733$) under tensile loading is studied. The dimensions, the displacement are given in both Fig. 7.1(a) and Eq. (7.1). The nodes in a finite element mesh with mesh size being 0.02, as depicted in Fig. 7.1, are leveraged as peridynamics material particles. The total number of material particles is 7,925. For comparison purposes, material point size convergence study is not performed in this study.

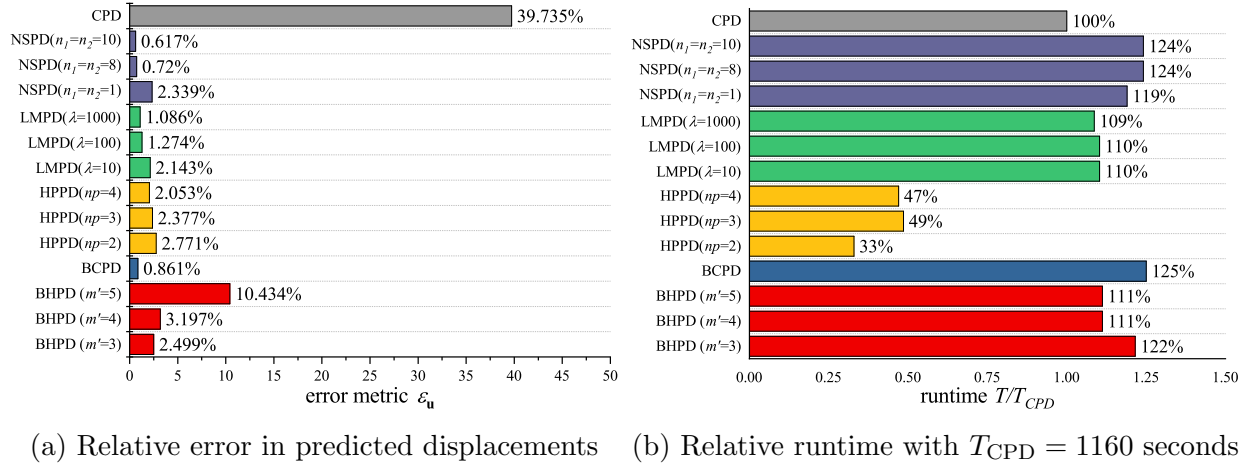


Figure 7.2: Comparison of prediction error and runtime among different formulations.

For the case of infinite plate size, the analytical solutions of displacements in the x- and y-direction for the problem are given as [15]

$$\begin{aligned} u_x(r, \theta) &= \frac{Ta}{8\mu} \left[\frac{r}{a} (\kappa + 1) \cos \theta + 2 \frac{a}{r} ((1 + \kappa) \cos \theta + \cos 3\theta) - 2 \frac{a^3}{r^3} \cos 3\theta \right] \\ u_y(r, \theta) &= \frac{Ta}{8\mu} \left[\frac{r}{a} (\kappa - 3) \sin \theta + 2 \frac{a}{r} ((1 - \kappa) \sin \theta + \sin 3\theta) - 2 \frac{a^3}{r^3} \sin 3\theta \right] \end{aligned} \quad (7.1)$$

where $\kappa = (3 - \nu) / (1 + \nu)$ for plane stress conditions, μ is the shear modulus, (r, θ) is a polar coordinate system with the origin at the hole center (see Fig. 7.1a), a is hole radius, and T is a scale factor that represents the magnitude of the external force. The length of the plate $L = 2$ is selected so that the analytical solution for infinite plate size can be reasonably used as reference solution for this study. The adaptive dynamic relaxation algorithm [44] is adopted in this study, and the scale factor T is linearly increased to 10^4 in the first 1,000 time steps and remains constant until the displacement field converges to a given tolerance. Displacement boundary conditions consistent with the above displacement fields (Eq. 7.1) are applied to the four sides of the plate.

To measure the error of the prediction against the analytical solution, the following metric is used to measure the error of the whole simulation domain:

$$\mathcal{E}_{|u|} = \frac{\int_{\Omega} ||\mathbf{u}_{AS}| - |\mathbf{u}_{PD}|| dV}{\int_{\Omega} |\mathbf{u}_{AS}| dV} \quad (7.2)$$

where the subscript PD refers to the quantity computed from peridynamics while AS refers to that from analytical solution.

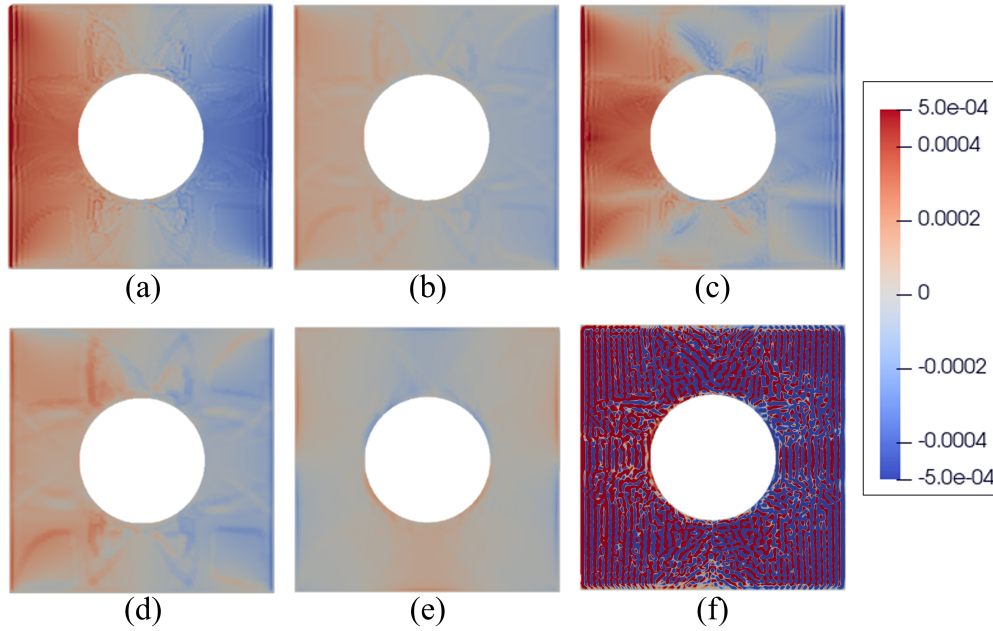


Figure 7.3: Comparison of absolute error in predicted x -displacement for different models: (a) BHPD with $m' = 3$, (b) BCPD, (c) HPPD with $np = 4$, (d) LMPD with $\lambda = 1000$, (e) NSPD with $n_1 = n_2 = 10$, and (f) CPD.

The error metric $\mathcal{E}_{|\mathbf{u}|}$ for different bond-associated models is presented and compared in Fig. 7.2a. It should be noted that the bond-associated horizon is characterized as $\delta_h = m' \times \Delta\bar{X}$, where $\Delta\bar{X}$ is an average material point spacing. As can be seen, all the bond-associated models predict accurate deformation fields, with the global error ranging from 0.617% to 2.771%. While the CPD model exhibits a significantly higher error of 39.735% due to the existence of material instability in the model. Among these bond-associated models, the NSPD and BCPD models predict the most accurate deformation fields, the LMPD and HPPD models predict less accurate results, and the BHPD model predicts the least accurate results. It can also be seen that the different model parameters play critical role in the prediction accuracy. From the parametric analysis, the error in BHPD increases as size of bond-associated horizon m' increases; in HPPD, the error decreases with increasing number of partitions np ; in LMPD, the error reduces as penalty factor λ increases; and in NSPD, the error decreases with increasing values of n_1 and n_2 .

To compare the computational efficiency among the bond-associated models, the total runtime required for each model to yield the results reported in Fig. 7.2a is measured and summarized in Fig. 7.2b. The models were implemented using the same algorithm, and simulations were executed on a desktop equipped with an AMD Ryzen 9 5950X 16-core processor. For comparison, the runtime of CPD model is taken as the baseline and normalized to 100%. Based on this reference, the average runtime of other models are as follows:

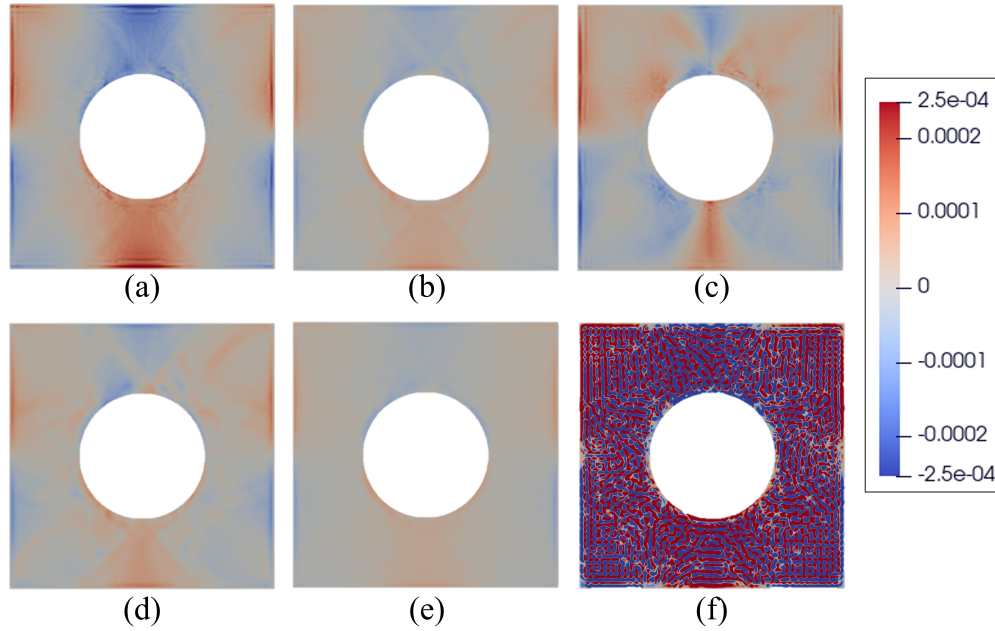


Figure 7.4: Comparison of absolute error in predicted y -displacement for different models: (a) BHPD with $m' = 3$, (b) BCPD, (c) HPPD with $np = 4$, (d) LMPD with $\lambda = 1000$, (e) NSPD with $n_1 = n_2 = 10$, and (f) CPD.

