ASPECTS OF CONSTITUTIVE MODELING IN CONTINUUM-KINEMATICS-INSPIRED PERIDYNAMICS

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Aspects of Constitutive Modeling in Continuum-Kinematics-Inspired Peridynamics
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We certify that we have read this thesis and that in our opinion it is fully adequate, in scope and in quality, as a thesis for the degree of Master of Science.

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ABSTRACT

ASPECTS OF CONSTITUTIVE MODELING IN CONTINUUM-KINEMATICS-INSPIRED PERIDYNAMICS

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Continuum-kinematics-inspired Peridynamics (CPD) has been recently proposed as a geometrically exact formulation of peridynamics (PD) that is also thermodynamically and variationally consistent. Unlike the original formulation of PD, CPD can accurately capture the Poisson effect. CPD consists of one-, two- and three-neighbor interactions. The isotropic CPD formulation of non-local elasticity therefore involves three material constants associated with length, area and volume. This manuscript aims to establish the relationships between the material parameters of CPD and isotropic linear elasticity for two- and three-dimensional problems. Two alternatives for the CPD energy density are introduced. Analytical solutions of the energy densities for affine deformations are derived. It is shown that the three material parameters of CPD reduce to two independent parameters in the linearized framework, and can be expressed in terms of any pairs of isotropic linear elasticity constants, such as Lamé parameters. The analysis here provides a physical interpretation for the first Lamé constant. Finally, the admissible ranges for CPD material parameters are established.

Keywords: Continuum-kinematics-inspired peridynamics, Non-local elasticity, Elastic material parameters, Peridynamics.

ÖZET

SÜREKLİ-ORTAMLAR KİNEMATİĞİNDEN İLHAM ALAN PERİDİNAMİK İÇİN YAPISAL MODELLEME

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Sürekli-ortamlar kinematiğinden ilham alan Peridinamik (CPD), yakın zamanda, termodinamik olarak tutarlı olan, geometrik olarak doğru bir peridinamik (PD) formülasyonu olarak önerilmiştir. Orijinal PD formülasyonunun aksine, CPD Poisson etkisini doğru bir şekilde yakalayabilir. CPD bir, iki ve üç komşu etkileşimlerinden oluşur. Yerel olmayan elastisitenin izotropik CPD formülasyonu bu nedenle uzunluk, alan ve hacim değişimi ile ilişkili üç malzeme sabiti içerir. Bu yazı, iki ve üç boyutlu problemler için CPD'nin malzeme parametreleri ile izotropik, doğrusal elastisite arasındaki ilişkileri kurmayı amaçlamaktadır. CPD enerji yoğunluğu için iki alternatif sunulmuştur. Afin deformasyonlar için enerji yoğunluklarının analitik çözümleri bulunmuştur. CPD'nin üç malzeme parametresinin, doğrusallaştırılmış çerçevede iki bağımsız parametreye indirgendiği ve Lamé parametreleri gibi herhangi bir çift izotropik, doğrusal elastisite sabiti cinsinden ifade edilebileceği gösterilmiştir. İlk Lamé sabiti için fiziksel bir yorum sağlanmıştır. Son olarak, CPD malzeme parametreleri için kabul edilebilir aralıklar belirlenmiştir.

Anahtar sözcükler: Sürekli-ortamlar kinematiğinden ilham alan peridinamik, Yerel olmayan elastikiyet, Elastik malzeme parametreleri, Peridinamik.

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Chapter 1

Introduction

Understanding, modeling, and tuning the behavior of materials is, without question, at the core of engineering sciences. From building spacecraft resistant to extreme temperatures and stresses to designing computer chips with millions of transistors, today's technological advancements necessitate a deep understanding of material behavior, along with mathematical models able to predict complex material response. In material modeling, the widespread approach is Classical Continuum Mechanics (CCM), which is a formulation that assumes materials are continuous objects, rather than of particulate nature, with contact interactions that are inherently local. Continuum-Kinematics-Inspired Peridynamics (CPD) is a non–local approach to mathematically model the behavior of materials, and in particular soft elastic solids [2]. In CPD, the behavior of each material point is dictated by its interactions with other material points in its vicinity. This enables CPD to model the deformation of bodies due to non-local field, e.g., thermal, electric or magnetic, as well as discontinuities, such as cracks in a material, where CCM falls short.

The predecessor of CPD, Peridynamics (PD), is a non-local approach to formulating continuum mechanics [3, 4] that does not include the concepts of stress and strain commonly employed in CCM. PD, with its integro-differential governing equations, is well suited to solving problems involving discontinuities, and

has been used in works involving fractures and interfaces. However, PD is not limited to material failure problems and has an extensive range of applications and studies, see for example [5–21], among others. For a more comprehensive summary of PD theory, applications, and related studies, see the review [22].

Although PD possesses various advantages due to its non-locality, the initial PD theory [3] suffered from a key shortcoming. The Poisson effect could not be accurately captured as the theory solely accounted for bond-based interactions. As a result, the formulation was unable to capture the behavior of materials having Poisson ratios other than $\frac{1}{4}$. To address this, state-based PD [23] was developed, along with a correspondence model that connected the material properties of state-based PD to those of CCM. Nevertheless, as the kinematics were not adequately preserved, this approach generated other shortcomings such as displacement oscillations and zero energy modes [24, 25]. To ameliorate the problem, a stability requirement was presented [25], however the underlying correspondence state-based formulation remained unchanged. The source of numerical oscillations was further addressed in [26, 27]. CPD, on the other hand, does not suffer from the shortcomings of bond- or state-based PD. CPD is a variationally consistent formulation of PD at large deformations that extends the bond-based approach of original PD while preserving the kinematics of the problem in the spirit of classical continuum mechanics. At the heart of CPD is one, two and three-neighbor interactions, that capture the length, area and volume changes that occur in the domain as a result of deformation. Therefore, CPD introduces three material constants, C_1, C_2 and C_3, that correspond to the resistances to the changes of length, area and volume, respectively. The horizon size δ, which corresponds to the range in which the points are considered neighbors, also comes into effect as a parameter that dictates the span of non-local effects. For a vanishing horizon, CPD kinematic measures recover the three invariants of classical finite deformation continuum mechanics, namely $\operatorname{Tr} \boldsymbol{F}$, $\operatorname{Cof} \boldsymbol{F}$ and $\operatorname{Det} \boldsymbol{F}$, with $\boldsymbol{F}$ being the deformation gradient.

It is well understood that CCM requires two material parameters to fully define the response of an isotropic, linear elastic material. The focus of this manuscript is to bridge the material parameters of CPD and CCM in the linear

elastic, isotropic setting for purely two-dimensional and three-dimensional cases. It must be emphasized that CPD, in principle, is not limited to linear, elastic or isotropic problems. However, such limitations are imposed here only in order to establish relationships between the material parameters of CPD and elastic constants of CCM for linear isotropic elasticity. The key features and novelties of this manuscript are as follows:

- Harmonic, and super-harmonic energy densities are introduced.
- The representations of the linearized measures of deformation for two- and three-dimensional problems, i.e. length, area, and volume change, are unified.
- The two- and three-dimensional integrals of the harmonic energy densities of CPD are solved analytically in the linear setting.
- The two- and three-dimensional integrals of the super-harmonic energy densities of CPD are solved analytically in the non-linear setting.
- The analysis unravels how the three CPD materials parameters reduce to only two independent parameters in the linearized setting, which in turn allows to relate these CPD coefficients to the Lamé constants..
- The results demonstrate how the CPD material parameters allow for combinations that qualify as either length-preserving, area-preserving, or volume-preserving, which extends our understanding of classical incompressibility.
- The admissible ranges for CPD material parameters to fulfill point-wise stability are established and compared to their CCM counterparts.
- The contribution provides an understanding of the physical interpretation of the first Lamé parameter, which has been a long-standing open question.

The manuscript is organized as follows. First, the theory of CPD is introduced in Chapter 2, with an overview of the notation, kinematics, and governing equations of the problem. The proofs of the key lemmas invoked throughout

the manuscript are given in Chapter 3. Chapter 4 analyzes the harmonic energy density, wherein the linearized measures of deformation are unified, the energy densities are integrated and the material parameter relations are established and discussed in detail. Chapter 5 focuses on the super-harmonic energy density, going through the integration of the energy densities in the large deformation regime and deriving the material parameter relations once more. Finally, Chapter 6 concludes the work and provides further outlook.

This manuscript is a compilation of the works of the author in the past years, therefore substantial portions of this work are contained in the following publications [1, 28–30]:

- A. Javili, E. Ekiz, , A. T. McBride, , and P. Steinmann, "Continuum-kinematics-inspired peridynamics: Thermo-mechanical problems," *Continuum Mechanics and Thermodynamics*, vol. 33, pp. 2039–2063, 2021.
- E. Ekiz and A. Javili, "The variational explanation of poisson's ratio in bond-based peridynamics and extension to nonlinear poisson's ratio," *Journal of Peridynamics and Nonlocal Modeling*, Nov 2021.
- E. Ekiz, P. Steinmann, and A. Javili, "Relationships between the material parameters of continuum-kinematics-inspired peridynamics and isotropic linear elasticity for two-dimensional problems," *International Journal of Solids and Structures*, vol. 238, p. 111366, 2022.
- E. Ekiz, P. Steinmann, and A. Javili, "From two- to three-dimensional continuum-kinematics-inspired peridynamics: More than just another dimension," *Mechanics of Materials*, vol. 173, p. 104417, 2022.

Chapter 2

Theory

We begin our analysis by defining the kinematics of the problem. Next, we go over the governing equations for the quasi-static, conservative problem. Finally, the contributions from one-, two- and three-neighbor interactions are given and the stored energy is defined. Before continuing with the kinematics, we introduce the common notations and definitions in Section 2.1. The analysis in this manuscript consists of two, parallel studies of the CPD framework, in two- and three-dimensional settings. The two-dimensional problem consists of a two-dimensional domain limited to a two-dimensional space. Therefore it should be differentiated from the plane-strain and plane-stress discussions commonly employed for two-dimensional analyses, as they are not purely two-dimensional, but rather degenerate three-dimensional cases. Additionally, as the concepts of strain and stress are absent, and must remain absent in the CPD formulation, plane-strain and plane-stress assumptions become inapplicable. More precisely, two-dimensional CPD should be compared to the surface elasticity theory of Gurtin and Murdoch [31].

2.1 Notation and definitions

Throughout the manuscript, the following notation and definitions hold unless stated otherwise for special cases. Scalars are written in non-bold, non-italic letters, while vectors are written in bold. Scalars and vectors that reside in the material and spatial configurations are denoted by upper-case and lower-case letters, respectively. For instance, X and x refer to scalars, while $\boldsymbol{X}$ and $\boldsymbol{x}$ refer to vectors, in the material and spatial configurations, respectively. Second order tensors are shown with a bold, calligraphic font, $\boldsymbol{\mathcal{X}}$, and fourth order tensors are shown with $\mathbb{X}$. Tensors of second order and higher are denoted with capital letters, regardless of their configuration, as the majority in this manuscript reside in the material configuration, with rare exceptions being two point tensors, such as the deformation gradient $\boldsymbol{\mathcal{F}}$. Einstein summation convention is adopted, with the occasional use of index notation. Single contraction, or dot product, is defined as $\{\bullet\} \cdot \{\circ\} = [\{\bullet\}]_{...i} [\{\circ\}]_{i...}$ between any two first order (vectors) or higher order tensors. That is, the single contraction of (i) vectors, $\boldsymbol{a} \cdot \boldsymbol{b} = [\boldsymbol{a}]_i [\boldsymbol{b}]_i$, yields a scalar, (ii) a second order tensor and a vector $\boldsymbol{\mathcal{A}} \cdot \boldsymbol{b}$, yields a vector $[\boldsymbol{\mathcal{A}} \cdot \boldsymbol{b}]_i = [\boldsymbol{\mathcal{A}}]_{ij} [\boldsymbol{b}]_j$, (iii) two second order tensors $\boldsymbol{\mathcal{A}} \cdot \boldsymbol{\mathcal{B}}$, yields a second order tensor $[\boldsymbol{\mathcal{A}} \cdot \boldsymbol{\mathcal{B}}]_{ik} = [\boldsymbol{\mathcal{A}}]_{ij} [\boldsymbol{\mathcal{B}}]_{jk}$, and so on. Double contraction is defined as $\{\bullet\} : \{\circ\} = [\{\bullet\}]_{...ij} [\{\circ\}]_{ij...}$ between any two second or higher order tensors. The double contraction of two second order tensors, $\boldsymbol{\mathcal{A}} : \boldsymbol{\mathcal{B}} = [\boldsymbol{\mathcal{A}}]_{ij} [\boldsymbol{\mathcal{B}}]_{ij}$, gives a scalar. In a similar fashion, the quadruple contraction is defined between any fourth or higher order tensors, as $\{\bullet\} :: \{\circ\} = [\{\bullet\}]_{...ijkl} [\{\circ\}]_{ijkl...}$, with the quadruple contraction of two fourth order tensors, $\mathbb{A} :: \mathbb{B} = [\mathbb{A}]_{ijkl} [\mathbb{B}]_{ijkl}$, yielding a scalar. The tensor product is denoted by $\{\bullet\} \otimes \{\circ\}$, and gives (i) a second order tensor from two vectors, $[\boldsymbol{a} \otimes \boldsymbol{b}]_{ij} = [\boldsymbol{a}]_i [\boldsymbol{b}]_j$, (ii) a fourth order tensor from two second order tensors, $[\boldsymbol{\mathcal{A}} \otimes \boldsymbol{\mathcal{B}}]_{ijkl} = [\boldsymbol{\mathcal{A}}]_{ij} [\boldsymbol{\mathcal{B}}]_{kl}$, and so forth. Two non-standard tensor operators, $\{\bullet\} \overline{\otimes} \{\circ\}$ and $\{\bullet\} \underline{\otimes} \{\circ\}$, are also used between two second order tensors, such that $[\boldsymbol{\mathcal{A}} \overline{\otimes} \boldsymbol{\mathcal{B}}]_{ijkl} = [\boldsymbol{\mathcal{A}}]_{ik} [\boldsymbol{\mathcal{B}}]_{jl}$ and $[\boldsymbol{\mathcal{A}} \underline{\otimes} \boldsymbol{\mathcal{B}}]_{ijkl} = [\boldsymbol{\mathcal{A}}]_{il} [\boldsymbol{\mathcal{B}}]_{jk}$. The cross product between two vectors is denoted as $\boldsymbol{a} \times \boldsymbol{b} = \boldsymbol{\varepsilon} : [\boldsymbol{a} \otimes \boldsymbol{b}]$, where $\boldsymbol{\varepsilon}$ is the third order Levi–Civita permutation tensor. The Kronecker delta operator is defined as δ_{ij}, and follows the rule $\delta_{ij} = 0$, if $i \neq j$, and $\delta_{ij} = 1$, if $i = j$. The superscripts $\{\bullet\}^{\mathrm{I}}$, $\{\bullet\}^{\mathrm{II}}$ and $\{\bullet\}^{\mathrm{III}}$ correspond to the first, second and third neighbors of a

point. Similarly, the superscripts $\{\bullet\}^{\mathrm{I}}$, $\{\bullet\}^{\mathrm{I/II}}$ and $\{\bullet\}^{\mathrm{I/II/III}}$ correspond to one-, two- and three-neighbor interactions, that are related to the first, first and second, and finally first, second and third neighbors of a point, respectively. The subscripts $\{\bullet\}_{\mathrm{2D}}$ and $\{\bullet\}_{\mathrm{3D}}$ refer to the real space the object lives in, that is either two-dimensional, $\mathbb{R}^2$, or three-dimensional, $\mathbb{R}^3$. The notation $\mathcal{Lin}\{\bullet\}$ expresses the linearization of the argument $\{\bullet\}$ at the initial configuration. Lastly, $\mathrm{Tr}\{\bullet\}$, $\mathrm{Cof}\{\bullet\}$ and $\mathrm{Det}\{\bullet\}$ stand for the trace, cofactor and determinant operations. For second order tensors, trace is defined as $\mathrm{Tr}\,\boldsymbol{\mathcal{A}} = \boldsymbol{\mathcal{I}} : \boldsymbol{\mathcal{A}}$, where $\boldsymbol{\mathcal{I}}$ is the second order identity tensor. The cofactor of a second order tensor is alternatively denoted by $\{\bullet\}^{\#}$, and is defined such that $\mathrm{Cof}\,\boldsymbol{\mathcal{A}} = \boldsymbol{\mathcal{A}}^{\#} = \mathrm{Det}\,\boldsymbol{\mathcal{A}}\,\boldsymbol{\mathcal{A}}^{-\mathrm{T}}$, where $\boldsymbol{\mathcal{A}}^{-\mathrm{T}}$ is the inverse-transpose of the tensor $\boldsymbol{\mathcal{A}}$.

2.2 Kinematics

The discussion at hand is restricted to the quasi-static case, where time is only a history parameter that orders the sequence of events. Consider two cases; (i) a two dimensional (2D) continuum surface in 2D space, and (ii) a three dimensional (3D) continuum body in 3D space. The surface, and the body, occupy the material configurations $\mathcal{S}_0 \subset \mathbb{R}^2$ and $\mathcal{B}_0 \subset \mathbb{R}^3$, at time $t = 0$, respectively. Both domains are mapped to their respective spatial configurations at time $t \in \mathbb{T}$, via nonlinear deformation maps $\boldsymbol{y}_{\mathrm{2D}}$ and $\boldsymbol{y}_{\mathrm{3D}}$, such that $\boldsymbol{x}_{\mathrm{2D}} = \boldsymbol{y}_{\mathrm{2D}}(\boldsymbol{X}_{\mathrm{2D}}, t) : \mathcal{S}_0 \times \mathbb{T} \to \mathcal{S}_t$, and $\boldsymbol{x}_{\mathrm{3D}} = \boldsymbol{y}_{\mathrm{3D}}(\boldsymbol{X}_{\mathrm{3D}}, t) : \mathcal{B}_0 \times \mathbb{T} \to \mathcal{B}_t$, as shown in Fig. 2.1. Here, $\boldsymbol{X}_{\{\bullet\}}$ and $\boldsymbol{x}_{\{\bullet\}}$ denote points in the material and spatial configurations, respectively.

Remark on the notation *In discussing both cases we shall come across shared mathematical operators, functions or structures, such as $\boldsymbol{y}_{2D}$ and $\boldsymbol{y}_{3D}$, that are conceptually identical. Moving forward, the subscripts $\{\bullet\}_{2D}$ and $\{\bullet\}_{3D}$ are omitted for such objects, for the sake of brevity. Most often the real space an object belongs to can easily be inferred from the context, and any general remark holds for both 2D and 3D problems. For objects that require clarification, the subscripts will be adopted occasionally to avoid confusion.* □

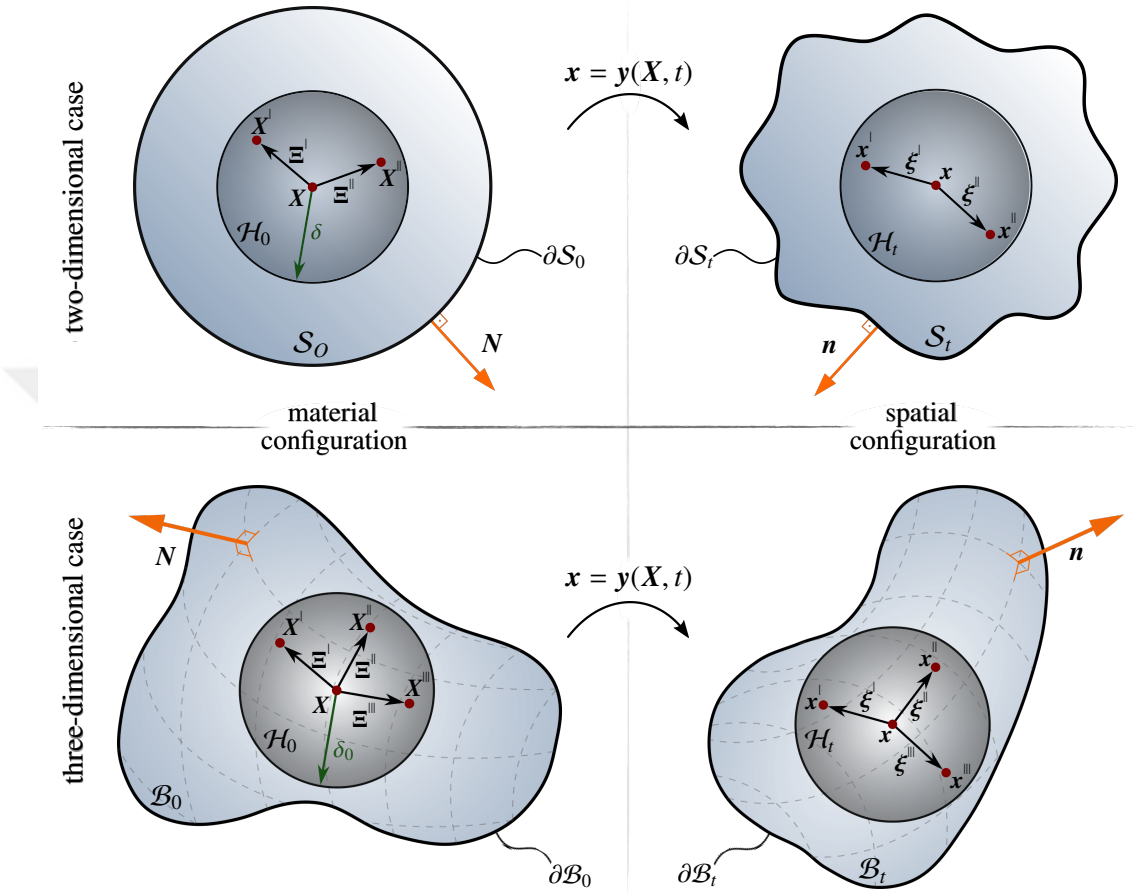

Figure 2.1: Motion of the continuum domains within the two-dimensional (top) and three-dimensional (bottom) CPD formulations.

The non-locality feature of CPD dictates that any point $\boldsymbol{X}$ in the material configuration can interact with other points in its finite neighborhood $\mathcal{H}_0(\boldsymbol{X})$, commonly referred to as the *horizon* of $\boldsymbol{X}$. The horizon is, generally, either a circle in 2D or a sphere in 3D with point $\boldsymbol{X}$ at the center, as illustrated in Fig. 2.1. The *measure* of the horizon, which corresponds to the radius of the circular or spherical neighborhood at $\boldsymbol{X}$, is denoted $\delta_0 := \text{meas}(\mathcal{H}_0)$. The mapping of $\mathcal{H}_0$ to the spatial configuration through the deformation map $\boldsymbol{y}$ gives the spatial horizon $\mathcal{H}_t = \boldsymbol{y}(\mathcal{H}_0, t)$. In the infinitesimal neighborhood limit, the horizons $\mathcal{H}_0$ and $\mathcal{H}_t$ coincide with the points $\boldsymbol{X}$ and $\boldsymbol{x}$, respectively. We identify the neighbors within the horizon through superscripts. The points $\{\boldsymbol{X}^{\mathrm{I}}, \boldsymbol{X}^{\mathrm{II}}, \boldsymbol{X}^{\mathrm{III}}\} \in \mathcal{H}_0(\boldsymbol{X})$ correspond to the first, second and third neighbors of $\boldsymbol{X}$, respectively. The points $\{\boldsymbol{x}^{\mathrm{I}}, \boldsymbol{x}^{\mathrm{II}}, \boldsymbol{x}^{\mathrm{III}}\} \in \mathcal{H}_t(\boldsymbol{x})$ denote the spatial counterparts of $\boldsymbol{X}^{\mathrm{I}}$, $\boldsymbol{X}^{\mathrm{II}}$ and

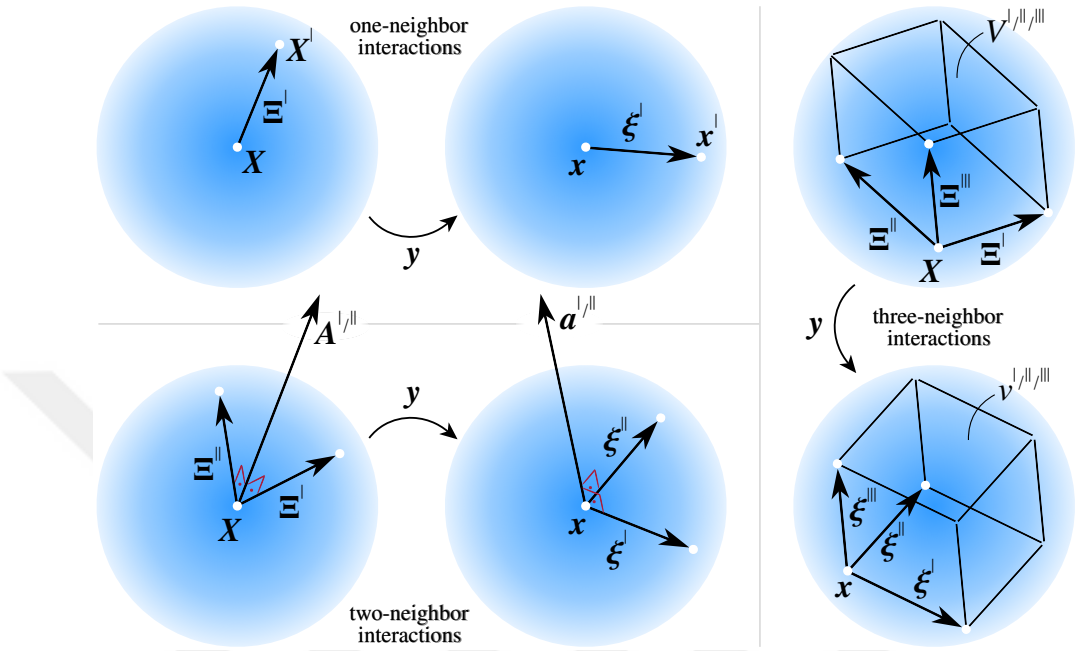

Figure 2.2: One-, two- and three-neighbor interactions, and their respective relative measures of deformation.

$\boldsymbol{X}^{|||}$, mapped through the nonlinear deformation map. The finite line elements, $\{\boldsymbol{\Xi}^{|}, \boldsymbol{\Xi}^{||}, \boldsymbol{\Xi}^{|||}\}$ and $\{\boldsymbol{\xi}^{|}, \boldsymbol{\xi}^{||}, \boldsymbol{\xi}^{|||}\}$, represent the relative positions between a point and its neighbor, in the material and spatial configurations respectively, and are illustrated in Fig. 2.1.

In the name of the formulation lies the key characteristic of CPD, its exact kinematics inspired by CCM. Inspired by the three *local kinematic measures* of relative deformation in 3D, namely the deformation gradient $\boldsymbol{\mathcal{F}} := \operatorname{Grad} \boldsymbol{y}$, its cofactor $\boldsymbol{\mathcal{F}}^{\#} := \operatorname{Cof} \boldsymbol{\mathcal{F}}$ and its determinant $J := \operatorname{Det} \boldsymbol{\mathcal{F}}$, three *non-local kinematic measures* of relative deformation, namely $\boldsymbol{\xi}^{|}$, $\boldsymbol{a}^{|/||}$ and $v^{|/||/|||}$ are introduced for the purposes of CPD [2]. The *first relative deformation measure*

$$\boldsymbol{\xi}^{|} = \boldsymbol{x}^{|} - \boldsymbol{x}\,, \tag{2.1}$$

serves to define *one-neighbor interactions* and mimics the linear map $\boldsymbol{\mathcal{F}}$ of the infinitesimal line element $\mathrm{d}\boldsymbol{X}$ in the material configuration to its spatial counterpart $\mathrm{d}\boldsymbol{x}$, as in the limit of an infinitesimal neighborhood, the relation $\boldsymbol{\xi}^{|} = \boldsymbol{\mathcal{F}} \cdot \boldsymbol{\Xi}^{|}$

Table 2.1: Summary of the CPD kinematics.

two-dimensional case					
one-neighbor interactions		two-neighbor interactions		three-neighbor interactions	
$\boldsymbol{\Xi}^{\mathrm{I}} = \boldsymbol{X}^{\mathrm{I}} - \boldsymbol{X}$	$\boldsymbol{\xi}^{\mathrm{I}} = \boldsymbol{x}^{\mathrm{I}} - \boldsymbol{x}$	$\boldsymbol{A}^{\mathrm{I/II}} = \boldsymbol{\Xi}^{\mathrm{I}} \times \boldsymbol{\Xi}^{\mathrm{II}}$	$\boldsymbol{a}^{\mathrm{I/II}} = \boldsymbol{\xi}^{\mathrm{I}} \times \boldsymbol{\xi}^{\mathrm{II}}$	$V^{\mathrm{I/II/III}} = \boldsymbol{\Xi}^{\mathrm{I}} \cdot [\boldsymbol{\Xi}^{\mathrm{II}} \times \boldsymbol{\Xi}^{\mathrm{III}}]$	$v^{\mathrm{I/II/III}} = \boldsymbol{\xi}^{\mathrm{I}} \cdot [\boldsymbol{\xi}^{\mathrm{II}} \times \boldsymbol{\xi}^{\mathrm{III}}]$
$\Xi^{\mathrm{I}} = \lVert\boldsymbol{\Xi}^{\mathrm{I}}\rVert$	$\xi^{\mathrm{I}} = \lVert\boldsymbol{\xi}^{\mathrm{I}}\rVert$	$A^{\mathrm{I/II}} = \lVert\boldsymbol{A}^{\mathrm{I/II}}\rVert$	$a^{\mathrm{I/II}} = \lVert\boldsymbol{a}^{\mathrm{I/II}}\rVert$	$V := \lVert V^{\mathrm{I/II/III}}\rVert = \lVert V^{\mathrm{III/I/II}}\rVert$ $= \lVert V^{\mathrm{II/III/I}}\rVert = \lVert V^{\mathrm{III/II/I}}\rVert$ $= \lVert V^{\mathrm{I/III/II}}\rVert = \lVert V^{\mathrm{II/I/III}}\rVert$	$v := \lVert v^{\mathrm{I/II/III}}\rVert = \lVert v^{\mathrm{III/I/II}}\rVert$ $= \lVert v^{\mathrm{II/III/I}}\rVert = \lVert v^{\mathrm{III/II/I}}\rVert$ $= \lVert v^{\mathrm{I/III/II}}\rVert = \lVert v^{\mathrm{II/I/III}}\rVert$
$L := \Xi^{\mathrm{I}}$	$l := \xi^{\mathrm{I}}$	$A := A^{\mathrm{I/II}} = A^{\mathrm{II/I}}$	$a := a^{\mathrm{I/II}} = a^{\mathrm{II/I}}$		
three-dimensional case					

holds [2]. The *second relative deformation measure*

$$\boldsymbol{a}^{\mathrm{I/II}} = [\boldsymbol{x}^{\mathrm{I}} - \boldsymbol{x}] \times [\boldsymbol{x}^{\mathrm{II}} - \boldsymbol{x}]\,, \tag{2.2}$$

serves as the main element in defining *two-neighbor interactions*, and mirrors the linear map $\boldsymbol{\mathcal{F}}^{\#}$ of the infinitesimal vectorial area element $\mathrm{d}\boldsymbol{A}$ in the material configuration to its spatial counterpart $\mathrm{d}\boldsymbol{a}$. Similarly, in the infinitesimal limit we recover the relation $\boldsymbol{a}^{\mathrm{I/II}} = \boldsymbol{\mathcal{F}}^{\#} \cdot \boldsymbol{A}^{\mathrm{I/II}}$. *The third relative deformation measure*

$$v^{\mathrm{I/II/III}} = [\boldsymbol{x}^{\mathrm{I}} - \boldsymbol{x}] \cdot \Big[[\boldsymbol{x}^{\mathrm{II}} - \boldsymbol{x}] \times [\boldsymbol{x}^{\mathrm{III}} - \boldsymbol{x}] \Big]\,, \tag{2.3}$$

is the main element in defining *three-neighbor interactions* and is reminiscent of the linear map J from the infinitesimal volume element $\mathrm{d}V$ in the material configuration to its spatial counterpart $\mathrm{d}v$. Once again, the relation $v^{\mathrm{I/II/III}} = J\, V^{\mathrm{I/II/III}}$ is obtained in the infinitesimal limit, recovering the kinematics of CCM. The three relative deformation measures of the different interactions are illustrated in Fig. 2.2. Table 2.1 summarizes the kinematics of CPD.