BHPD requires approximately 115% of the CPD runtime, BCPD 125%, HPPD 43%, LMPD 110%, and NSPD 122%. These results indicate that, although some bond-associated models incur higher computational time, particularly the BHPD, HPPD and LMPD models, they offer improved accuracy and stability. On the other hand, the HPPD model demonstrates significantly better computational efficiency while still addressing the zero-energy mode issue and yields reasonably accurate results, highlighting its potential as a practical and efficient alternative to the conventional formulation for elastic deformation problems. It is worth noting that although the CPD formulation requires less computing time per step, it needs significantly more steps to achieve convergence due to existence of material instability. In contrast, bond-associated formulations takes longer computing time per step but generally requires less solution steps to converge. Consequently, certain bond-associated formulations can achieve comparable or even better performance than the CPD formulation in terms of computational efficiency.

The detailed absolute error distribution of the displacement fields, $u_{x,AS} - u_{x,PD}$ and $u_{y,AS} - u_{y,PD}$, are shown in Fig. 7.3 and Fig. 7.4, respectively. As can be seen from these results, the CPD model exhibits significant oscillation in the predicted displacement fields, due to the existence of material instability. The absolute errors of CPD model exceed the bounds of the bond-associated models that shown in the legend. For all bond-associated models, the distribution of the absolute errors shows that the NSPD model has the most accurate pre-

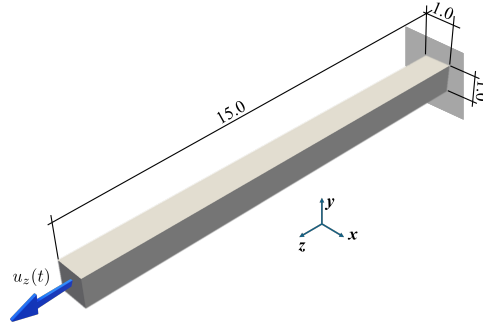


Figure 7.5: Schematic diagram of elastic bar subjected to z-direction displacement load.

diction, followed by the BCPD model and the LMPD model. The HPPD and BHPD models predict the less accurate displacements distribution among the bond-associated models.

In summary, for modeling elastic deformation problems, the NSPD is the most predictive, followed by the BCPD, the LMPD, the HPPD and the BHPD models. In terms of computational efficiency, the HPPD is the most efficient. The BHPD and LMPD models take slightly less computational time than the NSPD and the BCPD models. There is material instability in the CPD model.

7.2 Elastic Wave Propagation Modeling

In this subsection, the performance of bond-associated models is assessed and compared for modeling 3D elastic wave propagation problems. An elastic bar with dimensions of $1.0 \times 1.0 \times 15.0$ under dynamic loading is considered. See Fig. 7.5 for reference. The mesh spacing used in this example is $\Delta X = \Delta Y = \Delta Z = 0.05$, resulting in 21, 21, and 315 material particles along the x , y and z directions, respectively. The first layer of material particles at one end of the elastic bar in the z -direction is fixed, while the other end is applied with a displacement of the following form

$$u_z(t) = 0.01 \times \sin(40\pi t) \quad (7.3)$$

for a period of time $t_{apply} = 0.05$. The total simulation time is $t_{total} = 0.35$, and time step size of $\Delta t = 10^{-4}$ is used. The Verlet method is used for time integration. To minimize the effect of the transverse wave on the longitudinal wave due to Poisson's effect, the material Poisson's ratio used in this example is $\nu = 0.0$. For reference, FEA results were also obtained, using 120,000 ($20 \times 20 \times 300$) 8-node hexahedral elements with element sides of $L_e = 0.05$. For the HPPD model, a single partition number of $np = 8$ was used in this example.

The displacement in the z -direction at the center point $(0.5, 0.5, 7.5)$ is extracted and plotted along with FEA solution to assess the accuracy and stability of various peridynamic bond-associated models. The comparison results are presented in Fig. 7.6. In the case of

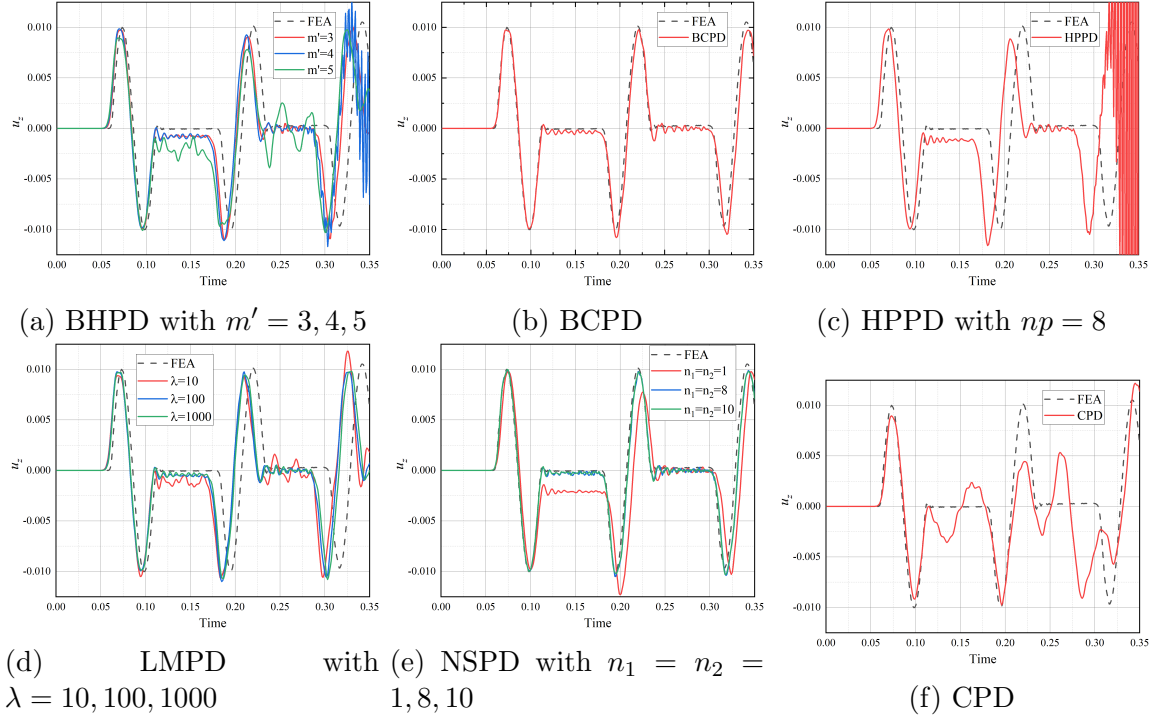


Figure 7.6: Time history of displacement u_z at the center point for various bond-associated models.

the CPD model (Fig. 7.6f), the displacement history curve exhibits a very large discrepancy with FEA results after the passage of the first elastic wave. This large discrepancy manifests the material instability in the model. The BHPD model (Fig. 7.6a) shows improvement over the CPD model, especially as the parameter m' decreases from 5 to 3. As m' decreases, the discrepancy with FEA results decreases, indicating smaller size sub-horizons help suppress the material instability. However, a phase shift is observed for the reflected wave, with displacement peaks occurring earlier than those in the FEA result during the second passage of the wave through the target location. The BCPD model (Fig. 7.6b) yields a much smoother displacement history compared to the BHPD model. The predicted displacement history curve aligns well with the FEA results in amplitude and without obvious phase shift for the reflected wave, demonstrating this model's ability to eliminate material instability while achieving accuracy. The HPPD model (Fig. 7.6c) with $np = 8$ sub-horizons predicts a displacement history that initially tracks the FEA results but later the reflected wave diverges with significant phase shift and eventually leads to spurious oscillation. After a complete cycle of wave propagation, the material points fluctuate erratically, reflecting numerical instability in the model during later simulation stage with reflected wave. Similar oscillations were observed in the BHPD model, but less severe than the HPPD model. This later stage spurious oscillation in both sub-horizon-based models will be investigated later. In

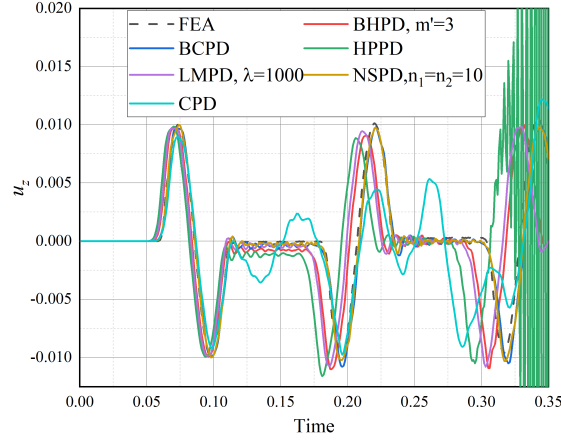


Figure 7.7: Summary and comparison of wave propagation predictions using various bond-associated models.

the LMPD model (Fig. 7.6d), increasing the penalty factor λ from 10 to 1,000 gradually improves material stability. While the predictions for smaller λ values are oscillatory and deviates from FEA results, the large penalty factor $\lambda = 1,000$ significantly improves the smoothness of the curve. However, even with large penalty factor λ , phase shift still exists. Finally, the NSPD model (Fig. 7.6e) shows great agreement with the FEA results as the parameters n_1 and n_2 increase. With $n_1 = n_2 = 10$, the displacement history curve almost overlaps with the FEA results in both amplitude and phase, indicating high accuracy of the model compared to the FEA results.

The optimum predictions of bond-associated models are summarized and compared in Fig. 7.7. As can be seen, except for the CPD and HPPD models, the material instability issue is eliminated in most bond-associated models. The phase shift of reflected wave exists in both the sub-horizon-based models, i.e., BHPD and HPPD, and the LMPD model. The spurious oscillation in the reflected wave exists in the HPPD model.

As computationally tested in this study, one simple but effective way to eliminate the phase shift of the reflected wave and spurious oscillation in the simulation is to use a constant influence function (Eq.(2.8)). In this study, $c = 1$ is adopted.