Remark on the linear mappings in 2D *The proof of CPD recovering the kinematics of CCM in the infinitesimal neighborhood limit is given in [2] for the 3D case. In the 2D case, as we assume the domain is a surface residing in a 2D space, there are no three-neighbor combinations that yields non-zero volumes, therefore we omit three-neighbor interactions in 2D. While the definitions of the remaining deformation measures* $\boldsymbol{\xi}^{\mathrm{I}}$ *and* $\boldsymbol{a}^{\mathrm{I/II}}$ *are conceptually identical to the*

3D case, their linear mappings, e.g. associated with an affine deformation, need clarification. The deformation gradient $\boldsymbol{\mathcal{F}}$ in the 2D setting is naturally a 2D tensor, and should not to be confused with a 3D tensor that enforces plane strain. For instance, the following deformation gradients

$$[\boldsymbol{\mathcal{F}}_{2D}] = \begin{bmatrix} 1+\lambda & 0 \\ 0 & 1+\lambda \end{bmatrix} \quad , \quad [\boldsymbol{\mathcal{F}}_{3D}] = \begin{bmatrix} 1+\lambda & 0 & 0 \\ 0 & 1+\lambda & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{2.4}$$

are fundamentally different, although they seem identical at first glance, as there is no change along the third direction in $\boldsymbol{\mathcal{F}}_{3D}$. With $\boldsymbol{\mathcal{F}}_{3D}$, $Det\,\boldsymbol{\mathcal{F}}_{3D}$ corresponds to a volume mapping, while there is no concept of volume in the 2D formulation. By contrast, $Det\,\boldsymbol{\mathcal{F}}_{2D}$ produces a scalar area mapping, that is $a^{|\nearrow|} = Det\,\boldsymbol{\mathcal{F}}_{2D}\, A^{|\nearrow|}$. The cofactor of $\boldsymbol{\mathcal{F}}_{2D}$ is rendered inane here, as the areal vectors $\boldsymbol{A}^{|\nearrow|}$ and $\boldsymbol{a}^{|\nearrow|}$ cannot exist in a vectorial form in the 2D setting, since cross-product is not defined in 2D space. More specifically, as $\boldsymbol{A}^{|\nearrow|}$ and $\boldsymbol{a}^{|\nearrow|}$ are both results of a cross product operation between two vectors on the same plane, they should be normal to the said plane, along a direction that simply does not exist in the purely 2D setting. Their norms $A^{|\nearrow|}$ and $a^{|\nearrow|}$, however, are well defined and rather easy to calculate by assuming that $\boldsymbol{\Xi}$'s and $\boldsymbol{\xi}$'s are 3D vectors with their third components zero, performing the cross product on them, and finally calculating the norm of the resulting vectors. Therefore in the 2D formulation, at the infinitesimal neighborhood limit, we recover the following mappings $\boldsymbol{\xi}^{|} = \boldsymbol{\mathcal{F}} \cdot \boldsymbol{\Xi}^{|}$ and $a^{|\nearrow|} = Det\,\boldsymbol{\mathcal{F}}\, A^{|\nearrow|}$. □

2.3 Governing equations

Though the CPD framework is suitable for and has been adopted to non-conservative problems [1, 32], the analysis in this contribution utilizes the quasi-static, conservative assumption. Accordingly, we proceed to go over the linear and angular momentum balances of the formulation. The governing equations of CCM and CPD can both be written in global or point-wise forms as needed. A

notable difference between the two formulations is, however, that the point-wise form of CCM is local, while the point-wise form of CPD is non-local, having the form of an integral over the horizon. A more rigorous discussion on the topic can be found in [2]. The global form of the linear momentum balance in the material configuration for a quasi-static case reads

$$\begin{cases} \text{2D}: & \displaystyle\int_{\mathcal{S}_0} \boldsymbol{b}_0^{\text{int}}\,\mathrm{d}A + \int_{\mathcal{S}_0} \boldsymbol{b}_0^{\text{ext}}\,\mathrm{d}A = \boldsymbol{0} \qquad \text{with} \qquad \boldsymbol{b}_0^{\text{int}} = \int_{\mathcal{H}_0} \boldsymbol{p}^{\shortmid}\,\mathrm{d}A^{\shortmid}\,, \\ & \left[\boldsymbol{b}_0^{\text{int}}\right] = \mathrm{N/m^2} \quad , \quad \left[\boldsymbol{b}_0^{\text{ext}}\right] = \mathrm{N/m^2} \quad , \quad \left[\boldsymbol{p}^{\shortmid}\right] = \mathrm{N/m^4}\,, \\ \text{3D}: & \displaystyle\int_{\mathcal{B}_0} \boldsymbol{b}_0^{\text{int}}\,\mathrm{d}V + \int_{\mathcal{B}_0} \boldsymbol{b}_0^{\text{ext}}\,\mathrm{d}V = \boldsymbol{0} \qquad \text{with} \qquad \boldsymbol{b}_0^{\text{int}} = \int_{\mathcal{H}_0} \boldsymbol{p}^{\shortmid}\,\mathrm{d}V^{\shortmid}\,, \\ & \left[\boldsymbol{b}_0^{\text{int}}\right] = \mathrm{N/m^3} \quad , \quad \left[\boldsymbol{b}_0^{\text{ext}}\right] = \mathrm{N/m^3} \quad , \quad \left[\boldsymbol{p}^{\shortmid}\right] = \mathrm{N/m^6}\,, \end{cases} \tag{2.5}$$

where $\boldsymbol{b}_0^{\text{int}}$ and $\boldsymbol{b}_0^{\text{ext}}$ denote the internal and external point-wise force densities, respectively, in the material configuration, with $\boldsymbol{p}^{\shortmid}$ being the neighbor-wise force density.

Remark on the various densities *The use of the term "density" is rather sloppy here, and corresponds to a measure of quantity per space of various dimensions rather than the commonly used definition of quantity per volume. For the correct technical definition, the units of the various densities should be considered. Per* $\mathrm{m^2}$ *and* $\mathrm{m^3}$ *correspond to per area and per volume, while* $\mathrm{m^4}$ *and* $\mathrm{m^6}$ *correspond to per area squared and per volume squared, and lastly* $\mathrm{m^6}$ *and* $\mathrm{m^9}$ *correspond to per area cubed and per volume cubed densities, respectively. The distinciton between per volume squared and per area cubed densities can be made by referring to the space they reside in, i.e. 2D or 3D.* □

Note that the global balance (2.5) not only holds over the entire material configuration, but it is also valid for any *arbitrary* cutout from the domain and therefore it can be localized. After localization, the point-wise linear momentum

balance of CPD reads

$$\begin{cases} \text{2D}: & \displaystyle\int_{\mathcal{H}_0} \boldsymbol{p}^{\shortmid}\,\mathrm{d}A^{\shortmid} + \boldsymbol{b}_0^{\text{ext}} = \boldsymbol{0} \qquad \text{with} \qquad \boldsymbol{p}^{\shortmid} = \boldsymbol{p}_1^{\shortmid} + \boldsymbol{p}_2^{\shortmid}\,, \\ \text{3D}: & \displaystyle\int_{\mathcal{H}_0} \boldsymbol{p}^{\shortmid}\,\mathrm{d}V^{\shortmid} + \boldsymbol{b}_0^{\text{ext}} = \boldsymbol{0} \qquad \text{with} \qquad \boldsymbol{p}^{\shortmid} = \boldsymbol{p}_1^{\shortmid} + \boldsymbol{p}_2^{\shortmid} + \boldsymbol{p}_3^{\shortmid}\,, \end{cases} \tag{2.6}$$

where $\boldsymbol{p}_1^{\shortmid}$, $\boldsymbol{p}_2^{\shortmid}$ and $\boldsymbol{p}_3^{\shortmid}$ are the contributions due to one-, two- and three-neighbor interactions that originate from the neighbor-wise energy densities ψ_1, ψ_2 and ψ_3, elaborated further in the following section. In a similar fashion, using the global form of the quasi-static moment balance, after some mathematical steps and localization [2], we arrive at the angular momentum balance in point-wise form

$$\begin{cases} \text{2D}: & \displaystyle\int_{\mathcal{H}_0} \boldsymbol{\xi}^{\shortmid} \times \boldsymbol{p}^{\shortmid}\,\mathrm{d}A^{\shortmid} = \boldsymbol{0} \qquad \text{with} \qquad \boldsymbol{p}^{\shortmid} = \boldsymbol{p}_1^{\shortmid} + \boldsymbol{p}_2^{\shortmid}\,, \\ \text{3D}: & \displaystyle\int_{\mathcal{H}_0} \boldsymbol{\xi}^{\shortmid} \times \boldsymbol{p}^{\shortmid}\,\mathrm{d}V^{\shortmid} = \boldsymbol{0} \qquad \text{with} \qquad \boldsymbol{p}^{\shortmid} = \boldsymbol{p}_1^{\shortmid} + \boldsymbol{p}_2^{\shortmid} + \boldsymbol{p}_3^{\shortmid}\,, \end{cases} \tag{2.7}$$

Note that the governing equations of CPD are derived in a variationally and thermodynamically consistent manner in [2] wherein the authors have shown how admissible energy densities can be chosen such that they a priori satisfy the conservation of angular momentum.

2.4 Stored energy

For the non-dissipative, elastic framework, the energy stored inside the body Π is comprised of the potentials due to one, two and three-neighbor interactions, Π_1, Π_2 and Π_3, respectively, as

$$\begin{cases} \text{2D}: & \Pi = \Pi_1 + \Pi_2\,, \\ \text{3D}: & \Pi = \Pi_1 + \Pi_2 + \Pi_3\,, \end{cases} \tag{2.8}$$

Table 2.2: Summary of the CPD energies.

one-neighbor interactions	two-neighbor interactions	three-neighbor interactions
2D neighbor-wise energy densities		
$\psi_1 = \psi_1(\xi^{\mid}) \quad , \quad [\psi_1] = \mathrm{N{\cdot}m/m^4}$	$\psi_2 = \psi_2\,(a^{\mid/\mid\mid}) \quad , \quad [\psi_2] = \mathrm{N{\cdot}m/m^6}$	—
3D neighbor-wise energy densities		
$\psi_1 = \psi_1(\xi^{\mid}) \quad , \quad [\psi_1] = \mathrm{N{\cdot}m/m^6}$	$\psi_2 = \psi_2\,(a^{\mid/\mid\mid}) \quad , \quad [\psi_2] = \mathrm{N{\cdot}m/m^9}$	$\psi_3 = \psi_3\,(\lvert v^{\mid/\mid\mid/\mid\mid\mid}\rvert) \quad , \quad [\psi_3] = \mathrm{N{\cdot}m/m^{12}}$
2D point-wise energy densities per area with dimension $\mathrm{N{\cdot}m/m^2}$		
$\Psi_1 = \int_{\mathcal{H}_0} \psi_1 \,\mathrm{d}A^{\mid}$	$\Psi_2 = \int_{\mathcal{H}_0}\int_{\mathcal{H}_0} \psi_2 \,\mathrm{d}A^{\mid}\,\mathrm{d}A^{\mid\mid}$	—
3D point-wise energy densities per volume with dimension $\mathrm{N{\cdot}m/m^3}$		
$\Psi_1 = \int_{\mathcal{H}_0} \psi_1 \,\mathrm{d}V^{\mid}$	$\Psi_2 = \int_{\mathcal{H}_0}\int_{\mathcal{H}_0} \psi_2 \,\mathrm{d}V^{\mid}\,\mathrm{d}V^{\mid\mid}$	$\Psi_3 = \int_{\mathcal{H}_0}\int_{\mathcal{H}_0}\int_{\mathcal{H}_0} \psi_3 \,\mathrm{d}V^{\mid}\,\mathrm{d}V^{\mid\mid}\,\mathrm{d}V^{\mid\mid\mid}$
2D stored energies with dimension $\mathrm{N{\cdot}m}$		
$\Pi_1 = \frac{1}{2}\int_{\mathcal{S}_0} \Psi_1 \,\mathrm{d}A$	$\Pi_2 = \frac{1}{3}\int_{\mathcal{S}_0} \Psi_2 \,\mathrm{d}A$	—
3D stored energies with dimension $\mathrm{N{\cdot}m}$		
$\Pi_1 = \frac{1}{2}\int_{\mathcal{B}_0} \Psi_1 \,\mathrm{d}V$	$\Pi_2 = \frac{1}{3}\int_{\mathcal{B}_0} \Psi_2 \,\mathrm{d}V$	$\Pi_3 = \frac{1}{4}\int_{\mathcal{B}_0} \Psi_3 \,\mathrm{d}V$

that will be explored further in the remainder of this section. A summary of the stored energies, along with the various energy density definitions that are derived in the consequtive sections are provided in Table 2.2.

2.4.1 One-neighbor interactions

To obtain Π_1, the stored energy due to one-neighbor interactions, we first define the neighbor-wise energy density ψ_1. This energy density between every pair of neighbors is a function of the first relative deformation measure $\boldsymbol{\xi}^{\mid}$. To satisfy material frame indifference, ψ_1 should only depend on the magnitude of $\boldsymbol{\xi}^{\mid}$, and thus it becomes a function of $\xi^{\mid} := |\boldsymbol{\xi}^{\mid}|$ as

$$\begin{cases} \text{2D}: \quad \psi_1 = \psi_1(\xi^{\mid}) \qquad \text{with} \qquad [\psi_1] = \mathrm{N{\cdot}m/m^4}\,, \\ \text{3D}: \quad \psi_1 = \psi_1(\xi^{\mid}) \qquad \text{with} \qquad [\psi_1] = \mathrm{N{\cdot}m/m^6}\,. \end{cases} \tag{2.9}$$

The integral of ψ_1 over the horizon yields the point-wise energy density Ψ_1 that is due to one-neighbor interactions as

$$\begin{cases} \text{2D}: \quad \Psi_1 = \displaystyle\int_{\mathcal{H}_0} \psi_1 \, \mathrm{d}A^{\shortmid} \qquad \text{with} \qquad [\Psi_1] = \mathrm{N{\cdot}m/m^2}\,, \\ \\ \text{3D}: \quad \Psi_1 = \displaystyle\int_{\mathcal{H}_0} \psi_1 \, \mathrm{d}V^{\shortmid} \qquad \text{with} \qquad [\Psi_1] = \mathrm{N{\cdot}m/m^3}\,. \end{cases} \tag{2.10}$$

Lastly, to obtain Π_1, Ψ_1 is integrated over the domain,

$$\begin{cases} \text{2D}: \quad \Pi_1 = \dfrac{1}{2}\displaystyle\int_{\mathcal{S}_0} \Psi_1 \, \mathrm{d}A \qquad \Rightarrow \qquad \Pi_1 = \dfrac{1}{2}\displaystyle\int_{\mathcal{S}_0}\int_{\mathcal{H}_0} \psi_1 \, \mathrm{d}A^{\shortmid} \, \mathrm{d}A\,, \\ \\ \text{3D}: \quad \Pi_1 = \dfrac{1}{2}\displaystyle\int_{\mathcal{B}_0} \Psi_1 \, \mathrm{d}V \qquad \Rightarrow \qquad \Pi_1 = \dfrac{1}{2}\displaystyle\int_{\mathcal{B}_0}\int_{\mathcal{H}_0} \psi_1 \, \mathrm{d}V^{\shortmid} \, \mathrm{d}V\,, \end{cases} \tag{2.11}$$

where the factor one-half prevents the double counting of the contributions from the neighbor pairs. The variation of Π_1 reads

$$\begin{cases} \text{2D}: \quad \delta\Pi_1 = \displaystyle\int_{\mathcal{S}_0}\int_{\mathcal{H}_0} \boldsymbol{p}_1^{\shortmid} \cdot \delta\boldsymbol{\xi}^{\shortmid} \, \mathrm{d}A^{\shortmid} \, \mathrm{d}A\,, \\ \\ \text{3D}: \quad \delta\Pi_1 = \displaystyle\int_{\mathcal{B}_0}\int_{\mathcal{H}_0} \boldsymbol{p}_1^{\shortmid} \cdot \delta\boldsymbol{\xi}^{\shortmid} \, \mathrm{d}V^{\shortmid} \, \mathrm{d}V\,, \end{cases} \tag{2.12}$$

in which

$$\begin{cases} \text{2D}: \quad \boldsymbol{p}_1^{\shortmid} := \dfrac{\partial\psi_1}{\partial\boldsymbol{\xi}^{\shortmid}} \quad , \quad \left[\boldsymbol{p}_1^{\shortmid}\right] = \mathrm{N{\cdot}m/m^4}\,, \\ \\ \text{3D}: \quad \boldsymbol{p}_1^{\shortmid} := \dfrac{\partial\psi_1}{\partial\boldsymbol{\xi}^{\shortmid}} \quad , \quad \left[\boldsymbol{p}_1^{\shortmid}\right] = \mathrm{N{\cdot}m/m^6}\,, \end{cases} \tag{2.13}$$

where $\boldsymbol{p}_1^{\shortmid}$ is the force density due to one-neighbor interactions.