The simulation results obtained using the unit influence function are shown in Fig. 7.8. For comparison purposes, the results of the NSPD model are also included in the figure. As can be seen, adopting the constant influence function not only eliminates the phase shift in reflected wave in the BHPD, HPPD and LMPD models but also removes the spurious oscillation in the BHPD and HPPD models. This adjustment leads to a more physically consistent wave propagation behavior and improved alignment with FEA results. For the BCPD model using two different spherical influence functions, the difference between the results is subtle. The material instability persists in the CPD model for using constant influence function.

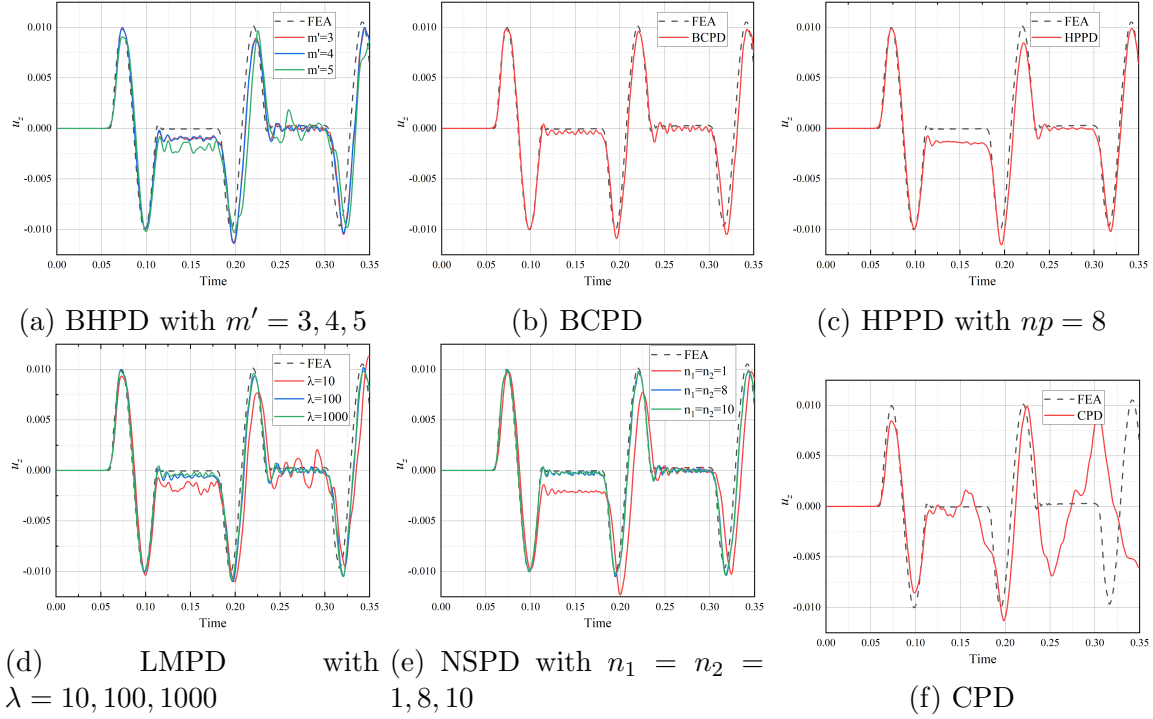


Figure 7.8: Time history of displacement u_z at the center point for various bond-associated models with unit influence function.

The optimum curves produced by various bond-associated models with constant influence function are plotted in Fig. 7.9. For comparison purposes, the results of the NSPD model are also included in the figure. In contrast to the results shown in Fig. 7.7, where notable discrepancies exist between the models and the FEA results, the displacement history curves in Fig. 7.9 exhibit nearly identical behavior, except the CPD model where material instability persists irrespective of whatever spherical influence function being used. The differences between the bond-associated models and the FEA results become negligible, highlighting the critical role of influence function symmetry in ensuring both accuracy and stability in dynamic simulations using the bond-associated models for a given horizon size.

A possible explanation for the phase shift of the reflected wave in the bond-associated models is provided as follows. The cause of the phase shift lies in the local non-symmetry of the influence function. To better explain this, a 1D example is demonstrated in Fig. 7.10. For the sake of clear illustration, the sub-horizon-based model is utilized in this example, and other bond-associated formulations can be examined in the same fashion. Consider two elastic waves: one propagating from left to right and the other from right to left. If the two waves are symmetric with respect to a material point $\mathbf{X}'$, a neighbor in the neighborhood of $\mathbf{X}$, then the deformation gradients they produce at $\mathbf{X}'$ should satisfy the relation $\mathbf{F}^{(1)}(\mathbf{X}') = -\mathbf{F}^{(2)}(\mathbf{X}')$, where $\mathbf{F}^{(1)}$ and $\mathbf{F}^{(2)}$ correspond to the two waves, respectively. However, if the

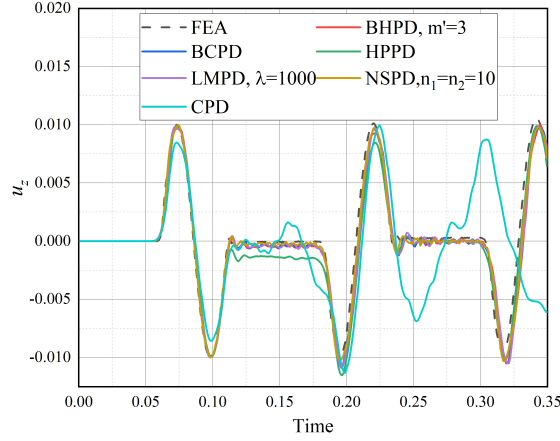


Figure 7.9: Summary and comparison of wave propagation predictions using various bond-associated models with unit influence function.

influence function lacks symmetry with respect to $\mathbf{X}'$ (which is coined as *local non-symmetry* with respect to $\mathbf{X}'$), such as the variable spherical influence function given in Eq. (2.7), the integrals involving ω^{SHPD} and $\mathbf{y}'$ yield different results, and by extension the nonlocal deformation gradients computed by Eq. (2.7) become unequal, as demonstrated in Fig. 7.10. This discrepancy results in different stress measures and, consequently, different bond force density states. These inconsistencies ultimately manifest as phase shift in the reflected elastic wave propagation. In conclusion, the local non-symmetric influence function adopted in calculating bond-associated deformation gradient effectively introduces “artificial” resistance forces into the system, which ultimately leads to the phase shift in reflected elastic wave modeled using the bond-associated models.

However, when the constant influence function given in Eq. (2.8) is used, the local symmetry within the sub-horizon and global symmetry within the material point horizon both are preserved. Hence, $\mathbf{F}^{(1)}(\mathbf{X}') = -\mathbf{F}^{(2)}(\mathbf{X}')$ is satisfied for the two waves passing through $\mathbf{X}'$. Therefore, there is no phase shift in the reflected wave.

In summary, for bond-associated models, the influence function significantly affects the wave propagation modeled using these models. Using variable spherical influence function in the SHPD and LMPD models, it results in phase shift in the reflected wave. However, using constant influence function can eliminate phase shift and significantly improve the performance of the SHPD and LMPD models. The BCPD model produces accurate results irrespective of the influence function, while the NSPD model has the best performance for elastic wave propagation problems among the bond-associated models due to the symmetry nature of the non-spherical influence functions with respect to $\mathbf{X}'$. Material instability exists in the CPD model irrespective of what spherical influence functions being used.

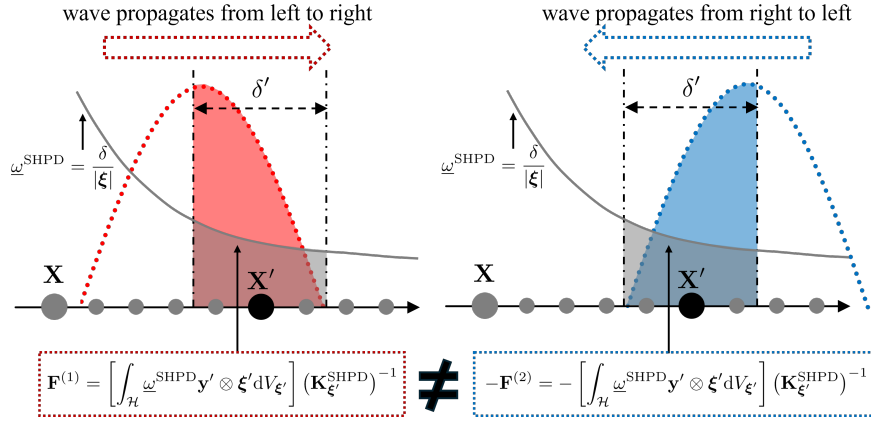


Figure 7.10: Schematic explanation for phase shift in sub-horizon-based models using variable spherical influence function.

7.3 Finite Elastoplastic Deformation Analysis

In this example, an elastoplastic problem under finite deformation is studied to assess the performance of the proposed NSPD formulation for modeling finite inelastic deformation problems. Specifically, a tensile test with applied displacements on a dog-bone shaped thin plated is modeled. The detailed geometric information and applied boundary conditions are given in Figure 7.11. The applied displacements on the top and bottom edges are $\bar{u}_y = +0.005$ and $\bar{u}_y = -0.005$ respectively while $\bar{u}_x = 0$, which results in total of 10% nominal strain in the y -direction. The same discretization (see Figure 7.11) with total number of 33,340 4-node quadrilateral (Q4) elements is used for both FE and NSPD simulations. The spacing factor is $n = 3$ and the exponents of influence function is set to $n_1 = n_2 = 8$.

The model predictions are verified against FE solutions obtained using the MOOSE framework. Recently developed plane stress model [16] that treats the out-of-plane strain as an independent variable in addition to the displacements is used to obtain both FE and NSPD results. The total Lagrangian formulation along with the incremental co-rotational formulation proposed by Rashid [64] have been used to model finite deformation problems in MOOSE. More formulation details can be found at [1].

The contour plots of the predicted x -displacement u_x , out-of-plane strain ϵ_{zz} and effective plastic strain $\bar{\epsilon}_p$ fields from both FE and NSPD simulations are shown in Figure 7.12. As can be seen, these three fields predicted by PD using the proposed formulation and bond-associated influence function agree very well with the FE results. However, clear strain localization has been observed in the out-of-plane strain and effective plastic strain fields obtained using NSPD. Similar phenomenon has been observed in other PD simulations for finite strain problems, such as [78, 79]. FE solutions don't show the similar strain localization pattern. The comparison of stress components between NSPD and FE results are shown in Figure 7.13. It is clear that the weighted average stress components from the bond-associated

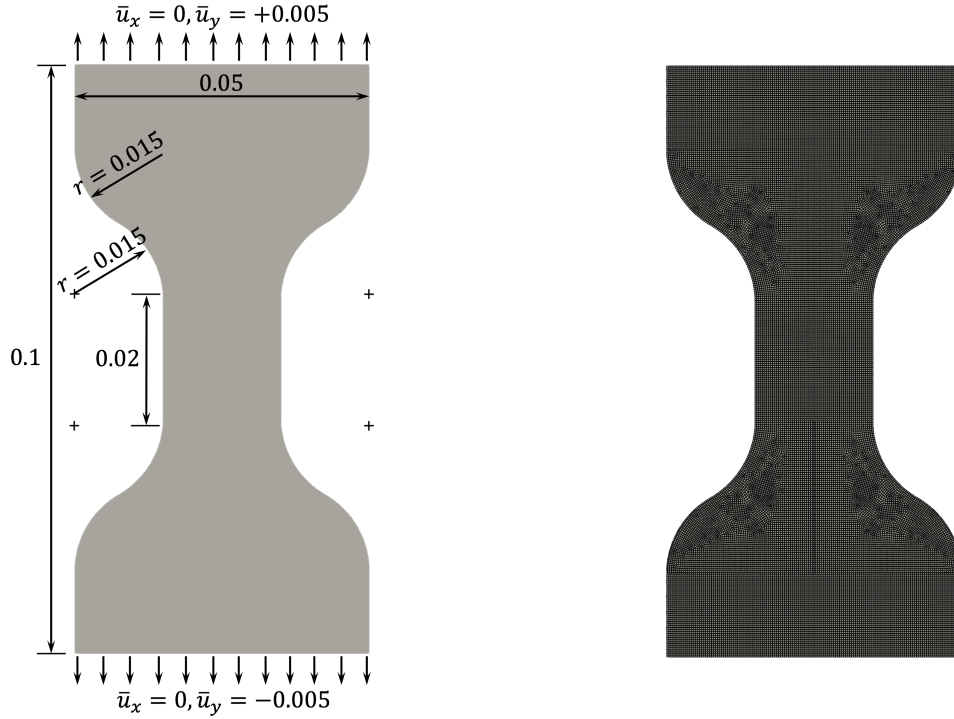


Figure 7.11: Dog-bone shaped thin plate under uni-axial displacement loading and the finite element discretization using 33,340 Q4 elements.

stress components match very well with the FE results. The strain localization can also be observed in the predicted stress fields of normal components.

The comparison of reaction force on the bottom edge between NSPD and FE results are shown in Figure 7.14. The normalized total reaction force of the y -axis is obtained by dividing the real reaction force by the plate thickness to avoid showing different values for different thickness. As can be seen from the total force-displacement curves, the predicted reaction force on the bottom edge matches very well with the FE result. However, the comparison of nodal force-displacement curves show discrepancy between NSPD prediction and FE result for the maximum nodal force on the bottom edge after the start of plastic deformation. The discrepancy increases with the increase of applied displacement. Nonetheless, the minimum nodal forces match very well between PD prediction and FE result for the whole loading profile. The average nodal force curves are the same as the total force curves on the bottom edge.

From this study, it is concluded that the proposed state-based model using the bond-associated influence function is highly predictive for finite elastoplastic deformation problems. Strain localization can be captured using the peridynamics model.

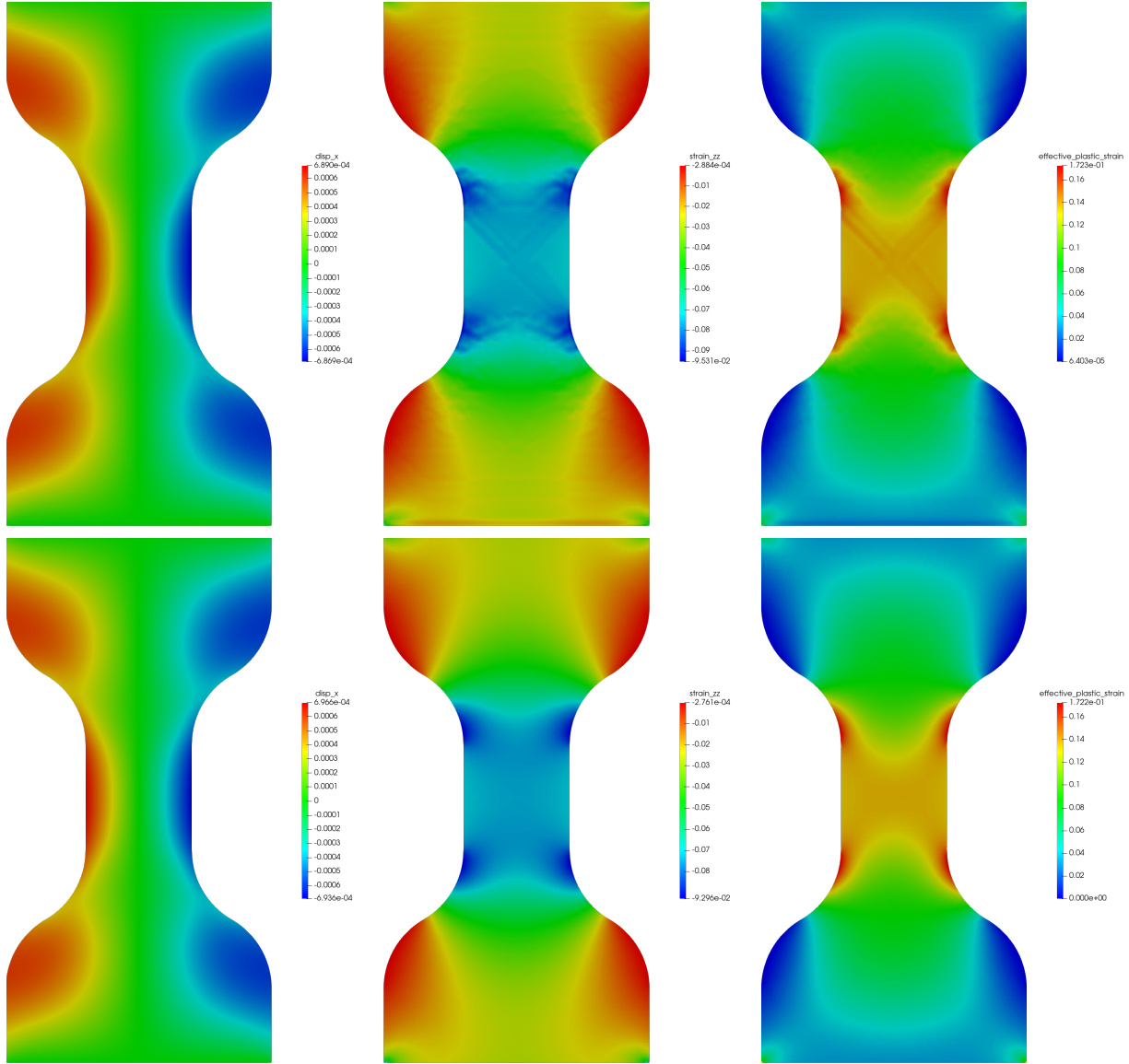


Figure 7.12: Comparison of PD and FE results: displacement u_x , strain ϵ_{zz} and effective plastic strain $\bar{\epsilon}_p$ (top row: PD; bottom row: FE).