2.4.2 Two-neighbor interactions

Again, we start by defining the neighbor-wise energy density ψ_2, a function of the magnitude of the second relative deformation measure $a^{|/||} := |\boldsymbol{a}^{|/||}|$,

$$\begin{cases} \text{2D}: \quad \psi_2 = \psi_2\left(a^{|/||}\right) & \text{with} \quad [\psi_2] = \text{N}\cdot\text{m}/\text{m}^6\,, \\ \text{3D}: \quad \psi_2 = \psi_2\left(a^{|/||}\right) & \text{with} \quad [\psi_2] = \text{N}\cdot\text{m}/\text{m}^9\,, \end{cases} \tag{2.14}$$

ensuring that the material frame indifference is fulfilled a priori. The double integral of ψ_2 over the horizon yields the point-wise energy density due to two-neighbor interactions Ψ_2 as

$$\begin{cases} \text{2D}: \quad \Psi_2 = \displaystyle\int_{\mathcal{H}_0}\int_{\mathcal{H}_0} \psi_2 \,\mathrm{d}A^{|}\,\mathrm{d}A^{||} & \text{with} \quad [\Psi_2] = \text{N}\cdot\text{m}/\text{m}^2\,, \\ \text{3D}: \quad \Psi_2 = \displaystyle\int_{\mathcal{H}_0}\int_{\mathcal{H}_0} \psi_2 \,\mathrm{d}V^{|}\,\mathrm{d}V^{||} & \text{with} \quad [\Psi_2] = \text{N}\cdot\text{m}/\text{m}^3\,, \end{cases} \tag{2.15}$$

Lastly, Ψ_2 is integrated over the domain to get the energy due to two-neighbor interactions, Π_2. That is

$$\begin{cases} \text{2D}: \ \Pi_2 = \dfrac{1}{3}\displaystyle\int_{\mathcal{S}_0} \Psi_2 \,\mathrm{d}A \quad \Rightarrow \quad \Pi_2 = \dfrac{1}{3}\int_{\mathcal{S}_0}\int_{\mathcal{H}_0}\int_{\mathcal{H}_0} \psi_2 \,\mathrm{d}A^{|}\,\mathrm{d}A^{||}\,\mathrm{d}A\,, \\ \text{3D}: \ \Pi_2 = \dfrac{1}{3}\displaystyle\int_{\mathcal{B}_0} \Psi_2 \,\mathrm{d}V \quad \Rightarrow \quad \Pi_2 = \dfrac{1}{3}\int_{\mathcal{B}_0}\int_{\mathcal{H}_0}\int_{\mathcal{H}_0} \psi_2 \,\mathrm{d}V^{|}\,\mathrm{d}V^{||}\,\mathrm{d}V\,, \end{cases} \tag{2.16}$$

where the factor one-third prevents the triple counting of neighbor triplets. Taking the variation of Π_2 it follows that

$$\begin{cases} \text{2D}: \quad \delta\Pi_2 = \displaystyle\int_{\mathcal{S}_0}\int_{\mathcal{H}_0} \boldsymbol{p}_2^{|}\cdot\delta\boldsymbol{\xi}^{|}\,\mathrm{d}A^{|}\,\mathrm{d}A\,, \\ \text{3D}: \quad \delta\Pi_2 = \displaystyle\int_{\mathcal{B}_0}\int_{\mathcal{H}_0} \boldsymbol{p}_2^{|}\cdot\delta\boldsymbol{\xi}^{|}\,\mathrm{d}V^{|}\,\mathrm{d}V\,, \end{cases} \tag{2.17}$$

with

$$\begin{cases} \text{2D}: \quad \boldsymbol{p}_2^{\,\mid} := \displaystyle\int_{\mathcal{H}_0} 2\,\boldsymbol{\xi}^{\mid\mid} \times \frac{\partial \psi_2}{\partial \boldsymbol{a}^{\mid/\mid\mid}}\,\mathrm{d}A^{\mid\mid} \quad , \quad \left[\boldsymbol{p}_2^{\,\mid}\right] = \mathrm{N{\cdot}m/m^4}\,, \\ \text{3D}: \quad \boldsymbol{p}_2^{\,\mid} := \displaystyle\int_{\mathcal{H}_0} 2\,\boldsymbol{\xi}^{\mid\mid} \times \frac{\partial \psi_2}{\partial \boldsymbol{a}^{\mid/\mid\mid}}\,\mathrm{d}V^{\mid\mid} \quad , \quad \left[\boldsymbol{p}_2^{\,\mid}\right] = \mathrm{N{\cdot}m/m^6}\,, \end{cases} \tag{2.18}$$

wherein the force density due to two-neighbor interactions is denoted $\boldsymbol{p}_2^{\,\mid}$.

2.4.3 Three-neighbor interactions

Note that three-neighbor interactions are specific to the 3D case, therefore the following remarks apply to the 3D case only. Just as before, we begin with defining the neighbor-wise energy density due to three-neighbor interactions ψ_3, now a function of the third relative deformation measure $v^{\mid/\mid\mid/\mid\mid\mid}$. That is

$$\psi_3 = \psi_3\ (|v^{\mid/\mid\mid/\mid\mid\mid}|) \qquad \text{with} \qquad [\psi_3] = \mathrm{N{\cdot}m/m^{12}}\,. \tag{2.19}$$

Expressing ψ_3 as a function of $|v^{\mid/\mid\mid/\mid\mid\mid}|$ rather than $v^{\mid/\mid\mid/\mid\mid\mid}$ guarantees that material frame indifference is fulfilled a priori. The triple integral of ψ_3 over the horizon yields the point-wise energy density Ψ_3 that is due to three-neighbor interactions as

$$\Psi_3 = \int_{\mathcal{H}_0}\int_{\mathcal{H}_0}\int_{\mathcal{H}_0} \psi_3\,\mathrm{d}V^{\mid}\,\mathrm{d}V^{\mid\mid}\,\mathrm{d}V^{\mid\mid\mid} \qquad \text{with} \qquad [\Psi_3] = \mathrm{N{\cdot}m/m^3}\,. \tag{2.20}$$

Finally, Ψ_3 is integrated over the body to get Π_3, the energy due to three-neighbor interactions.

$$\Pi_3 = \frac{1}{4}\int_{\mathcal{B}_0} \Psi_3\,\mathrm{d}V \quad \Rightarrow \quad \Pi_3 = \frac{1}{4}\int_{\mathcal{B}_0}\int_{\mathcal{H}_0}\int_{\mathcal{H}_0}\int_{\mathcal{H}_0} \psi_3\,\mathrm{d}V^{\mid}\,\mathrm{d}V^{\mid\mid}\,\mathrm{d}V^{\mid\mid\mid}\,\mathrm{d}V\,, \tag{2.21}$$

where the factor $\frac{1}{4}$ prevents the quadruple counting of energy-contributing neighbors. After some mathematical steps, the variation of Π_3 reads

$$\delta\Pi_3 = \int_{\mathcal{B}_0}\int_{\mathcal{H}_0} \boldsymbol{p}_3^{\,\mid} \cdot \delta\boldsymbol{\xi}^{\mid}\,\mathrm{d}V^{\mid}\,\mathrm{d}V\,, \tag{2.22}$$

with

$$\boldsymbol{p}_3^{\,\mathrm{I}} := \int_{\mathcal{H}_0}\int_{\mathcal{H}_0} 3\left[\boldsymbol{\xi}^{\mathrm{II}} \times \boldsymbol{\xi}^{\mathrm{III}}\right] \frac{\partial \psi_3}{\partial v^{\mathrm{I}/\mathrm{II}/\mathrm{III}}}\, \mathrm{d}V^{\mathrm{II}}\, \mathrm{d}V^{\mathrm{III}} \quad , \quad \left[\boldsymbol{p}_3^{\,\mathrm{I}}\right] = \mathrm{N/m^6}\,, \tag{2.23}$$

where $\boldsymbol{p}_3^{\,\mathrm{I}}$ is the force density due to three-neighbor interactions.

2.5 Proposed energy densities

Previously, the energy stored inside the body (2.8), denoted as Π, was established as the sum of the energy densities due to one-, two- and three-neighbor interactions, Ψ_1, Ψ_2 and Ψ_3. The stored energy can alternatively be written as

$$\begin{cases} \text{2D}: \quad \Pi = \displaystyle\int_{\mathcal{S}_0} \Psi_{\mathrm{CPD}}\, \mathrm{d}A \qquad \text{with} \qquad \Psi_{\mathrm{CPD}} := \frac{1}{2}\,\Psi_1 + \frac{1}{3}\,\Psi_2\,, \\ \text{3D}: \quad \Pi = \displaystyle\int_{\mathcal{B}_0} \Psi_{\mathrm{CPD}}\, \mathrm{d}V \qquad \text{with} \qquad \Psi_{\mathrm{CPD}} := \frac{1}{2}\,\Psi_1 + \frac{1}{3}\,\Psi_2 + \frac{1}{4}\,\Psi_3\,. \end{cases} \tag{2.24}$$

The neighbor-wise energy densities of one-, two- and three-neighbor interactions, discussed in Sections 2.4.1, 2.4.2 and 2.4.3, were stated to be functions of ξ^{I}, $a^{\mathrm{I}/\mathrm{II}}$ and $|v^{\mathrm{I}/\mathrm{II}/\mathrm{III}}|$, or simply l, a and v respectively, see Table 2.1. To this end, we propose harmonic potentials that fulfill this requirement as

$$\psi_1 = \frac{1}{2}\,C_1\,L\,\varepsilon_l^2 \quad , \qquad \psi_2 = \frac{1}{2}\,C_2\,A\,\varepsilon_a^2 \quad , \qquad \psi_3 = \frac{1}{2}\,C_3\,V\,\varepsilon_v^2\,, \tag{2.25}$$

where C_1, C_2 and C_3 are elastic constants that correspond to the resistances to length, area and volume change, respectively. The deformation measures ε_l, ε_a and ε_v are named the *length, area* and *volume strains*, respectively. Next, we propose two different definitions of strain, *linear strain* $\varepsilon_{\{\bullet\}}$ and *non-linear strain* $E_{\{\bullet\}}$, that is

$$\begin{aligned} &\varepsilon_l := \lambda_l - 1\,, && \varepsilon_a := \lambda_a - 1\,, && \varepsilon_v := \lambda_v - 1\,, \\ &E_l := \frac{1}{2}\left[\lambda_l^2 - 1\right]\,, && E_a := \frac{1}{2}\left[\lambda_a^2 - 1\right]\,, && E_v := \frac{1}{2}\left[\lambda_v^2 - 1\right]\,, \end{aligned} \tag{2.26}$$

where, λ_l, λ_a and λ_v are the *length, area* and *volume stretches*, defined as

$$\lambda_l := l/L \qquad , \qquad \lambda_a := a/A \qquad , \qquad \lambda_v := v/V \, . \tag{2.27}$$

Thus, we propose and investigate two options for the energy densities, *harmonic*

$$\psi_1 = \frac{1}{2} C_1 \, L \, \varepsilon_l^2 \, , \quad \psi_2 = \frac{1}{2} C_2 \, A \, \varepsilon_a^2 \, , \quad \psi_3 = \frac{1}{2} C_3 \, V \, \varepsilon_v^2 \, , \tag{2.28}$$

and *super-harmonic*

$$\psi_1 = \frac{1}{2} C_1 \, L \, E_l^2 \, , \quad \psi_2 = \frac{1}{2} C_2 \, A \, E_a^2 \, , \quad \psi_3 = \frac{1}{2} C_3 \, V \, E_v^2 \, , \tag{2.29}$$

to be explored in the coming sections.

Remark on the proposed energy densities and their associated strains *The proposed energies of CPD are merely two options, and are valid for both small and finite deformation problems. Though they seem rather simple functions of the strains, the results of using these different definitions of strain are not trivial. Chronologically, we began our analysis with the harmonic definition, as it is identical to bond-based peridynamics in one-neighbor interactions. However, as we will see in the coming sections, the integrals of these harmonic potentials proved impossible to analytically calculate without an additional linearization of the strains and thus assuming the deformations are small. Though this is a valid assumption when dealing with material parameter relationships in the linear elastic setting, we were still interested in the analytical solutions of the integrals at large deformations. This motivated us to investigate alternative strain measures, one being the super-harmonic option, which proved possible to integrate without the linearization step. Three important points should be noted here:*

- *The linear strain is reminiscent of the one-dimensional, small deformation definition of strain,*

$$\boldsymbol{\varepsilon} := \frac{1}{2} \left[\boldsymbol{\mathcal{F}}^T + \boldsymbol{\mathcal{F}} \right] - \boldsymbol{\mathcal{I}} \qquad , \qquad \textit{for 1D} \qquad \Rightarrow \qquad \varepsilon = \lambda - 1 \, ,$$

  where $\boldsymbol{\varepsilon}$ is the small deformation strain tensor,

- *The non-linear strain is reminiscent of the one-dimensional, finite deformation definition of strain*

$$\boldsymbol{E} := \frac{1}{2}\left[\boldsymbol{\mathcal{C}} - \boldsymbol{\mathcal{I}}\right] \qquad , \qquad \textit{for 1D} \qquad \Rightarrow \qquad E = \frac{1}{2}\left[\lambda^2 - 1\right]$$

where $\boldsymbol{\mathcal{C}} := \boldsymbol{\mathcal{F}}^T \cdot \boldsymbol{\mathcal{F}}$ *is the Right Cauchy-Green deformation tensor, and* $\boldsymbol{E}$ *is the Lagrangian (Green) strain tensor.*

- *The linearization of the non-linear strains at the reference configuration recover the linear strains, therefore we expect to get identical material parameter relations for both options in a linear elasticity analysis.* □

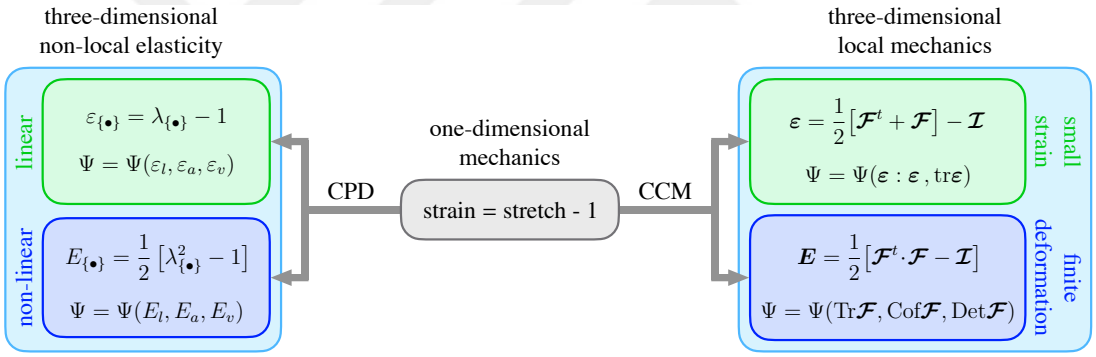

Figure 2.3: The different strain concepts of CPD, CCM and one-dimensional mechanics. The strains of CPD, similar to one-dimensional mechanics, are scalars and are valid in both small and finite deformation analyses. Whereas in CCM, strain is a tensor with different definitions in small and finite deformation frameworks, with the energy density being a function of the small deformation strain tensor $\boldsymbol{\varepsilon}$, and $\boldsymbol{\mathcal{F}}$, respectively.