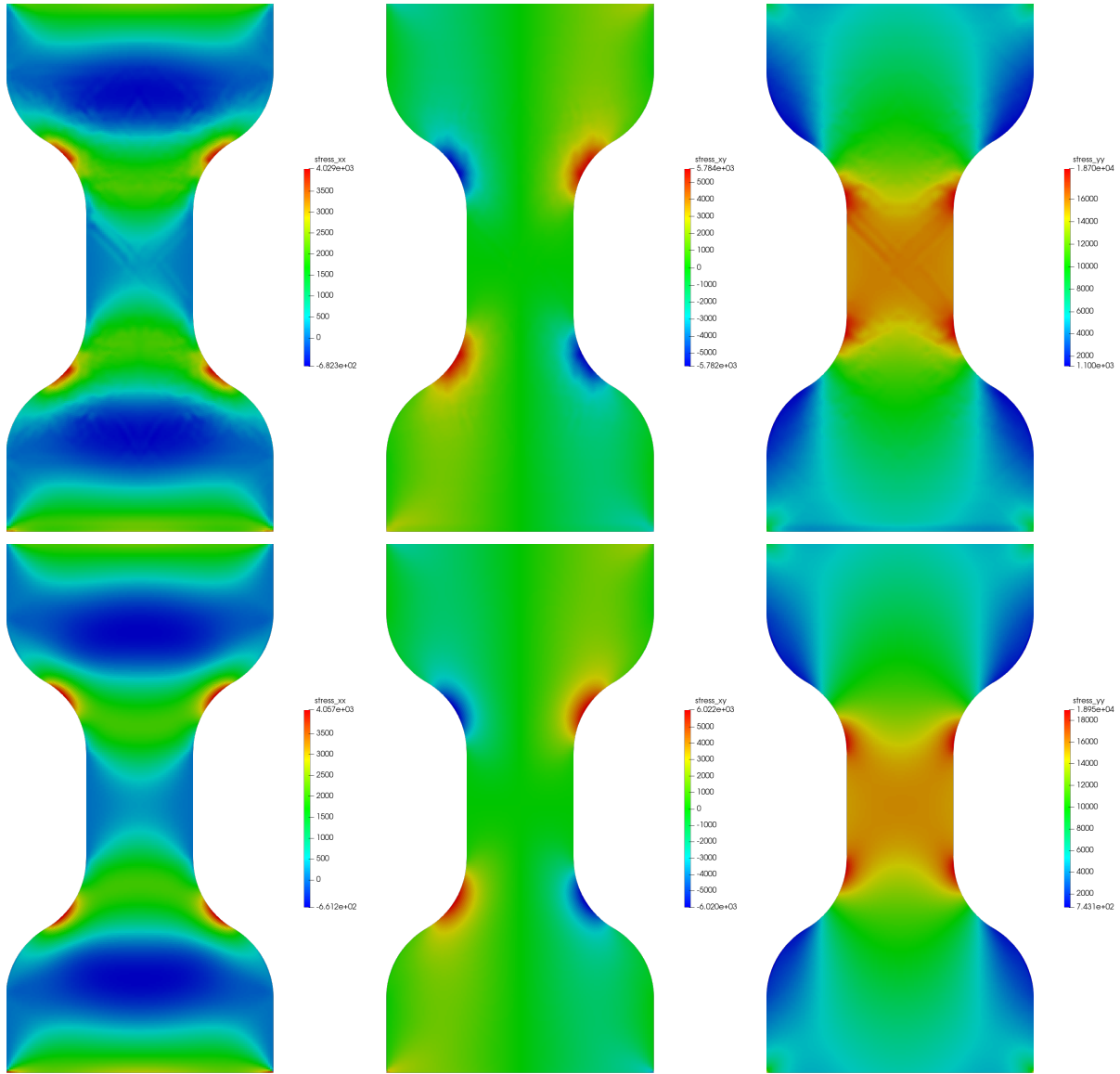


Figure 7.13: Comparison of PD and FE results: stresses σ_{xx} , σ_{xy} and σ_{yy} (top row: PD; bottom row: FE).

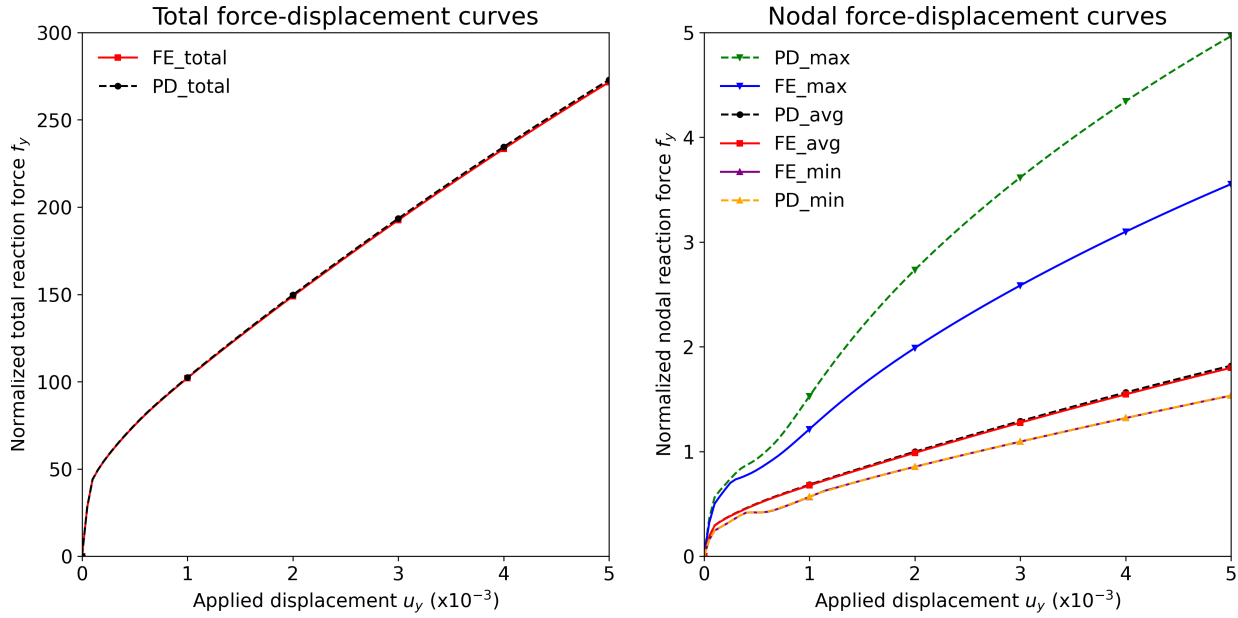


Figure 7.14: Comparison of PD and FE results: force-displacement curves of the bottom edge.

7.4 Linear elastic fracture analysis

In this example, a classical linear elastic single-edge-notch-tension problem is investigated to demonstrate the applicability of the proposed NSPD formulation to fracture problems. As shown in Fig. 7.15, a two-dimensional single-edge-notch plate is subjected to tension on both sides. A uniform grid structure with spacing of 0.02 is used to discretize the domain, which results in total of 10,174 material points. The notch is created by removing material points based on its dimensions (see Fig. 7.15). Similarly, the spacing factor of $n = 3$ is used and the exponents of the influence function is set to be $n_1 = n_2 = 8$. The plane strain model is used. To achieve a quasi-static process, the loading velocity is set to 5×10^{-8} /step and the simulation runs for a total of 4000 steps. The adaptive dynamic relaxation integrator [37] is adopted.

For modeling fracture using material correspondence model, it has been a common practice that broken bonds are excluded from the computation of the shape tensor and nonlocal deformation gradient [17, 46, 24, 84]. As a result, this approach often leads to a singular shape tensor due to insufficient number of non-broken bonds left for a material point after bond breakage. In this study, we propose an alternative approach to address this issue by treating bond failure as an integral part of the constitutive law for each bond. Take the bond failure criterion adopted in this problem as an example: if the maximum principal stress computed for a given bond exceeds the threshold value σ_c , the bond is considered broken and the stress for this bond is set to zero. For fracture problems, quantities such as

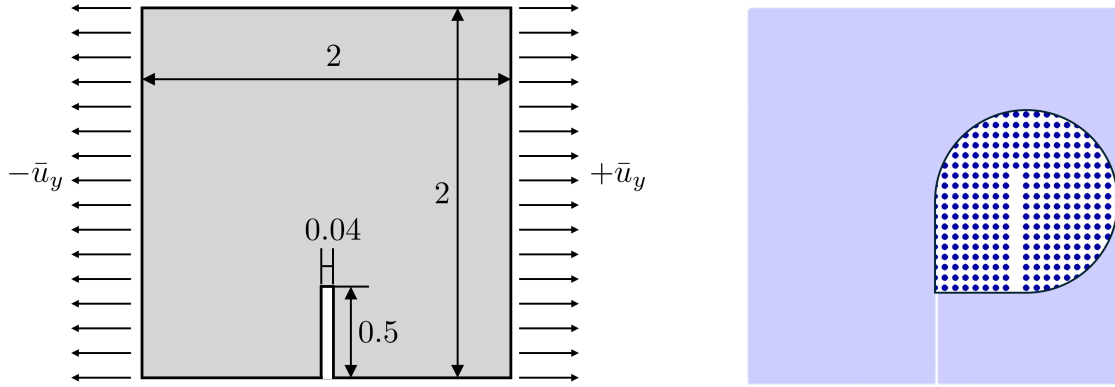


Figure 7.15: A single-edge-notch elastic plate under tension and uniform discretization using 10,174 material points.

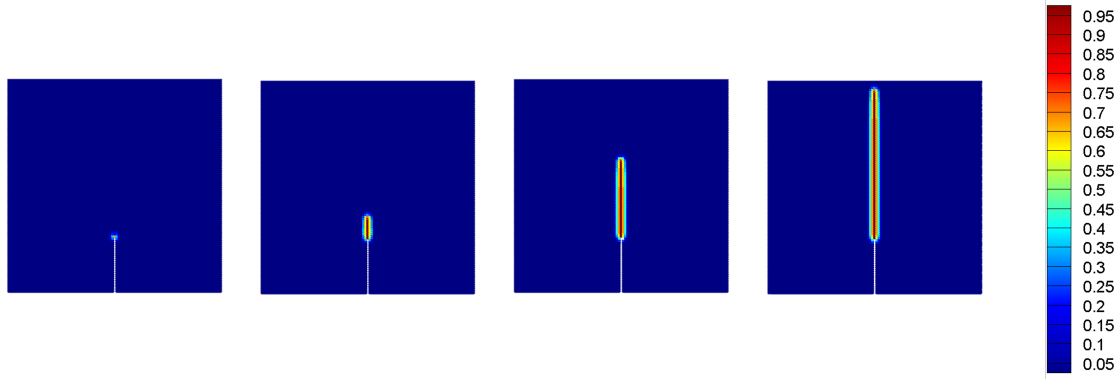


Figure 7.16: Crack initiation and propagation for the single-edge-notch-tension problem. The length of crack is $l = 0.06, 0.26, 0.88$ and 1.40 respectively from left to right.

damage index and stress for a material point are computed as average values from all bonds.

The process of crack initiation and propagation is illustrated in Fig. 7.16. Notably, the material damage forms a continuous field. Consistent with the theory of linear elastic fracture mechanics for Mode-I fracture, the crack initiates at the tip of the pre-existing notch and propagates along the direction of the notch until completely separates the plate into two halves.

The stress distributions of σ_{xx} , σ_{xy} and σ_{yy} are depicted in Fig. 7.17. As the crack develops, a noticeable stress concentration can be observed at the crack tip. For linear elastic material subjected to Mode-I loading with an edge notch, there exists an analytical asymptotic solution for the stress concentration [80, 3]. These stress fields are proportional

to

$$\sigma_{xx} \propto \cos \frac{\theta}{2} \left(1 - \sin \frac{\theta}{2} \sin \frac{3\theta}{2} \right) \quad (7.4)$$

$$\sigma_{xy} \propto \cos \frac{\theta}{2} \left(1 + \sin \frac{\theta}{2} \sin \frac{3\theta}{2} \right) \quad (7.5)$$

$$\sigma_{yy} \propto \cos \frac{\theta}{2} \sin \frac{\theta}{2} \cos \frac{3\theta}{2} \quad (7.6)$$

where θ is the angle cylindrical coordinate at the crack tip. To further verify the proposed formulation, the stress components obtained through numerical simulation are compared with their analytical solutions. At each time step, the position of the crack tip is firstly located. Next, a circular region with a radius of 0.2 at the crack tip is identified. The stress values of the material points on the edge of the circular region are then extracted. To draw a straightforward comparison, the stress fields are normalized. Specifically, the numerical solutions for σ_{xx} , σ_{xy} and σ_{yy} are scaled to match the range of the corresponding analytical solutions presented above. The resulting normalized stress components corresponding to crack length of 0.06, 0.26, 0.88 and 1.40 are plotted in Fig. 7.18 together with the analytical solution. As shown in the Fig. 7.18, the stress fields generally agree with the analytical solution during crack propagation. However, in certain regions, the abrupt stress changes are not accurately captured. This discrepancy arises from the non-local nature of peridynamics, and can be mitigated by using a smaller grid spacing and horizon. A systematic study on this will be performed in future work.