Remark on the strain concept in CPD as opposed to CCM *In contrast to CCM, the "strains" in CPD are not associated with the gradient of the displacement field. In three-dimensional non-local elasticity associated with CPD, "strains" are scalar values defined through the geometrical changes prevalent on the body, irrespective of the deformation amount. The energy densities of CPD is a function of these strains* ε_l, ε_a *and* ε_v, *or* E_l, E_a *and* E_v, *that are not necessarily small. Whereas in CCM, there are different strain measures defined for small and large deformations, schematically illustrated in Fig. 2.3.*[1] *The energy density of*

[1]For finite deformations, the Seth–Hill family of strain tensors constitute infinitely many strain measures, although they all boil down to only one strain measure for small strain elasticity.

small strain elasticity is a function of the small deformation (infinitesimal) strain tensor $\boldsymbol{\varepsilon}$, while the energy density of finite deformation elasticity is a function of $\boldsymbol{\mathcal{F}}$, or its rotation-free counterpart $\boldsymbol{\mathcal{C}}$, and more specifically its trace, cofactor and determinant. This demonstrates that CPD furnishes a more unified formulation applicable to both small and finite deformation analyses. □

To derive the material parameter relations, we will proceed to express the point-wise energy densities, or Ψ_{CPD}, in terms of $\boldsymbol{\mathcal{F}}$, the linear mapping associated with a prescribed affine deformation; that is $\boldsymbol{\xi}^{|} = \boldsymbol{\mathcal{F}} \cdot \boldsymbol{\Xi}^{|}$. This shared mapping will enable us to make a connection between CPD and isotropic linear elasticity later. At this point, the point-wise energy densities of CPD are non-local, in the form of integrals over the horizon. Explicit solutions of these integrals are required to derive the material parameter relationships in the coming sections, which will shortly prove demanding to calculate. To make the procedure more straightforward to follow, the following section goes over the derivations of the common integrals that will appear in the different energy densities. Afterwards, with the key lemmas at hand, we will proceed to integrate the harmonic, and super-harmonic energy densities, in 2D and 3D.

Chapter 3

Key Lemmas

Before tackling the proofs of the key lemmas, let us introduce the mathematical objects that repeatedly appear in the upcoming derivations. Starting with the vector $\boldsymbol{\Xi}^{|}$, we decompose it into its magnitude $\Xi^{|}$ and its direction vector $\hat{\boldsymbol{\Xi}}^{|}$ as

$$\boldsymbol{\Xi}^{|} = \Xi^{|}\,\hat{\boldsymbol{\Xi}}^{|} \qquad \text{with} \qquad |\hat{\boldsymbol{\Xi}}^{|}| = 1. \tag{3.1}$$

Next, we define the vector $\hat{\boldsymbol{N}}$,

$$\hat{\boldsymbol{N}} := \frac{\hat{\boldsymbol{\Xi}}^{|} \times \hat{\boldsymbol{\Xi}}^{||}}{|\hat{\boldsymbol{\Xi}}^{|} \times \hat{\boldsymbol{\Xi}}^{||}|}, \tag{3.2}$$

which is a unit vector normal to the plane spanned by $\hat{\boldsymbol{\Xi}}^{|}$ and $\hat{\boldsymbol{\Xi}}^{||}$. Finally, vectors have the components

$$\left[\hat{\boldsymbol{\Xi}}^{\{\bullet\}}\right] = \begin{bmatrix} \cos\Theta^{\{\bullet\}} \\ \sin\Theta^{\{\bullet\}} \end{bmatrix} \qquad , \qquad \left[\hat{\boldsymbol{\Xi}}^{\{\bullet\}}\right] = \begin{bmatrix} \sin\Phi^{\{\bullet\}}\cos\Theta^{\{\bullet\}} \\ \sin\Phi^{\{\bullet\}}\sin\Theta^{\{\bullet\}} \\ \cos\Phi^{\{\bullet\}} \end{bmatrix}, \tag{3.3}$$

in 2D and 3D, respectively. Equipped with these preliminaries, we move on to the key lemmas and their proofs. The summary of the lemmas are given at the end of the section, in Table 3.1

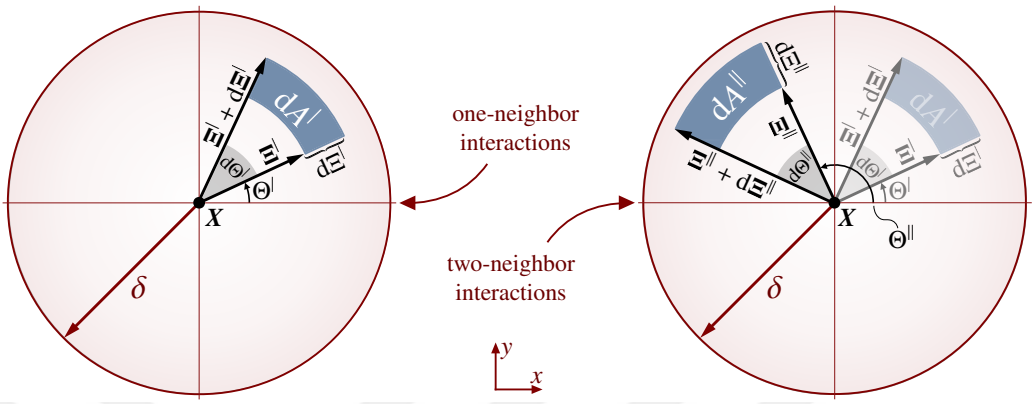

Figure 3.1: The polar coordinate system utilized for the integrals over the horizon in 2D due to one-neighbor (left) and two-neighbor (right) interactions, where $\mathrm{d}A^{|} := \Xi^{|}\,\mathrm{d}\Xi^{|}\,\mathrm{d}\Theta^{|}$ and $\mathrm{d}A^{||} := \Xi^{||}\,\mathrm{d}\Xi^{||}\,\mathrm{d}\Theta^{||}$.

Remark on the integrals over the horizon *The polar coordinate systems that are used for the 2D and 3D cases are illustrated in Fig. 3.1 and Fig. 3.2, respectively. We denote the integrals over the horizon as*

$$\begin{cases} \text{2D}: & \displaystyle\int_{\mathcal{H}_0^{\{\bullet\}}} \{\circ\}\,\mathrm{d}A^{\{\bullet\}}\,, \\ \text{3D}: & \displaystyle\int_{\mathcal{H}_0^{\{\bullet\}}} \{\circ\}\,\mathrm{d}V^{\{\bullet\}}\,, \end{cases} \tag{3.4}$$

in which

$$\begin{cases} \text{2D}: & \displaystyle\int_{\mathcal{H}_0^{\{\bullet\}}} := \int_{\Theta^{\{\bullet\}}=0}^{\Theta^{\{\bullet\}}=2\pi} \int_{\Xi^{\{\bullet\}}=0}^{\Xi^{\{\bullet\}}=\delta}\,, \quad \mathrm{d}A^{\{\bullet\}} := \Xi^{\{\bullet\}}\,\mathrm{d}\Xi^{\{\bullet\}}\,\mathrm{d}\Theta^{\{\bullet\}}\,, \\ \text{3D}: & \displaystyle\int_{\mathcal{H}_0^{\{\bullet\}}} := \int_{\Theta^{\{\bullet\}}=0}^{\Theta^{\{\bullet\}}=2\pi} \int_{\Phi^{\{\bullet\}}=0}^{\Phi^{\{\bullet\}}=\pi} \int_{\Xi^{\{\bullet\}}=0}^{\Xi^{\{\bullet\}}=\delta}\,, \\ & \mathrm{d}V^{\{\bullet\}} := {\Xi^{\{\bullet\}}}^2 \sin\Phi^{\{\bullet\}}\,\mathrm{d}\Xi^{\{\bullet\}}\,\mathrm{d}\Phi^{\{\bullet\}}\,\mathrm{d}\Theta^{\{\bullet\}}\,, \end{cases} \tag{3.5}$$

with the former covering the area of a circle, and the latter covering the volume of a sphere. For the rest of this section we shall utilize simplified integrals with

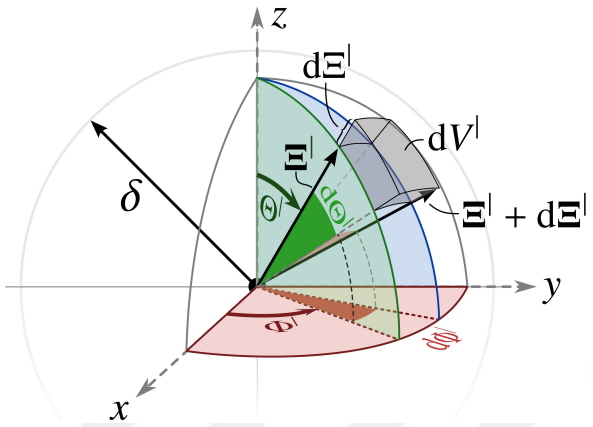

Figure 3.2: The polar coordinate system utilized for the integrals over the horizon in 3D due to one-neighbor interactions, where $\mathrm{d}V^{|} := {\Xi^{|}}^2 \sin\Phi^{|}\,\mathrm{d}\Xi^{|}\,\mathrm{d}\Phi^{|}\,\mathrm{d}\Theta^{|}$. The same schematic representation can be used for two and three-neighbor interactions where $\mathrm{d}V^{||} := {\Xi^{||}}^2 \sin\Phi^{||}\,\mathrm{d}\Xi^{||}\,\mathrm{d}\Phi^{||}\,\mathrm{d}\Theta^{||}$ and $\mathrm{d}V^{|||} := {\Xi^{|||}}^2 \sin\Phi^{|||}\,\mathrm{d}\Xi^{|||}\,\mathrm{d}\Phi^{|||}\,\mathrm{d}\Theta^{|||}$, respectively.

the notation

$$\begin{cases} \text{2D}: \displaystyle\int_{\hat{\mathcal{H}}_0^{\{\bullet\}}} := \int_{\Theta^{\{\bullet\}}=0}^{\Theta^{\{\bullet\}}=2\pi} & , \quad \mathrm{d}\hat{A}^{\{\bullet\}} := \mathrm{d}\Theta^{\{\bullet\}}\,, \\ \text{3D}: \displaystyle\int_{\hat{\mathcal{H}}_0^{\{\bullet\}}} := \int_{\Theta^{\{\bullet\}}=0}^{\Theta^{\{\bullet\}}=2\pi}\int_{\Phi^{\{\bullet\}}=0}^{\Phi^{\{\bullet\}}=\pi} & , \quad \mathrm{d}\hat{V}^{\{\bullet\}} := \sin\Phi^{\{\bullet\}}\,\mathrm{d}\Phi^{\{\bullet\}}\,\mathrm{d}\Theta^{\{\bullet\}}\,, \end{cases} \tag{3.6}$$

omitting the integrals over Ξ, as the complexity lies in the angular integrals. This is possible due to the form of the integrands we will deal with, which allows Ξ to be extracted and integrated separately. Note, Ξ will be accounted for during the actual integrations of the energy densities in the following sections. □

Lemma 1.

$$\int_{\hat{\mathcal{H}}_0^{|}} |\hat{\boldsymbol{\Xi}}^{|}|\, d\hat{A}^{|} = 2\pi$$

Proof.

$$\int_{\Theta^{|}=0}^{\Theta^{|}=2\pi} 1 \, \mathrm{d}\Theta^{|} = 2\pi \, .$$

□

Lemma 2.

$$\boxed{\int_{\hat{\mathcal{H}}_0{}^{|}} \left| \hat{\boldsymbol{\Xi}}^{|} \right| \, d\hat{V}^{|} = 4\pi}$$

Proof.

$$\int_{\Theta^{|}=0}^{\Theta^{|}=2\pi} \int_{\Phi^{|}=0}^{\Phi^{|}=\pi} 1 \, \sin\Phi^{|} \, \mathrm{d}\Phi^{|} \, \mathrm{d}\Theta^{|} = 4\pi \, .$$

□

Lemma 3.

$$\boxed{\int_{\hat{\mathcal{H}}_0{}^{||}} \int_{\hat{\mathcal{H}}_0{}^{|}} \left| \hat{\boldsymbol{\Xi}}^{|} \times \hat{\boldsymbol{\Xi}}^{||} \right| \, d\hat{A}^{|} \, d\hat{A}^{||} = 8\pi}$$

Proof.

$$\int_{\Theta^{||}=0}^{\Theta^{||}=2\pi} \underbrace{\int_{\Theta^{|}=0}^{\Theta^{|}=2\pi} \underbrace{\left| \hat{\boldsymbol{\Xi}}^{|} \times \hat{\boldsymbol{\Xi}}^{||} \right|}_{f} \, \mathrm{d}\Theta^{|}}_{g} \, \mathrm{d}\Theta^{||} \, , \quad \text{where} \quad f = f(\Theta^{|}, \Theta^{||}) \quad \text{and} \quad g = g(\Theta^{||}) \, .$$

Here, g proves to be in fact independent of $\Theta^{||}$ as the integral is axisymmetric, making a full rotation of $\Theta^{|}$ from 0 to 2π. More specifically, for any given $\Theta^{||} = \Theta_0^{||}$, g renders the same value. Note that this property is associated with the geometrical nature of the problem, and is valid despite g formally being a function of $\Theta^{||}$. Thus the integral of f over $\Theta^{|}$ can be evaluated for any value of

$\Theta^{\shortparallel}$. Taking $\Theta^{\shortparallel} = 0$, we carry out the integral of f as

$$\left[\hat{\boldsymbol{\Xi}}^{\shortparallel}\right] = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad , \qquad \left|\hat{\boldsymbol{\Xi}}^{\shortmid} \times \hat{\boldsymbol{\Xi}}^{\shortparallel}\right| = \left|\sin\Theta^{\shortmid}\right| ,$$

and therefore

$$g = \int_{\Theta^{\shortmid}=0}^{\Theta^{\shortmid}=2\pi} f \, \mathrm{d}\Theta^{\shortmid} = \int_{\Theta^{\shortmid}=0}^{\Theta^{\shortmid}=2\pi} \left|\sin\Theta^{\shortmid}\right| \mathrm{d}\Theta^{\shortmid} = 4 \, .$$

Finally, taking the integral of g over $\Theta^{\shortparallel}$ yields

$$\int_{\Theta^{\shortparallel}=0}^{\Theta^{\shortparallel}=2\pi} g \, \mathrm{d}\Theta^{\shortparallel} = \int_{\Theta^{\shortparallel}=0}^{\Theta^{\shortparallel}=2\pi} 4 \, \mathrm{d}\Theta^{\shortparallel} = 8\pi \, .$$

□

Lemma 4.

$$\boxed{\int_{\hat{\mathcal{H}}_0{}^{\shortparallel}} \int_{\hat{\mathcal{H}}_0{}^{\shortmid}} \left|\hat{\boldsymbol{\Xi}}^{\shortmid} \times \hat{\boldsymbol{\Xi}}^{\shortparallel}\right| \, d\hat{V}^{\shortmid} \, d\hat{V}^{\shortparallel} = 4\pi^3}$$

Proof.

$$\int_{\Theta^{\shortparallel}=0}^{\Theta^{\shortparallel}=2\pi} \int_{\Phi^{\shortparallel}=0}^{\Phi^{\shortparallel}=\pi} \underbrace{\int_{\Theta^{\shortmid}=0}^{\Theta^{\shortmid}=2\pi} \int_{\Phi^{\shortmid}=0}^{\Phi^{\shortmid}=\pi} \underbrace{\left|\hat{\boldsymbol{\Xi}}^{\shortmid} \times \hat{\boldsymbol{\Xi}}^{\shortparallel}\right|}_{f} \sin\Phi^{\shortmid} \, \mathrm{d}\Phi^{\shortmid} \, \mathrm{d}\Theta^{\shortmid}}_{g} \sin\Phi^{\shortparallel} \, \mathrm{d}\Phi^{\shortparallel} \, \mathrm{d}\Theta^{\shortparallel} \, ,$$

where $f = f(\Phi^{\shortmid}, \Theta^{\shortmid}, \Phi^{\shortparallel}, \Theta^{\shortparallel})$ and $g = g(\Phi^{\shortparallel}, \Theta^{\shortparallel})$. Though the integral over g is a function of $\Theta^{\shortparallel}$ and $\Phi^{\shortparallel}$, or in a geometrical sense a function of $\hat{\boldsymbol{\Xi}}^{\shortparallel}$, the integrals inside g that are over $\Theta^{\shortmid}$ and $\Phi^{\shortmid}$ are axisymmetric, such that $\hat{\boldsymbol{\Xi}}^{\shortmid}$ makes a full rotation in space in the shape of a sphere. This geometrical feature leads to g itself being independent of the starting position of $\hat{\boldsymbol{\Xi}}^{\shortparallel}$, and thus independent of $\Theta^{\shortparallel}$ and $\Phi^{\shortparallel}$. Making use of this property, we can evaluate the integral for any $\hat{\boldsymbol{\Xi}}^{\shortparallel}$,

with any value of $\Theta^{||}$ and $\Phi^{||}$. Doing so, we set $\Theta^{||} = 0$ and $\Phi^{||} = 0$, such that

$$\left[\hat{\boldsymbol{\Xi}}^{||}\right] = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \quad \left[\hat{\boldsymbol{\Xi}}^{|} \times \hat{\boldsymbol{\Xi}}^{||}\right] = \begin{bmatrix} \sin\Theta^{|}\sin\Phi^{|} \\ -\sin\Theta^{|}\cos\Phi^{|} \\ 0 \end{bmatrix} \quad \Rightarrow \quad \left|\hat{\boldsymbol{\Xi}}^{|} \times \hat{\boldsymbol{\Xi}}^{||}\right| = \left|\sin\Phi^{|}\right|.$$

As $\sin\Phi^{|}$ itself is positive when $\Phi^{|}$ is between 0 to π, we are left with

$$\int_{\Theta^{||}=0}^{\Theta^{||}=2\pi}\int_{\Phi^{||}=0}^{\Phi^{||}=\pi}\int_{\Theta^{|}=0}^{\Theta^{|}=2\pi}\int_{\Phi^{|}=0}^{\Phi^{|}=\pi} \sin^2\Phi^{|}\,\mathrm{d}\Phi^{|}\,\mathrm{d}\Theta^{|}\,\sin\Phi^{||}\,\mathrm{d}\Phi^{||}\,\mathrm{d}\Theta^{||} = 4\pi^3\,.$$

□

Lemma 5.

$$\int_{\hat{\mathcal{H}}_0{}^{|}} \hat{\boldsymbol{\Xi}}^{|} \otimes \hat{\boldsymbol{\Xi}}^{|}\; d\hat{A}^{|} = \pi\boldsymbol{\mathcal{I}}$$

Proof.

$$\int_{\Theta^{|}=0}^{\Theta^{|}=2\pi} \underbrace{\hat{\boldsymbol{\Xi}}^{|} \otimes \hat{\boldsymbol{\Xi}}^{|}}_{\boldsymbol{\mathcal{G}}}\,\mathrm{d}\Theta^{|} = \int_{\Theta^{|}=0}^{\Theta^{|}=2\pi} \begin{bmatrix} \cos^2\Theta^{|} & \cos\Theta^{|}\sin\Theta^{|} \\ \cos\Theta^{|}\sin\Theta^{|} & \sin^2\Theta^{|} \end{bmatrix} \mathrm{d}\Theta^{|} = \begin{bmatrix} \pi & 0 \\ 0 & \pi \end{bmatrix},$$

which, written in tensor form, is $\pi\boldsymbol{\mathcal{I}}$, where $\boldsymbol{\mathcal{I}}$ is the second order identity tensor in 2D. Note, we expected to find an isotropic and symmetric tensor as the result, due to the axisymmetry property of the integral. □

Lemma 6.

$$\int_{\hat{\mathcal{H}}_0{}^{|}} \hat{\boldsymbol{\Xi}}^{|} \otimes \hat{\boldsymbol{\Xi}}^{|}\; d\hat{V}^{|} = \frac{4}{3}\pi\boldsymbol{\mathcal{I}}$$

Proof.

$$\boldsymbol{\mathcal{G}} := \int_{\Theta^{|}=0}^{\Theta^{|}=2\pi}\int_{\Phi^{|}=0}^{\Phi^{|}=\pi} \hat{\boldsymbol{\Xi}}^{|} \otimes \hat{\boldsymbol{\Xi}}^{|}\,\sin\Phi^{|}\,\mathrm{d}\Phi^{|}\,\mathrm{d}\Theta^{|}\,,$$

where $\boldsymbol{\mathcal{G}}$ should be a second order, isotropic and symmetric tensor in 3D. Note that while $\hat{\boldsymbol{\Xi}}^{\shortmid} \otimes \hat{\boldsymbol{\Xi}}^{\shortmid}$ is symmetric, it is not necessarily an isotropic tensor, but the axisymmetric integration renders the resultant tensor $\boldsymbol{\mathcal{G}}$

$$[\boldsymbol{\mathcal{G}}] = \begin{bmatrix} G_{11} & G_{12} & G_{13} \\ G_{21} & G_{22} & G_{23} \\ G_{31} & G_{32} & G_{33} \end{bmatrix},$$

that is isotropic and possesses the properties

$$G_{11} = G_{22} = G_{33}\,,$$
$$G_{12} = G_{21} = G_{13} = G_{31} = G_{23} = G_{32}\,.$$

Calculating the components of $\boldsymbol{\mathcal{G}}$ gives

$$G_{11} = \int_{\Theta^{\shortmid}=0}^{\Theta^{\shortmid}=2\pi} \int_{\Phi^{\shortmid}=0}^{\Phi^{\shortmid}=\pi} \sin^3\Phi^{\shortmid} \cos^2\Theta^{\shortmid}\, \mathrm{d}\Phi^{\shortmid}\, \mathrm{d}\Theta^{\shortmid} = \frac{4\pi}{3}\,,$$
$$G_{12} = \int_{\Theta^{\shortmid}=0}^{\Theta^{\shortmid}=2\pi} \int_{\Phi^{\shortmid}=0}^{\Phi^{\shortmid}=\pi} \sin^3\Phi^{\shortmid} \cos\Theta^{\shortmid} \sin\Theta^{\shortmid}\, \mathrm{d}\Phi^{\shortmid}\, \mathrm{d}\Theta^{\shortmid} = 0\,,$$

or in tensor form

$$\boldsymbol{\mathcal{G}} = \frac{4}{3}\pi\, \boldsymbol{\mathcal{I}}\,,$$

where $\boldsymbol{\mathcal{I}}$ is the second order identity tensor in 3D. □

Lemma 7.

$$\boxed{\int_{\hat{\mathcal{H}}_0{}^{\shortmid}} \hat{\boldsymbol{\Xi}}^{\shortmid} \otimes \hat{\boldsymbol{\Xi}}^{\shortmid} \otimes \hat{\boldsymbol{\Xi}}^{\shortmid} \otimes \hat{\boldsymbol{\Xi}}^{\shortmid}\, d\hat{A}^{\shortmid} = \frac{1}{4}\pi\, \mathbb{I}}$$

Proof.

$$\mathbb{K} := \int_{\Theta^{\shortmid}=0}^{\Theta^{\shortmid}=2\pi} \hat{\boldsymbol{\Xi}}^{\shortmid} \otimes \hat{\boldsymbol{\Xi}}^{\shortmid} \otimes \hat{\boldsymbol{\Xi}}^{\shortmid} \otimes \hat{\boldsymbol{\Xi}}^{\shortmid}\, \mathrm{d}\Theta^{\shortmid}\,,$$

where $\mathbb{K}$ should be a fourth order, isotropic and symmetric tensor in 2D. Calculating the components of $\mathbb{K}$ yields

$$
\begin{aligned}
\left[\mathbb{K}\right]_{1111} &= \int_{\Theta^{|}=0}^{\Theta^{|}=2\pi} \cos^4\Theta^{|}\,\mathrm{d}\Theta^{|} = \frac{3}{4}\pi\,,\\
\left[\mathbb{K}\right]_{2222} &= \int_{\Theta^{|}=0}^{\Theta^{|}=2\pi} \sin^4\Theta^{|}\,\mathrm{d}\Theta^{|} = \frac{3}{4}\pi\,,\\
\left[\mathbb{K}\right]_{1122} &= \left[\mathbb{K}\right]_{2211} = \int_{\Theta^{|}=0}^{\Theta^{|}=2\pi} \sin^2\Theta^{|}\cos^2\Theta^{|}\,\mathrm{d}\Theta^{|} = \frac{1}{4}\pi\\
\left[\mathbb{K}\right]_{1212} &= \left[\mathbb{K}\right]_{2121} = \left[\mathbb{K}\right]_{1221} = \left[\mathbb{K}\right]_{2112} = \int_{\Theta^{|}=0}^{\Theta^{|}=2\pi} \sin^2\Theta^{|}\cos^2\Theta^{|}\,\mathrm{d}\Theta^{|} = \frac{1}{4}\pi\,,\\
\left[\mathbb{K}\right]_{1222} &= \left[\mathbb{K}\right]_{2122} = \left[\mathbb{K}\right]_{2212} = \left[\mathbb{K}\right]_{2221} = \int_{\Theta^{|}=0}^{\Theta^{|}=2\pi} \sin^3\Theta^{|}\cos\Theta^{|}\,\mathrm{d}\Theta^{|} = 0\,,\\
\left[\mathbb{K}\right]_{2111} &= \left[\mathbb{K}\right]_{1211} = \left[\mathbb{K}\right]_{1121} = \left[\mathbb{K}\right]_{1112} = \int_{\Theta^{|}=0}^{\Theta^{|}=2\pi} \sin\Theta^{|}\cos^3\Theta^{|}\,\mathrm{d}\Theta^{|} = 0\,.
\end{aligned}
$$

Remark on the properties of $\mathbb{K}$ *After integration,* $\mathbb{K}$ *reduces to just three different components from originally sixteen. This is not surprising as* $\mathbb{K}$ *is of isotropic and symmetric nature. These characteristics can further be illustrated via the use of Voigt notation as follows*

$$
\boldsymbol{K} = \begin{bmatrix} K_{11} & K_{12} & 0 \\ K_{12} & K_{11} & 0 \\ 0 & 0 & K_{33} \end{bmatrix}
$$

$$
\begin{aligned}
K_{11} = K_{22} &:= \left[\mathbb{K}\right]_{1111} = \left[\mathbb{K}\right]_{2222}\,,\\
K_{12} = K_{21} &:= \left[\mathbb{K}\right]_{1122} = \left[\mathbb{K}\right]_{2211}\,,\\
K_{13} = K_{31} &:= \left[\mathbb{K}\right]_{1112} = \left[\mathbb{K}\right]_{1121} = \left[\mathbb{K}\right]_{1211} = \left[\mathbb{K}\right]_{2111} = 0\,,\\
K_{23} = K_{32} &:= \left[\mathbb{K}\right]_{1222} = \left[\mathbb{K}\right]_{2122} = \left[\mathbb{K}\right]_{2212} = \left[\mathbb{K}\right]_{2221} = 0\,,\\
K_{33} &:= \left[\mathbb{K}\right]_{1212} = \left[\mathbb{K}\right]_{1221} = \left[\mathbb{K}\right]_{2121} = \left[\mathbb{K}\right]_{2112} = \tfrac{1}{2}[K_{11} - K_{12}]\,,
\end{aligned}
$$

where $\boldsymbol{K}$ *is a matrix with identical components to* $\mathbb{K}$ *calculated in the previous*

step.

Equipped with the components of $\mathbb{K}$, it can be shown that

$$\mathbb{K} = \frac{1}{4}\pi\,\mathbb{I} \qquad \text{with} \qquad \mathbb{I} := \boldsymbol{\mathcal{I}}\,\overline{\otimes}\,\boldsymbol{\mathcal{I}} + \boldsymbol{\mathcal{I}}\,\underline{\otimes}\,\boldsymbol{\mathcal{I}} + \boldsymbol{\mathcal{I}}\otimes\boldsymbol{\mathcal{I}}\,,$$

where $\mathbb{I}$ is a two-dimensional, fourth-order identity tensor. □

Lemma 8.

$$\boxed{\int_{\hat{\mathcal{H}}_0{}^{|}} \hat{\boldsymbol{\Xi}}^{|}\otimes\hat{\boldsymbol{\Xi}}^{|}\otimes\hat{\boldsymbol{\Xi}}^{|}\otimes\hat{\boldsymbol{\Xi}}^{|}\,d\hat{V}^{|} = \frac{4}{15}\pi\,\mathbb{I}}$$

Proof.

$$\mathbb{L} := \int_{\Theta^{|}=0}^{\Theta^{|}=2\pi}\int_{\Phi^{|}=0}^{\Phi^{|}=\pi} \hat{\boldsymbol{\Xi}}^{|}\otimes\hat{\boldsymbol{\Xi}}^{|}\otimes\hat{\boldsymbol{\Xi}}^{|}\otimes\hat{\boldsymbol{\Xi}}^{|}\sin\Phi^{|}\,\mathrm{d}\Phi^{|}\,\mathrm{d}\Theta^{|}\,.$$

Owing to the symmetric (both major and minor) structure of $\mathbb{L}$, where

$$\big[\mathbb{L}\big]_{ijkl} = \big[\mathbb{L}\big]_{klij} \qquad , \qquad \big[\mathbb{L}\big]_{ijkl} = \big[\mathbb{L}\big]_{jikl}\,,$$

we can write it in Voigt notation

$$\boldsymbol{L} = \begin{bmatrix} L_{11} & L_{12} & L_{13} & L_{14} & L_{15} & L_{16} \\ L_{21} & L_{22} & L_{23} & L_{24} & L_{25} & L_{26} \\ L_{31} & L_{32} & L_{33} & L_{34} & L_{35} & L_{36} \\ L_{41} & L_{42} & L_{43} & L_{44} & L_{45} & L_{46} \\ L_{51} & L_{52} & L_{53} & L_{54} & L_{55} & L_{56} \\ L_{61} & L_{62} & L_{63} & L_{64} & L_{65} & L_{66} \end{bmatrix}$$

$$\equiv \begin{bmatrix} \big[\mathbb{L}\big]_{1111} & \big[\mathbb{L}\big]_{1122} & \big[\mathbb{L}\big]_{1133} & \big[\mathbb{L}\big]_{1112} & \big[\mathbb{L}\big]_{1113} & \big[\mathbb{L}\big]_{1123} \\ \big[\mathbb{L}\big]_{2211} & \big[\mathbb{L}\big]_{2222} & \big[\mathbb{L}\big]_{2233} & \big[\mathbb{L}\big]_{2212} & \big[\mathbb{L}\big]_{2213} & \big[\mathbb{L}\big]_{2223} \\ \big[\mathbb{L}\big]_{3311} & \big[\mathbb{L}\big]_{3322} & \big[\mathbb{L}\big]_{3333} & \big[\mathbb{L}\big]_{3312} & \big[\mathbb{L}\big]_{3313} & \big[\mathbb{L}\big]_{3323} \\ \big[\mathbb{L}\big]_{1211} & \big[\mathbb{L}\big]_{1222} & \big[\mathbb{L}\big]_{1233} & \big[\mathbb{L}\big]_{1212} & \big[\mathbb{L}\big]_{1213} & \big[\mathbb{L}\big]_{1223} \\ \big[\mathbb{L}\big]_{1311} & \big[\mathbb{L}\big]_{1322} & \big[\mathbb{L}\big]_{1333} & \big[\mathbb{L}\big]_{1312} & \big[\mathbb{L}\big]_{1313} & \big[\mathbb{L}\big]_{1323} \\ \big[\mathbb{L}\big]_{2311} & \big[\mathbb{L}\big]_{2322} & \big[\mathbb{L}\big]_{2333} & \big[\mathbb{L}\big]_{2312} & \big[\mathbb{L}\big]_{2313} & \big[\mathbb{L}\big]_{2323} \end{bmatrix},$$

where the elements of the matrix $\boldsymbol{L}$ are defined from the components of the fourth order tensor $\mathbb{L}$. As $\mathbb{L}$ is composed of axisymmetric integrals over Φ and Θ, the resulting tensor is expected to be isotropic. This further simplifies the problem as $\boldsymbol{L}$ takes the form

$$\boldsymbol{L} = \begin{bmatrix} L_{11} & L_{12} & L_{13} & 0 & 0 & 0 \\ L_{21} & L_{22} & L_{23} & 0 & 0 & 0 \\ L_{31} & L_{32} & L_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & L_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & L_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & L_{66} \end{bmatrix}, \quad \begin{aligned} &L_{11} = L_{22} = L_{33}\,, \\ &L_{12} = L_{21} = L_{13} = L_{31} = L_{23} = L_{32}\,, \\ &L_{44} = L_{55} = L_{66} = \tfrac{1}{2}[L_{11} - L_{12}]\,, \end{aligned}$$

with the remaining components of $\boldsymbol{L}$, and with it $\mathbb{L}$, equal to zero. Calculating the non-zero components of $\boldsymbol{L}$ yields

$$\begin{aligned} L_{11} &= \int_{\Theta^{|}=0}^{\Theta^{|}=2\pi} \int_{\Phi^{|}=0}^{\Phi^{|}=\pi} \sin^5\Phi^{|} \sin^4\Theta^{|}\, \mathrm{d}\Phi^{|}\, \mathrm{d}\Theta^{|} = \frac{4}{5}\pi\,, \\ L_{12} &= \int_{\Theta^{|}=0}^{\Theta^{|}=2\pi} \int_{\Phi^{|}=0}^{\Phi^{|}=\pi} \sin^5\Phi^{|} \sin^2\Theta^{|} \cos^2\Theta^{|}\, \mathrm{d}\Phi^{|}\, \mathrm{d}\Theta^{|} = \frac{4}{15}\pi\,, \\ L_{44} &= \tfrac{1}{2}[L_{11} - L_{12}] = \frac{4}{15}\pi\,. \end{aligned}$$