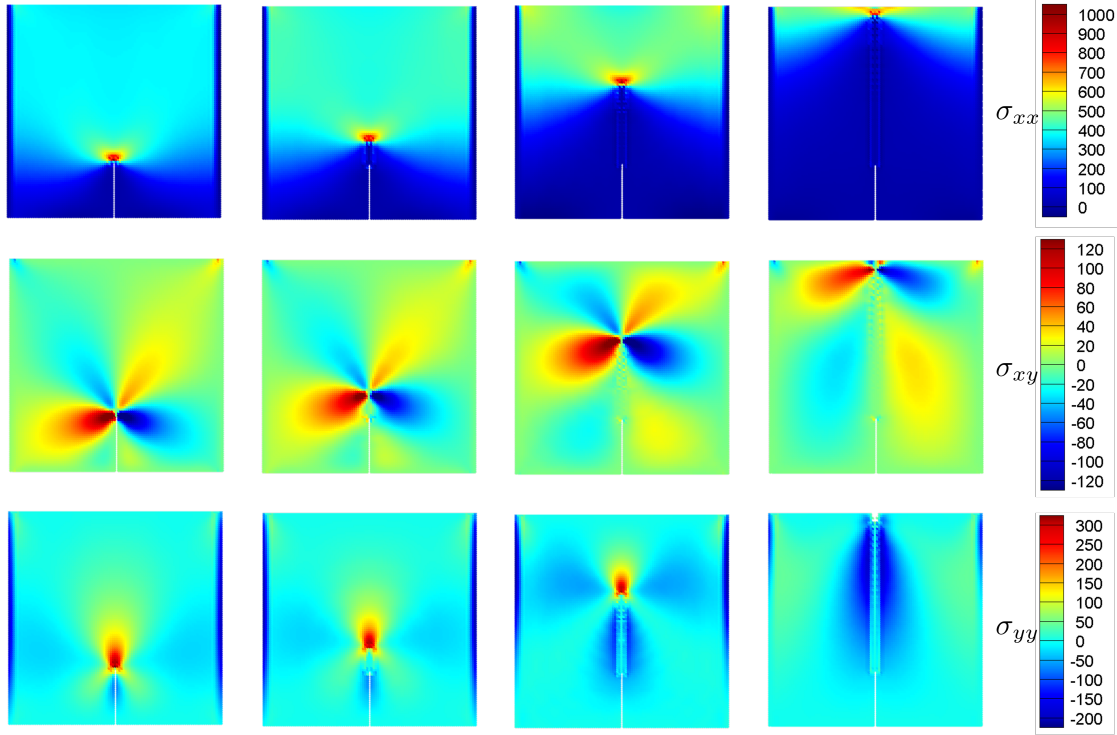


Figure 7.17: Stress distribution during the crack propagation process. The length of crack is $l = 0.06, 0.26, 0.88$ and 1.40 respectively from left to right.

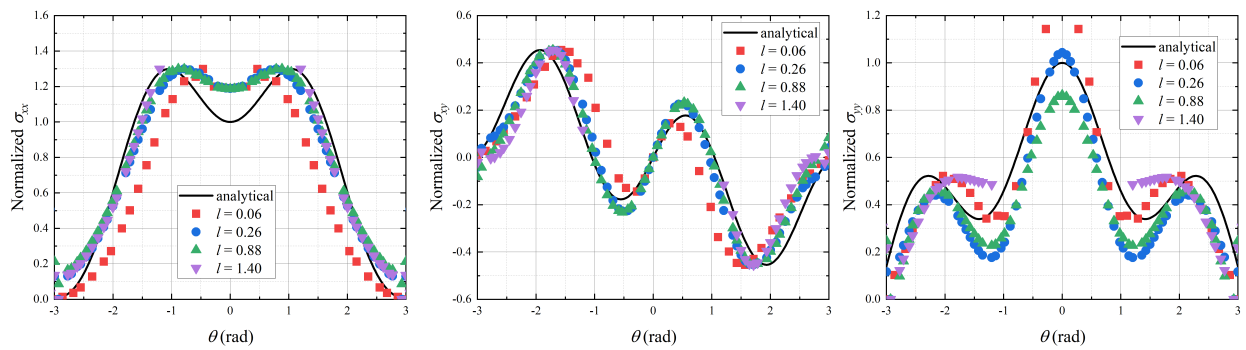


Figure 7.18: Distribution of σ_{xx} , σ_{xy} and σ_{yy} on a circle around crack tip with various crack length l

Chapter 8

Conclusions and future work

8.1 Conclusions

This dissertation presents a comprehensive development and extension of the peridynamic theory. Based on the bond-associated nonlocal deformation gradient, the bond-based models, i.e. nonlocal-deformation-field-driven bond-based models, and the state-based models, i.e. bond-associated state-based material correspondence models, have been established. A series of numerical examples have been conducted to evaluate the accuracy, robustness, and physical consistency of these formulations. The main contributions of this research can be summarized as follows:

1. A unified framework of bond-associated nonlocal deformation gradient was proposed to address the persistent zero-energy mode issues in peridynamic formulations and to enhance the accuracy of bond-level deformation characterization. This unified framework was developed through the introduction of two new state variables $\underline{\mathbf{A}}(\boldsymbol{\xi})$ and $\underline{\mathbf{B}}(\boldsymbol{\xi})$. By appropriately specifying these two state variables, various existing bond-associated deformation gradient can be recovered.
2. The adoption of bond-associated nonlocal deformation gradient enables precise calculation of deformation at both bond and material level. This provides a rigorous kinematic foundation for developing nonlocal-deformation-field-driven bond-based peridynamic models. In addition, a family of pairwise bond potential energy functions has been proposed to capture diverse material behaviors. This substantially broadens the scope of material models available for bond-based peridynamics.
3. Assuming equivalence of strain energy with the conventional continuum mechanics theory, the bond-associated state-based material correspondence models are derived. By choosing different values for the two state variables $\underline{\mathbf{A}}(\boldsymbol{\xi})$ and $\underline{\mathbf{B}}(\boldsymbol{\xi})$, the bond-associated force density states for corresponding bond-associated deformation gradients were recovered. Combined with the above-mentioned bond-associated deformation gradient, a generalized framework for bond-associated state-based models is established.

4. Rigorous proofs were provided to verify the balance of linear and angular momentum and the objectivity of stress for both bond-based models and state-based models. These theoretical proofs strengthen the physical soundness of the proposed formulations and ensure their consistency with the fundamental principles of continuum mechanics.
5. Extensive numerical studies were conducted to demonstrate the accuracy and versatility of the proposed models in capturing the static, dynamic, and fracture responses of materials and structures. The results confirm the robustness and predictive capability of the new formulations across a wide range of loading and boundary conditions.

Overall, this work contributes to the fundamental understanding and practical advancement of peridynamic theory. The methodologies and formulations developed herein not only resolve key theoretical challenges, but also provide a versatile foundation for future extensions in nonlinear material modeling, multiscale coupling, and computational efficiency improvements in peridynamic simulations.

8.2 Future work

While this dissertation establishes comprehensive and theoretically rigorous frameworks for both bond-based and state-based peridynamics using the bond-associated nonlocal deformation gradient, several avenues remain open for future exploration and development. These potential extensions span theoretical refinement, numerical enhancement, and multidisciplinary applications.

1. The current formulations primarily focus on pure solid mechanics problems. Future research can extend the bond-associated peridynamics theory to multi-physics systems. The bond-associated nonlocal deformation gradient naturally implies a corresponding nonlocal differential operator, which provides a foundation for formulating nonlocal governing partial differential equations across multiple physical fields. This allows seamless integration of thermal, moisture, or electromagnetic fields into the bond-associated framework. Consequently, the framework's capability in modeling thermo-mechanical, poro-mechanical, and electro-mechanical interactions can be further enhanced, which is critical for describing the behavior of advanced materials such as smart composites, energy storage materials, and biological tissues.
2. The bond-based formulation provides a natural bridge between bond-level interactions and macroscopic constitutive laws. Future work may focus on developing bond-level constitutive models that capture complex inelastic behaviors such as plasticity, viscoelasticity, and phase transformations. Furthermore, coupling the bond-associated framework with experimental or data-driven material characterization techniques, such as digital image correlation and Bayesian-based inverse discovery of constitutive law, could enable automatic calibration of peridynamic material parameters directly from observed deformation fields.

3. Although the proposed formulations achieve consistency and stability, their computational cost remains significant for large-scale simulations. Future efforts could explore efficient discretization strategies, such as adaptive horizon adjustment to reduce computational expense. In addition, parallel implementations on high-performance computing platforms and GPU acceleration will be essential to extend the applicability of the proposed frameworks to realistic engineering-scale problems.
4. Direct incorporation of classical damage mechanics models into bond-associated state-based formulations for modeling material failure will be investigated. Since bond-associated formulation significantly improves the accuracy of bond-level quantities, such as deformation gradient, strain and stress tensors, it paves the way to directly adopt the classical damage mechanics model to peridynamics and develop bond-level material failure model. Adopting classical damage models into the bond-associated framework is expected to mitigate the issue of damage localization and provide more physical and interpretable criteria for bond failure.