These three components of $\boldsymbol{L}$ are sufficient to define every non-zero component of $\mathbb{L}$, that is

$$\mathbb{L} = \frac{4}{15}\pi\,\mathbb{I} \qquad \text{with} \qquad \mathbb{I} := \boldsymbol{\mathcal{I}} \overline{\otimes}\, \boldsymbol{\mathcal{I}} + \boldsymbol{\mathcal{I}} \underline{\otimes}\, \boldsymbol{\mathcal{I}} + \boldsymbol{\mathcal{I}} \otimes \boldsymbol{\mathcal{I}}\,,$$

where $\mathbb{I}$ is a three-dimensional, fourth-order identity tensor. □

Lemma 9.

$$\int_{\hat{\mathcal{H}}_0{}^{|||}} \int_{\hat{\mathcal{H}}_0{}^{||}} \int_{\hat{\mathcal{H}}_0{}^{|}} \left| \hat{\boldsymbol{\Xi}}^{|} \cdot \left[\hat{\boldsymbol{\Xi}}^{||} \times \hat{\boldsymbol{\Xi}}^{|||} \right] \right| d\hat{V}^{|}\, d\hat{V}^{||}\, d\hat{V}^{|||} = 8\pi^4$$

Proof.

$$\int_{\hat{\mathcal{H}}_0{}^{\mathrm{III}}} \underbrace{\int_{\hat{\mathcal{H}}_0{}^{\mathrm{II}}} \int_{\hat{\mathcal{H}}_0{}^{\mathrm{I}}} \left| \hat{\boldsymbol{\Xi}}^{\mathrm{I}} \cdot \left[\hat{\boldsymbol{\Xi}}^{\mathrm{II}} \times \hat{\boldsymbol{\Xi}}^{\mathrm{III}} \right] \right| \mathrm{d}\hat{V}^{\mathrm{I}}\, \mathrm{d}\hat{V}^{\mathrm{II}}}_{f}\, \mathrm{d}\hat{V}^{\mathrm{III}}, \quad \text{where} \quad f(\Phi^{\mathrm{III}}, \Theta^{\mathrm{III}}) .$$

At first look, f seems to be a function of Φ^{III} and Θ^{III}, but upon further inspection we see that due to the geometrical nature of the problem, f is independent of Φ^{III} and Θ^{III}. That is, the integrals over Φ^{I}, Θ^{I}, Φ^{II} and Θ^{II} make axisymmetric rotations, covering the volume of two complete unit spheres corresponding to $\mathrm{d}V^{\mathrm{I}}$ and $\mathrm{d}V^{\mathrm{II}}$. As a result, the initial values of Φ^{III} and Θ^{III} do not affect the outcome of f, enabling us to assign arbitrary values to Φ^{III} and Θ^{III}. Assigning $\Phi^{\mathrm{III}} = 0$ and $\Theta^{\mathrm{III}} = 0$ leaves us with

$$\left[\hat{\boldsymbol{\Xi}}^{\mathrm{III}} \right] = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \quad , \quad \left[\hat{\boldsymbol{\Xi}}^{\mathrm{II}} \times \hat{\boldsymbol{\Xi}}^{\mathrm{III}} \right] = \begin{bmatrix} \sin\Theta^{\mathrm{I}} \sin\Phi^{\mathrm{I}} \\ -\sin\Theta^{\mathrm{I}} \cos\Phi^{\mathrm{I}} \\ 0 \end{bmatrix} ,$$

$$\begin{aligned} \left| \hat{\boldsymbol{\Xi}}^{\mathrm{I}} \cdot \left[\hat{\boldsymbol{\Xi}}^{\mathrm{II}} \times \hat{\boldsymbol{\Xi}}^{\mathrm{III}} \right] \right| &= \left| \sin\Phi^{\mathrm{I}} \sin\Phi^{\mathrm{II}} \left[\cos\Theta^{\mathrm{I}} \sin\Theta^{\mathrm{II}} - \sin\Theta^{\mathrm{I}} \cos\Theta^{\mathrm{II}} \right] \right| \\ &= \left| \sin\Phi^{\mathrm{I}} \sin\Phi^{\mathrm{II}} \sin\left(\Theta^{\mathrm{II}} - \Theta^{\mathrm{I}}\right) \right| , \end{aligned}$$

rendering

$$\begin{aligned} f &= \int_{\Theta^{\mathrm{II}}=0}^{\Theta^{\mathrm{II}}=2\pi} \int_{\Phi^{\mathrm{II}}=0}^{\Phi^{\mathrm{II}}=\pi} \int_{\Theta^{\mathrm{I}}=0}^{\Theta^{\mathrm{I}}=2\pi} \int_{\Phi^{\mathrm{I}}=0}^{\Phi^{\mathrm{I}}=\pi} \left| \sin\left(\Theta^{\mathrm{II}} - \Theta^{\mathrm{I}}\right) \right| \sin^2\Phi^{\mathrm{I}} \sin^2\Phi^{\mathrm{II}}\, \mathrm{d}\Phi^{\mathrm{I}}\, \mathrm{d}\Theta^{\mathrm{I}}\, \mathrm{d}\Phi^{\mathrm{II}}\, \mathrm{d}\Theta^{\mathrm{II}} \\ &= \frac{1}{4}\pi^2 \int_{\Theta^{\mathrm{II}}=0}^{\Theta^{\mathrm{II}}=2\pi} \int_{\Theta^{\mathrm{I}}=0}^{\Theta^{\mathrm{I}}=2\pi} \left| \sin\left(\Theta^{\mathrm{II}} - \Theta^{\mathrm{I}}\right) \right| \mathrm{d}\Theta^{\mathrm{I}}\, \mathrm{d}\Theta^{\mathrm{II}} . \end{aligned}$$

Again, the axisymmetry property of the integral over Θ^{I} renders it independent from the value of Θ^{II}, thus we can proceed with assigning an arbitrary value for Θ^{II}. Taking $\Theta^{\mathrm{II}} = 0$ results in

$$f = \frac{1}{4}\pi^2 \int_{\Theta^{\mathrm{II}}=0}^{\Theta^{\mathrm{II}}=2\pi} \int_{\Theta^{\mathrm{I}}=0}^{\Theta^{\mathrm{I}}=2\pi} \left| -\sin\Theta^{\mathrm{I}} \right| \mathrm{d}\Theta^{\mathrm{I}}\, \mathrm{d}\Theta^{\mathrm{II}} = \frac{1}{4}\pi^2 \int_{\Theta^{\mathrm{II}}=0}^{\Theta^{\mathrm{II}}=2\pi} 4\, \mathrm{d}\Theta^{\mathrm{II}} = 2\pi^3 .$$

Finally, integrating over f yields

$$\int_{\Theta^{|||}=0}^{\Theta^{|||}=2\pi} \int_{\Phi^{|||}=0}^{\Phi^{|||}=\pi} 2\pi^3 \sin\Phi^{|||}\, \mathrm{d}\Phi^{|||}\, \mathrm{d}\Theta^{|||} = 8\pi^4 \,.$$

□

Lemma 10.

$$\boxed{\int_{\hat{\mathcal{H}}_0{}^{||}} \int_{\hat{\mathcal{H}}_0{}^{|}} \left|\hat{\boldsymbol{\Xi}}^{|} \times \hat{\boldsymbol{\Xi}}^{||}\right| \hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}}\, d\hat{V}^{|}\, d\hat{V}^{||} = \frac{4}{3}\pi^3 \boldsymbol{\mathcal{I}}}$$

Proof.

$$\int_{\Theta^{||}=0}^{\Theta^{||}=2\pi} \int_{\Phi^{||}=0}^{\Phi^{||}=\pi} \underbrace{\int_{\Theta^{|}=0}^{\Theta^{|}=2\pi} \int_{\Phi^{|}=0}^{\Phi^{|}=\pi} \left|\hat{\boldsymbol{\Xi}}^{|} \times \hat{\boldsymbol{\Xi}}^{||}\right| \hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}}\, \sin\Phi^{|}\, \mathrm{d}\Phi^{|}\, \mathrm{d}\Theta^{|}}_{\boldsymbol{\mathcal{M}}} \sin\Phi^{||}\, \mathrm{d}\Phi^{||}\, \mathrm{d}\Theta^{||} \,,$$

Here, $\boldsymbol{\mathcal{M}}$ is independent of the initial values of $\Phi^{||}$ and $\Theta^{||}$ due to the axisymmetric integral over it, which enables us to assign arbitrary values to the components of $\boldsymbol{\mathcal{M}}$. Doing so, without loss of generality, we choose a $\hat{\boldsymbol{\Xi}}^{||}$ such that $\Phi^{||} = 0$ and $\Theta^{||} = 0$, leaving us with

$$\left[\hat{\boldsymbol{\Xi}}^{||}\right] = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \quad \left[\hat{\boldsymbol{\Xi}}^{|} \times \hat{\boldsymbol{\Xi}}^{||}\right] = \begin{bmatrix} \sin\Theta^{|} \sin\Phi^{|} \\ -\sin\Theta^{|} \cos\Phi^{|} \\ 0 \end{bmatrix} \quad \Rightarrow \quad \left|\hat{\boldsymbol{\Xi}}^{|} \times \hat{\boldsymbol{\Xi}}^{||}\right| = \left|\sin\Phi^{|}\right|,$$

$$\left[\hat{\boldsymbol{N}}\right] = \begin{bmatrix} \sin\Theta^{|} \\ -\cos\Theta^{|} \\ 0 \end{bmatrix} \quad \Rightarrow \quad \left[\hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}}\right] = \begin{bmatrix} \sin^2\Theta^{|} & -\sin\Theta^{|}\cos\Theta^{|} & 0 \\ -\sin\Theta^{|}\cos\Theta^{|} & \cos^2\Theta^{|} & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

Using these relations, evaluating the integral in $\boldsymbol{\mathcal{M}}$ yields

$$[\boldsymbol{\mathcal{M}}] = \frac{\pi^2}{2} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

Note that $\boldsymbol{\mathcal{M}}$ happens to take this particular form since we have chosen $\hat{\boldsymbol{\Xi}}^{\shortparallel}$ such that $\Phi^{\shortparallel} = 0$ and $\Theta^{\shortparallel} = 0$. After some mathematical steps, it can be shown that, in general,

$$\boldsymbol{\mathcal{M}} = \frac{\pi^2}{2}\left[\boldsymbol{\mathcal{I}} - \hat{\boldsymbol{\Xi}}^{\shortparallel} \otimes \hat{\boldsymbol{\Xi}}^{\shortparallel}\right],$$

where $\boldsymbol{\mathcal{I}}$ is the second order, three-dimensional identity. Integrating over $\boldsymbol{\mathcal{M}}$,

$$\int_{\Theta^{\shortparallel}=0}^{\Theta^{\shortparallel}=2\pi}\int_{\Phi^{\shortparallel}=0}^{\Phi^{\shortparallel}=\pi} \frac{\pi^2}{2}\left[\boldsymbol{\mathcal{I}} - \hat{\boldsymbol{\Xi}}^{\shortparallel} \otimes \hat{\boldsymbol{\Xi}}^{\shortparallel}\right] \sin\Phi^{\shortparallel}\, \mathrm{d}\Phi^{\shortparallel}\, \mathrm{d}\Theta^{\shortparallel} =$$

$$\frac{\pi^2}{2}\boldsymbol{\mathcal{I}} \int_{\Theta^{\shortparallel}=0}^{\Theta^{\shortparallel}=2\pi}\int_{\Phi^{\shortparallel}=0}^{\Phi^{\shortparallel}=\pi} \sin\Phi^{\shortparallel}\, \mathrm{d}\Phi^{\shortparallel}\, \mathrm{d}\Theta^{\shortparallel} - \frac{\pi^2}{2}\int_{\Theta^{\shortparallel}=0}^{\Theta^{\shortparallel}=2\pi}\int_{\Phi^{\shortparallel}=0}^{\Phi^{\shortparallel}=\pi} \left[\hat{\boldsymbol{\Xi}}^{\shortparallel} \otimes \hat{\boldsymbol{\Xi}}^{\shortparallel}\right] \sin\Phi^{\shortparallel}\, \mathrm{d}\Phi^{\shortparallel}\, \mathrm{d}\Theta^{\shortparallel},$$

and utilizing Lemma 2 and Lemma 6 yields

$$\frac{\pi^2}{2}\boldsymbol{\mathcal{I}} \underbrace{\int_{\Theta^{\shortparallel}=0}^{\Theta^{\shortparallel}=2\pi}\int_{\Phi^{\shortparallel}=0}^{\Phi^{\shortparallel}=\pi} \sin\Phi^{\shortparallel}\, \mathrm{d}\Phi^{\shortparallel}\, \mathrm{d}\Theta^{\shortparallel}}_{4\pi} - \frac{\pi^2}{2}\underbrace{\int_{\Theta^{\shortparallel}=0}^{\Theta^{\shortparallel}=2\pi}\int_{\Phi^{\shortparallel}=0}^{\Phi^{\shortparallel}=\pi} \left[\hat{\boldsymbol{\Xi}}^{\shortparallel} \otimes \hat{\boldsymbol{\Xi}}^{\shortparallel}\right] \sin\Phi^{\shortparallel}\, \mathrm{d}\Phi^{\shortparallel}\, \mathrm{d}\Theta^{\shortparallel}}_{\frac{4}{3}\pi\boldsymbol{\mathcal{I}}}$$

$$= \frac{4}{3}\pi^3\boldsymbol{\mathcal{I}}.$$

□

Lemma 11.

$$\boxed{\int_{\hat{\mathcal{H}}_0{}^{\shortparallel}}\int_{\hat{\mathcal{H}}_0{}^{\shortmid}} \left|\hat{\boldsymbol{\Xi}}^{\shortmid} \times \hat{\boldsymbol{\Xi}}^{\shortparallel}\right| \hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}}\, d\hat{V}^{\shortmid}\, d\hat{V}^{\shortparallel} = \frac{4}{15}\pi^3\,\mathbb{I}}$$

Proof.

$$\underbrace{\int_{\hat{\mathcal{H}}_0{}^{\shortparallel}} \underbrace{\int_{\hat{\mathcal{H}}_0{}^{\shortmid}} \left|\hat{\boldsymbol{\Xi}}^{\shortmid} \times \hat{\boldsymbol{\Xi}}^{\shortparallel}\right| \hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}}\, \mathrm{d}\hat{V}^{\shortmid}}_{\mathbb{R}}\, \mathrm{d}\hat{V}^{\shortparallel}}_{\$}.$$

Notice that $\mathbb{R}$ has axisymmetric integrals over $\Theta^{|}$ and thus the outcome is independent of the initial values of $\Theta^{||}$ and $\Phi^{||}$, allowing us to assign them arbitrary values. Taking $\Theta^{||} = 0$ and $\Phi^{||} = 0$ yields

$$\left[\hat{\boldsymbol{\Xi}}^{||}\right] = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \qquad , \qquad \left[\hat{\boldsymbol{\Xi}}^{|} \times \hat{\boldsymbol{\Xi}}^{||}\right] = \begin{bmatrix} \sin\Theta^{|}\sin\Phi^{|} \\ -\sin\Theta^{|}\cos\Phi^{|} \\ 0 \end{bmatrix} ,$$

$$\Rightarrow \quad \left|\hat{\boldsymbol{\Xi}}^{|} \times \hat{\boldsymbol{\Xi}}^{||}\right| = \left|\sin\Phi^{|}\right| \qquad , \qquad \left[\hat{\boldsymbol{N}}\right] = \begin{bmatrix} \sin\Theta^{|} \\ -\cos\Theta^{|} \\ 0 \end{bmatrix} .$$

As $\hat{\boldsymbol{N}}$ is now solely a function of $\Theta^{|}$, so is $\hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}}$, allowing us to write $\mathbb{R}$ as the multiplication of two separate integrals

$$\mathbb{R} = \int_{\Theta^{|}=0}^{\Theta^{|}=2\pi} \hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}} \, \mathrm{d}\Theta^{|} \int_{\Phi^{|}=0}^{\Phi^{|}=\pi} \sin^2\Phi^{|} \, \mathrm{d}\Phi^{|} ,$$

in which the second integral reduces to $\pi/2$, resulting in

$$\mathbb{R} = \frac{\pi}{2} \int_{\Theta^{|}=0}^{\Theta^{|}=2\pi} \hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}} \, \mathrm{d}\Theta^{|} .$$