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Appendix A

Solutions of Four Integrals

A.1 Integrals in Two-Dimensional Case

Without loss of generality, the origin of the global coordinate system $(\mathbf{e}_1, \mathbf{e}_2)$ is set up at the point $\mathbf{X}$, which is the center of the horizon, as shown in Fig. A.1. Hence, the coordinates of one arbitrary point $\mathbf{X}'$ within the horizon can be expressed as

$$\mathbf{X}' = x_0 H \cos \alpha \mathbf{e}_1 + x_0 H \sin \alpha \mathbf{e}_2$$

where H is the radius of the horizon, x_0 is a nondimensional scalar ranging from 0 to 1, α is the angle between $\mathbf{e}_1$ and $\mathbf{XX}'$. The unit vector in the direction of $\mathbf{XX}'$ is denoted as

$$\mathbf{x} = \cos \alpha \mathbf{e}_1 + \sin \alpha \mathbf{e}_2$$

Another new coordinate system $(\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2)$ is set up at point X' with

$$\hat{\mathbf{e}}_1 = \cos \alpha \mathbf{e}_1 + \sin \alpha \mathbf{e}_2, \quad \hat{\mathbf{e}}_2 = -\sin \alpha \mathbf{e}_1 + \cos \alpha \mathbf{e}_2$$

The conversion matrix between the new local coordinates and the global coordinates is Q_{ij} , and it writes as

$$\hat{\mathbf{e}}_i = Q_{ij} \mathbf{e}_j, \quad \text{with} \quad [Q_{ij}] = \begin{bmatrix} \cos \alpha & \sin \alpha \\ -\sin \alpha & \cos \alpha \end{bmatrix} \quad (\text{A1})$$


$$\begin{aligned}\mathbf{N} &= \cos \theta \hat{\mathbf{e}}_1 + \sin \theta \hat{\mathbf{e}}_2 \\ &= \cos \theta Q_{1i} \mathbf{e}_i + \sin \theta Q_{2i} \mathbf{e}_i \\ &= N_1 \mathbf{e}_1 + N_2 \mathbf{e}_2\end{aligned}\tag{A2}$$
$$\hat{N}_1 = \cos \theta, \quad \hat{N}_2 = \sin \theta$$
$$N_i = Q_{ij} \hat{N}_j \quad (\text{A3})$$
$$\begin{aligned}
I_1 &= \int_{\mathcal{H}_X} \int_{\mathcal{H}_X} \mathbf{N} \otimes \mathbf{N} \otimes \mathbf{N} \otimes \mathbf{N} dV_{\mathbf{X}'} dV_{\mathbf{X}'} \\
&= \int_{\mathcal{H}_X} \int_0^{2\pi} \int_0^{\rho_1} N_i N_j N_k N_l \cdot r dr d\theta dV_{\mathbf{X}'} \\
&= \int_{\mathcal{H}_X} \int_0^{2\pi} N_i N_j N_k N_l \frac{1}{2} \rho_1^2 d\theta dV_{\mathbf{X}'} \\
&= \int_{\mathcal{H}_X} \int_0^{2\pi} Q_{ip} \hat{N}_p Q_{jq} \hat{N}_q Q_{kr} \hat{N}_r Q_{ls} \hat{N}_s \frac{1}{2} \rho_1^2 d\theta dV_{\mathbf{X}'} \\
&= \int_{\mathcal{H}_X} Q_{ip} Q_{jq} Q_{kr} Q_{ls} \int_0^{2\pi} \hat{N}_p \hat{N}_q \hat{N}_r \hat{N}_s \frac{1}{2} \rho_1^2 d\theta dV_{\mathbf{X}'} \tag{A4}
\end{aligned}$$

where ρ_1 is the distance from point $\mathbf{X}'$ to point $\mathbf{Y}$; $\mathbf{Y}$ is a point at the edge of horizon along direction $\mathbf{n}$, as shown in Fig. A.1. By applying the law of cosines to the triangle $\triangle \mathbf{X}\mathbf{X}'\mathbf{Y}$, ρ_1 can be computed as

$$\begin{aligned}\rho_1 &= H \left(-x_0 \cos \theta + \sqrt{1 - x_0^2 \sin^2 \theta} \right) \\ &= H \left(-x_0 \hat{N}_1 + \sqrt{1 - x_0^2 \hat{N}_2^2} \right)\end{aligned}\quad (\text{A5})$$

From Li et al.'s study [54, 55], it is found that when θ is in the range of 0 to 2π the integral of any odd functions $\mathcal{L}^{odd}(\hat{N}_i)$ w.r.t. $\hat{N}_i$ is zero while the integral of even function $\mathcal{L}^{even}(\hat{N}_i)$ is non-zero, i.e.

$$\int_0^{2\pi} \mathcal{L}^{odd}(\hat{N}_i) d\theta = 0, \quad \text{and} \quad \int_0^{2\pi} \mathcal{L}^{even}(\hat{N}_i) d\theta \neq 0$$

This leads to

$$\begin{aligned}& \int_{\mathcal{H}_X} Q_{ip} Q_{jq} Q_{kr} Q_{ls} \int_0^{2\pi} \hat{N}_p \hat{N}_q \hat{N}_r \hat{N}_s \frac{1}{2} \rho_1^2 d\theta dV_{\mathbf{X}'} \\ &= \int_0^{2\pi} Q_{ip} Q_{jq} Q_{kr} Q_{ls} \int_0^1 \int_0^{2\pi} \mathcal{L}^{even}(\hat{N}_i) d\theta x_0 H \cdot H dx_0 d\alpha\end{aligned}\quad (\text{A6})$$

where

$$\begin{aligned}\mathcal{L}^{even}(\hat{N}_i) &:= \left[\hat{N}_p \hat{N}_q \hat{N}_r \hat{N}_s \frac{1}{2} \rho_1^2 \right]^{even} \\ &= \hat{N}_p \hat{N}_q \hat{N}_r \hat{N}_s \frac{1}{2} H^2 \left[1 + x_0^2 \hat{N}_1^2 - x_0^2 \hat{N}_2^2 \right]\end{aligned}\quad (\text{A7})$$

Thus the analytical solution to the integral I_1 can be obtained, as shown in Eq. (A8).

$$\begin{aligned}I_1 &= \int_0^{2\pi} Q_{ip} Q_{jq} Q_{kr} Q_{ls} \int_0^1 \int_0^{2\pi} \mathcal{L}^{even}(\hat{N}_i) d\theta x_0 H \cdot H dx_0 d\alpha \\ &= \frac{\pi^2 H^4}{8} (\delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk})\end{aligned}\quad (\text{A8})$$

Following the same methodology, the solution to the second integral I_2 can also be achieved, i.e.

$$\begin{aligned}I_2 &= \int_{\mathcal{H}_X} \int_{\mathcal{H}_X} \mathbf{N} \otimes \mathbf{N} dV_{\mathbf{X}''} dV_{\mathbf{X}'} \\ &= \int_{\mathcal{H}_X} Q_{kr} Q_{ls} \int_0^{2\pi} \hat{N}_r \hat{N}_s \frac{1}{2} \rho_1^2 d\theta dV_{\mathbf{X}'} \\ &= \int_0^{2\pi} Q_{kr} Q_{ls} \int_0^1 \int_0^{2\pi} \mathcal{L}^{even}(\hat{N}_i) d\theta H^2 x_0 dx_0 d\alpha\end{aligned}\quad (\text{A9})$$

with

$$\begin{aligned}\mathcal{L}^{even}(\hat{N}_i) &:= \hat{N}_r \hat{N}_s \frac{1}{2} \rho_1^2 \\ &= \hat{N}_r \hat{N}_s \frac{1}{2} H^2 \left[1 + x_0^2 \hat{N}_1^2 - x_0^2 \hat{N}_2^2 \right]\end{aligned}\quad (\text{A10})$$

Hence we can obtain

$$I_2 = \frac{\pi^2 H^4}{2} \delta_{ij} \delta_{kl} \quad (\text{A11})$$

Using the fact that $V_{\mathcal{H}} = \pi H^2$ in two-dimensional configuration, we can conclude

$$I_1 = \int_{\mathcal{H}_X} \int_{\mathcal{H}_X} \mathbf{N} \otimes \mathbf{N} \otimes \mathbf{N} \otimes \mathbf{N} dV_{\mathbf{X}''} dV_{\mathbf{X}'} = \frac{V_{\mathcal{H}}^2}{8} (\mathbb{I}^{(2)} \otimes \mathbb{I}^{(2)} + 2\mathbb{I}^{(4s)}) \quad (\text{A12})$$

$$I_2 = \int_{\mathcal{H}_X} \int_{\mathcal{H}_X} \mathbf{N} \otimes \mathbf{N} dV_{\mathbf{X}''} dV_{\mathbf{X}'} = \frac{V_{\mathcal{H}}^2}{2} \mathbb{I}^{(2)} \quad (\text{A13})$$

A.2 Integrals in Three-Dimensional Case

Similar to Section A.1, we use two coordinate systems to solve the double integral in three-dimensional case, as shown in Fig. A.2. The orthonormal basis of global coordinates are $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ while the counterpart of local coordinates is $(\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3)$. The relation between the local and global systems can be denoted by two angles (α, β) as follows,

$$\begin{aligned}\hat{\mathbf{e}}_1 &= \cos \alpha \cos \beta \mathbf{e}_1 + \cos \alpha \sin \beta \mathbf{e}_2 - \sin \alpha \mathbf{e}_3 \\ \hat{\mathbf{e}}_2 &= -\sin \beta \mathbf{e}_1 + \cos \beta \mathbf{e}_2 + 0 \mathbf{e}_3 \\ \hat{\mathbf{e}}_3 &= \cos \beta \sin \alpha \mathbf{e}_1 + \sin \beta \sin \alpha \mathbf{e}_2 + \cos \alpha \mathbf{e}_3\end{aligned}\quad (\text{A14})$$

It should be noted that the vector $\hat{\mathbf{e}}_3$ aligns with the unit vector in the direction of $\mathbf{X}\mathbf{X}'$, i.e. $\hat{\mathbf{e}}_3 = \mathbf{x}$. Rewriting above equations in tensor form, it is given as follows,

$$\hat{\mathbf{e}}_i = Q_{ij} \mathbf{e}_j, \quad \text{with} \quad [Q_{ij}] = \begin{bmatrix} \cos \alpha \cos \beta & \cos \alpha \sin \beta & -\sin \alpha \\ -\sin \beta & \cos \beta & 0 \\ \cos \beta \sin \alpha & \sin \beta \sin \alpha & \cos \alpha \end{bmatrix} \quad (\text{A15})$$

The unit vector $\mathbf{N}$ in the direction of $\boldsymbol{\xi} = \mathbf{X}'\mathbf{X}''$ can be expressed in both local and global coordinate systems as

$$\begin{aligned}\mathbf{N} &= \cos \phi \sin \theta \hat{\mathbf{e}}_1 + \sin \phi \sin \theta \hat{\mathbf{e}}_2 + \cos \theta \hat{\mathbf{e}}_3 \\ &= \cos \phi \sin \theta Q_{1i} \mathbf{e}_i + \sin \phi \sin \theta Q_{2i} \mathbf{e}_i + \cos \theta Q_{3i} \mathbf{e}_i \\ &= N_1 \mathbf{e}_1 + N_2 \mathbf{e}_2 + N_3 \mathbf{e}_3\end{aligned}\quad (\text{A16})$$

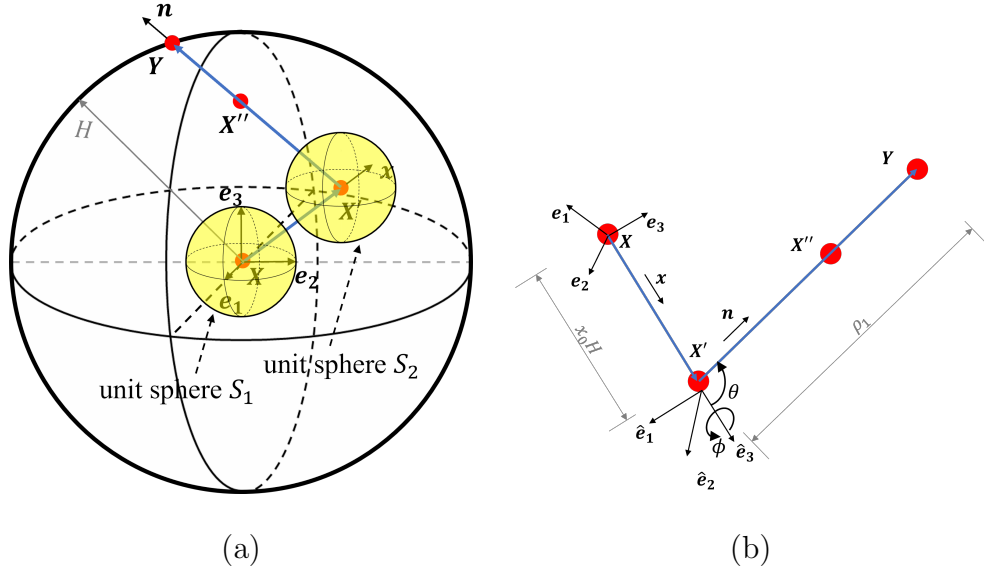


Figure A.2: geometric relation of material points within three-dimensional horizon

if we denote

$$\hat{N}_1 = \cos \phi \sin \theta, \quad \hat{N}_2 = \sin \phi \sin \theta, \quad \hat{N}_3 = \cos \theta$$

then we will have

$$N_i = Q_{ij} \hat{N}_j \quad (\text{A17})$$

where $\hat{N}_i$ is only related to the angle (ϕ, θ) while Q_{ij} is only dependent on (α, β)

Therefore, the integral I_3 can be decomposed as

$$\begin{aligned} I_3 &= \int_{\mathcal{H}_X} \int_{\mathcal{H}_X} \mathbf{N} \otimes \mathbf{N} \otimes \mathbf{N} \otimes \mathbf{N} dV_{\mathbf{X}''} dV_{\mathbf{X}'} \\ &= \int_{\mathcal{H}_X} \int_{S_2} \int_0^{\rho_1} N_i N_j N_k N_l \cdot r^2 dr d\omega_2 dV_{\mathbf{X}'} \\ &= \int_{\mathcal{H}_X} \int_{S_2} N_i N_j N_k N_l \frac{1}{3} \rho_1^3 d\omega_2 dV_{\mathbf{X}'} \\ &= \int_{\mathcal{H}_X} Q_{ip} Q_{jq} Q_{kr} Q_{ls} \int_{S_2} \hat{N}_p \hat{N}_q \hat{N}_r \hat{N}_s \frac{1}{3} \rho_1^3 d\omega_2 dV_{\mathbf{X}'} \end{aligned} \quad (\text{A18})$$

where ρ_1 represents the distance from point $\mathbf{X}'$ to point $\mathbf{Y}$, and point $\mathbf{Y}$ locates at the surface of horizon along the direction of $\mathbf{X}'\mathbf{X}''$; ω_2 is the solid angle defined under local coordinate system, and S_2 is a unit sphere centered at point $\mathbf{X}'$. As shown in Fig. A.2(b),

ρ_1 can be computed by applying the law of cosines in $\triangle \mathbf{X}\mathbf{X}'\mathbf{Y}$ as follows,

$$\begin{aligned}\rho_1 &= H \left(-x_0 \cos \theta + \sqrt{1 - x_0^2 \sin^2 \theta} \right) \\ &= H \left(-x_0 \hat{N}_3 + \sqrt{1 - x_0^2 (\hat{N}_1^2 + \hat{N}_2^2)} \right)\end{aligned}\quad (\text{A19})$$

Similar to Eq. (A6), the odd functions with respect to $\hat{N}_i$ becomes zero while even functions gives non-zero results after integration. If we denote

$$\begin{aligned}\mathcal{L}(\hat{N}_i) &:= \hat{N}_p \hat{N}_q \hat{N}_r \hat{N}_s \frac{1}{3} \rho_1^3 \\ &= \hat{N}_p \hat{N}_q \hat{N}_r \hat{N}_s \frac{1}{3} H^3 \left(-x_0 \hat{N}_3 + \sqrt{1 - x_0^2 (\hat{N}_1^2 + \hat{N}_2^2)} \right)^3\end{aligned}\quad (\text{A20})$$

and naturally,

$$\begin{aligned}\mathcal{L}^{even}(\hat{N}_i) &:= \hat{N}_p \hat{N}_q \hat{N}_r \hat{N}_s \frac{1}{3} \rho_1^3 \\ &= \hat{N}_p \hat{N}_q \hat{N}_r \hat{N}_s \frac{1}{3} H^3 \sqrt{1 - x_0^2 (\hat{N}_1^2 + \hat{N}_2^2)} \left[1 - x_0^2 \hat{N}_1^2 - x_0^2 \hat{N}_2^2 + 3x_0^2 \hat{N}_3^2 \right]\end{aligned}\quad (\text{A21})$$

then the analytical solution of the integral can be obtained as

$$\begin{aligned}I_3 &= \int_{\mathcal{H}_X} Q_{ip} Q_{jq} Q_{kr} Q_{ls} \int_{S_2} \hat{N}_p \hat{N}_q \hat{N}_r \hat{N}_s \frac{1}{3} \rho_1^3 d\omega_2 dV_{\mathbf{X}'} \\ &= \int_{S_1} Q_{ip} Q_{jq} Q_{kr} Q_{ls} \int_0^1 \int_{S_2} \mathcal{L}^{even}(\hat{N}_i) d\omega_2 H^3 x_0^2 dx_0 d\omega_1 \\ &= \frac{16\pi^2 H^6}{45} (\delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk})\end{aligned}\quad (\text{A22})$$

where ω_1 is the solid angle defined under global coordinate system and S_1 represents the unit sphere centered at point $\mathbf{X}$.

The fourth integral can be derived in a similar way,

$$\begin{aligned}I_4 &= \int_{\mathcal{H}_X} Q_{kr} Q_{ls} \int_{S_2} \hat{N}_r \hat{N}_s \frac{1}{3} \rho_1^3 d\omega_2 dV_{\mathbf{X}'} \\ &= \int_{S_1} Q_{kr} Q_{ls} \int_0^1 \int_{S_2} \mathcal{L}^{even}(\hat{N}_i) d\omega_2 H^3 x_0^2 dx_0 d\omega_1\end{aligned}\quad (\text{A23})$$

with

$$\begin{aligned}\mathcal{L}^{even}(\hat{N}_i) &:= \hat{N}_r \hat{N}_s \frac{1}{3} \rho_1^3 \\ &= \hat{N}_r \hat{N}_s \frac{1}{3} H^3 \sqrt{1 - x_0^2 (\hat{N}_1^2 + \hat{N}_2^2)} \left[1 - x_0^2 \hat{N}_1^2 - x_0^2 \hat{N}_2^2 + 3x_0^2 \hat{N}_3^2 \right]\end{aligned}\quad (\text{A24})$$

Therefore, the analytical solution should be

$$\begin{aligned}
 I_4 &= \int_{S_1} Q_{kr} Q_{ls} \int_0^1 \int_{S_2} \mathcal{L}^{even}(\hat{N}_i) d\omega_2 H^3 x_0^2 dx_0 d\omega_1 \\
 &= \frac{16\pi^2 H^6}{9} \delta_{ij}
 \end{aligned} \tag{A25}$$

Note that the volume of a perfect spherical horizon is $V_{\mathcal{H}}^2 = 4\pi H^3/3$, we conclude

$$I_3 = \int_{V_{\mathbf{X}}} \int_{V'_{\mathbf{X}}} \mathbf{N} \otimes \mathbf{N} \otimes \mathbf{N} \otimes \mathbf{N} dV_{\mathbf{X}'} dV_{\mathbf{X}} = \frac{V_{\mathcal{H}}^2}{5} (\mathbb{I}^{(2)} \otimes \mathbb{I}^{(2)} + 2\mathbb{I}^{(4s)}) \tag{A26}$$

$$I_4 = \int_{V_{\mathbf{X}}} \int_{V'_{\mathbf{X}}} \mathbf{N} \otimes \mathbf{N} dV_{\mathbf{X}'} dV_{\mathbf{X}} = V_{\mathcal{H}}^2 \mathbb{I}^{(2)} \tag{A27}$$