Remark *Note that the tensor $\hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}}$ is anisotropic as it is a function of $\Theta^{|}$, and thus direction dependent. As $\hat{\boldsymbol{\Xi}}^{||}$ is fixed, changing $\hat{\boldsymbol{\Xi}}^{|}$ results in a varying $\hat{\boldsymbol{N}}$ that remains on the plane orthogonal to $\hat{\boldsymbol{\Xi}}^{||}$. However, once it's integrated over $\Theta^{|}$, the resulting tensor $\mathbb{R}$ will be isotropic in the two-dimensional plane orthogonal to $\hat{\boldsymbol{\Xi}}^{||}$, as the axisymmetric integral will eliminate the direction dependence on $\Theta^{|}$. The isotropic part of $\mathbb{R}$, denoted by $\mathbb{R}^*$, is the usual two-dimensional isotropic fourth-order tensor on the plane orthogonal to $\hat{\boldsymbol{\Xi}}^{||}$. The components of $\mathbb{R}^*$, along with the components of $\mathbb{R}$ in terms of $\mathbb{R}^*$ are given in*

Voigt notation below.

$$\boldsymbol{R}^* = \begin{bmatrix} R^*_{11} & R^*_{12} & 0 \\ R^*_{21} & R^*_{22} & 0 \\ 0 & 0 & R^*_{33} \end{bmatrix} \quad , \quad \boldsymbol{R} = \begin{bmatrix} R_{11} = R^*_{11} & R_{12} = R^*_{12} & 0 & 0 & 0 & 0 \\ R_{21} = R^*_{21} & R_{22} = R^*_{22} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & R_{44} = R^*_{33} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Note that the particular ordering of the zero components of $\mathbb{R}$ *are a result of the fact that* $\hat{\boldsymbol{\Xi}}^{||}$ *here, without the loss of generality, is assumed to coincide with* $\boldsymbol{e}_3$*, as* $\Theta^{||}$ *and* $\Phi^{||}$ *were both previously set to 0.*

Now that $\mathbb{R}$ is a symmetric tensor with the components in Voigt notation

$$R_{11} = R_{22} := \big[\mathbb{R}\big]_{1111} = \big[\mathbb{R}\big]_{2222} = \frac{\pi}{2}\int_{\Theta^{|}=0}^{\Theta^{|}=2\pi} \sin^4\Theta^{|}\,\mathrm{d}\Theta^{|} = \frac{3}{8}\pi^2\,,$$

$$R_{12} = R_{21} := \big[\mathbb{R}\big]_{1122} = \big[\mathbb{R}\big]_{2211} = \frac{\pi}{2}\int_{\Theta^{|}=0}^{\Theta^{|}=2\pi} \sin^2\Theta^{|}\cos^2\Theta^{|}\,\mathrm{d}\Theta^{|} = \frac{1}{8}\pi^2\,,$$

$$R_{44} := \big[\mathbb{R}\big]_{1212} = \big[\mathbb{R}\big]_{1221} = \big[\mathbb{R}\big]_{2121} = \big[\mathbb{R}\big]_{2112} = \frac{\pi}{2}\int_{\Theta^{|}=0}^{\Theta^{|}=2\pi} \sin^2\Theta^{|}\cos^2\Theta^{|}\,\mathrm{d}\Theta^{|}$$
$$= \frac{1}{8}\pi^2\,,$$

as $\hat{\boldsymbol{\Xi}}^{||}$ is assumed to coincide with the basis vector $\boldsymbol{e}_3$, without the loss of generality, tensor $\mathbb{R}$ can also be written as

$$\mathbb{R} = \frac{\pi^2}{8}\big[\,\overline{\boldsymbol{\mathcal{I}}}\,\overline{\otimes}\,\overline{\boldsymbol{\mathcal{I}}} + \overline{\boldsymbol{\mathcal{I}}}\,\underline{\otimes}\,\overline{\boldsymbol{\mathcal{I}}} + \overline{\boldsymbol{\mathcal{I}}}\otimes\overline{\boldsymbol{\mathcal{I}}}\big] \qquad \text{where} \qquad \overline{\boldsymbol{\mathcal{I}}} = \boldsymbol{\mathcal{I}} - \hat{\boldsymbol{\Xi}}^{||}\otimes\hat{\boldsymbol{\Xi}}^{||}\,.$$

Now $\overline{\boldsymbol{\mathcal{I}}}$ can be expressed as

$$\big[\overline{\boldsymbol{\mathcal{I}}}\big] = \begin{bmatrix} 1-\sin^2\Phi^{||}\cos^2\Theta^{||} & -\sin^3\Phi^{||}\sin\Theta^{||}\cos\Theta^{||} & -\sin\Phi^{||}\cos\Phi^{||}\cos\Theta^{||} \\ -\sin^3\Phi^{||}\sin\Theta^{||}\cos\Theta^{||} & 1-\sin^2\Phi^{||}\sin^2\Theta^{||} & -\sin\Phi^{||}\cos\Phi^{||}\sin\Theta^{||} \\ -\sin\Phi^{||}\cos\Phi^{||}\cos\Theta^{||} & -\sin\Phi^{||}\cos\Phi^{||}\sin\Theta^{||} & 1-\cos^2\Phi^{||} \end{bmatrix}.$$

Moving on to the integration of $\mathbb{R}$, as the integrals over $\mathbb{R}$ are axisymmetric, the resulting tensor $\mathbb{S}$ is expected to be symmetric and isotropic. Thus it is sufficient to calculate just three of its components

$$\boldsymbol{S} = \begin{bmatrix} S_{11} & S_{12} & S_{13} & 0 & 0 & 0 \\ S_{21} & S_{22} & S_{23} & 0 & 0 & 0 \\ S_{31} & S_{32} & S_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & S_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & S_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & S_{66} \end{bmatrix} \quad \text{with} \quad \begin{aligned} & S_{11} = S_{22} = S_{33}\,, \\ & S_{12} = S_{21} = S_{13} = S_{31} = S_{23} = S_{32}\,, \\ & S_{44} = S_{55} = S_{66}\,, \end{aligned}$$

where the remaining components of $\boldsymbol{S}$, and with it $\mathbb{S}$, equal to zero. Calculating the non-zero components of $\boldsymbol{S}$ yields

$$\begin{aligned} \boldsymbol{S}_{11} &= \int_{\Theta^{||}=0}^{\Theta^{||}=2\pi} \int_{\Phi^{||}=0}^{\Phi^{||}=\pi} \left[\mathbb{R}\right]_{1111} \sin\Phi^{||}\,\mathrm{d}\Phi^{||}\,\mathrm{d}\Theta^{||} \\ &= \int_{\Theta^{||}=0}^{\Theta^{||}=2\pi} \int_{\Phi^{||}=0}^{\Phi^{||}=\pi} \frac{\pi^2}{8} 3 \left[\overline{\boldsymbol{\mathcal{I}}}\right]_{11} \left[\overline{\boldsymbol{\mathcal{I}}}\right]_{11} \sin\Phi^{||}\,\mathrm{d}\Phi^{||}\,\mathrm{d}\Theta^{||} = \frac{12}{15}\pi^3\,, \\ \boldsymbol{S}_{12} &= \int_{\Theta^{||}=0}^{\Theta^{||}=2\pi} \int_{\Phi^{||}=0}^{\Phi^{||}=\pi} \left[\mathbb{R}\right]_{1122} \sin\Phi^{||}\,\mathrm{d}\Phi^{||}\,\mathrm{d}\Theta^{||} \\ &= \int_{\Theta^{||}=0}^{\Theta^{||}=2\pi} \int_{\Phi^{||}=0}^{\Phi^{||}=\pi} \frac{\pi^2}{8} 2 \Big[\left[\overline{\boldsymbol{\mathcal{I}}}\right]_{12} \left[\overline{\boldsymbol{\mathcal{I}}}\right]_{12} + \left[\overline{\boldsymbol{\mathcal{I}}}\right]_{11} \left[\overline{\boldsymbol{\mathcal{I}}}\right]_{22} \Big] \sin\Phi^{||}\,\mathrm{d}\Phi^{||}\,\mathrm{d}\Theta^{||} = \frac{4}{15}\pi^3\,, \\ \boldsymbol{S}_{44} &= \tfrac{1}{2}\left[\boldsymbol{S}_{11} - \boldsymbol{S}_{12}\right] = \frac{4}{15}\pi^3\,. \end{aligned}$$

Equipped with the components of $\boldsymbol{S}$, it can be shown that $\mathbb{S}$ is

$$\mathbb{S} = \frac{4}{15}\pi^3\,\mathbb{I}\,.$$

□

Table 3.1: Summary of the key lemmas. The second-order identity $\boldsymbol{\mathcal{I}}$ stands for $\boldsymbol{\mathcal{I}}_{\text{2D}}$ in 2D space, and $\boldsymbol{\mathcal{I}}_{\text{3D}}$ in 3D space.

2D Space	3D Space
1. $\int_{\hat{\mathcal{H}}_0{}^{\mathrm{I}}} \lvert\hat{\boldsymbol{\Xi}}^{\mathrm{I}}\rvert \,\mathrm{d}\hat{A}^{\mathrm{I}} = 2\pi$	2. $\int_{\hat{\mathcal{H}}_0{}^{\mathrm{I}}} \lvert\hat{\boldsymbol{\Xi}}^{\mathrm{I}}\rvert \,\mathrm{d}\hat{V}^{\mathrm{I}} = 4\pi$
3. $\int_{\hat{\mathcal{H}}_0{}^{\mathrm{II}}} \int_{\hat{\mathcal{H}}_0{}^{\mathrm{I}}} \lvert\hat{\boldsymbol{\Xi}}^{\mathrm{I}} \times \hat{\boldsymbol{\Xi}}^{\mathrm{II}}\rvert \,\mathrm{d}\hat{A}^{\mathrm{I}} \,\mathrm{d}\hat{A}^{\mathrm{II}} = 8\pi$	4. $\int_{\hat{\mathcal{H}}_0{}^{\mathrm{II}}} \int_{\hat{\mathcal{H}}_0{}^{\mathrm{I}}} \lvert\hat{\boldsymbol{\Xi}}^{\mathrm{I}} \times \hat{\boldsymbol{\Xi}}^{\mathrm{II}}\rvert \,\mathrm{d}\hat{V}^{\mathrm{I}} \,\mathrm{d}\hat{V}^{\mathrm{II}} = 4\pi^3$
5. $\int_{\hat{\mathcal{H}}_0{}^{\mathrm{I}}} \hat{\boldsymbol{\Xi}}^{\mathrm{I}} \otimes \hat{\boldsymbol{\Xi}}^{\mathrm{I}} \,\mathrm{d}\hat{A}^{\mathrm{I}} = \pi \boldsymbol{\mathcal{I}}$	6. $\int_{\hat{\mathcal{H}}_0{}^{\mathrm{I}}} \hat{\boldsymbol{\Xi}}^{\mathrm{I}} \otimes \hat{\boldsymbol{\Xi}}^{\mathrm{I}} \,\mathrm{d}\hat{V}^{\mathrm{I}} = \frac{4}{3}\pi \boldsymbol{\mathcal{I}}$
7. $\int_{\hat{\mathcal{H}}_0{}^{\mathrm{I}}} \hat{\boldsymbol{\Xi}}^{\mathrm{I}} \otimes \hat{\boldsymbol{\Xi}}^{\mathrm{I}} \otimes \hat{\boldsymbol{\Xi}}^{\mathrm{I}} \otimes \hat{\boldsymbol{\Xi}}^{\mathrm{I}} \,\mathrm{d}\hat{A}^{\mathrm{I}} = \frac{1}{4}\pi \mathbb{I}$	8. $\int_{\hat{\mathcal{H}}_0{}^{\mathrm{I}}} \hat{\boldsymbol{\Xi}}^{\mathrm{I}} \otimes \hat{\boldsymbol{\Xi}}^{\mathrm{I}} \otimes \hat{\boldsymbol{\Xi}}^{\mathrm{I}} \otimes \hat{\boldsymbol{\Xi}}^{\mathrm{I}} \,\mathrm{d}\hat{V}^{\mathrm{I}} = \frac{4}{15}\pi \mathbb{I}$
no 2D counterparts	9. $\int_{\hat{\mathcal{H}}_0{}^{\mathrm{III}}} \int_{\hat{\mathcal{H}}_0{}^{\mathrm{II}}} \int_{\hat{\mathcal{H}}_0{}^{\mathrm{I}}} \left\lvert\hat{\boldsymbol{\Xi}}^{\mathrm{I}} \cdot \left[\hat{\boldsymbol{\Xi}}^{\mathrm{II}} \times \hat{\boldsymbol{\Xi}}^{\mathrm{III}}\right]\right\rvert \,\mathrm{d}\hat{V}^{\mathrm{I}} \,\mathrm{d}\hat{V}^{\mathrm{II}} \,\mathrm{d}\hat{V}^{\mathrm{III}} = 8\pi^4$
	10. $\int_{\hat{\mathcal{H}}_0{}^{\mathrm{II}}} \int_{\hat{\mathcal{H}}_0{}^{\mathrm{I}}} \lvert\hat{\boldsymbol{\Xi}}^{\mathrm{I}} \times \hat{\boldsymbol{\Xi}}^{\mathrm{II}}\rvert \,\hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}} \,\mathrm{d}\hat{V}^{\mathrm{I}} \,\mathrm{d}\hat{V}^{\mathrm{II}} = \frac{4}{3}\pi^3 \boldsymbol{\mathcal{I}}$
	11. $\int_{\hat{\mathcal{H}}_0{}^{\mathrm{II}}} \int_{\hat{\mathcal{H}}_0{}^{\mathrm{I}}} \lvert\hat{\boldsymbol{\Xi}}^{\mathrm{I}} \times \hat{\boldsymbol{\Xi}}^{\mathrm{II}}\rvert \,\hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}} \,\mathrm{d}\hat{V}^{\mathrm{I}} \,\mathrm{d}\hat{V}^{\mathrm{II}} = \frac{4}{15}\pi^3 \mathbb{I}$
$\int_{\hat{\mathcal{H}}_0^{\{\bullet\}}} := \int_{\Theta^{\{\bullet\}}=0}^{\Theta^{\{\bullet\}}=2\pi}$, $\mathrm{d}\hat{A}^{\{\bullet\}} := \mathrm{d}\Theta^{\{\bullet\}}$	$\int_{\hat{\mathcal{H}}_0^{\{\bullet\}}} := \int_{\Theta^{\{\bullet\}}=0}^{\Theta^{\{\bullet\}}=2\pi} \int_{\Phi^{\{\bullet\}}=0}^{\Phi^{\{\bullet\}}=\pi}$, $\mathrm{d}\hat{V}^{\{\bullet\}} := \sin\Phi^{\{\bullet\}} \,\mathrm{d}\Phi^{\{\bullet\}} \,\mathrm{d}\Theta^{\{\bullet\}}$
fourth-order identity $\mathbb{I} := \boldsymbol{\mathcal{I}} \overline{\otimes} \boldsymbol{\mathcal{I}} + \boldsymbol{\mathcal{I}} \underline{\otimes} \boldsymbol{\mathcal{I}} + \boldsymbol{\mathcal{I}} \otimes \boldsymbol{\mathcal{I}}$	

Chapter 4

Harmonic Model

In this chapter, we will derive the relationships between the material parameters of CCM, namely λ, μ, ν, κ and E, and the material parameters of harmonic CPD. To obtain the relations between the material parameters, we propose a method rooted in the postulated equivalence of the total point-wise energy density of harmonic CPD for the case of affine deformations, denoted as Ψ_{H}, and the linear elastic point-wise strain energy of CCM, which holds in both 2D and 3D,

$$\Psi_{\mathrm{CCM}} = \mu\, \boldsymbol{\varepsilon} : \boldsymbol{\varepsilon} + \frac{1}{2}\lambda \left[\boldsymbol{\varepsilon} : \boldsymbol{\mathcal{I}}\right]^2, \tag{4.1}$$

where $\boldsymbol{\varepsilon}$ is the strain tensor and $\boldsymbol{\mathcal{I}}$ is the second-order identity tensor. The first and second Lamé parameters are denoted as λ and μ, respectively. Unlike isotropic linear elasticity, CPD is intrinsically suited for finite deformations. In order to equate the energies of the two formulations, the energy densities of harmonic CPD should be evaluated at the reference configuration first. This can be done in two ways (i) linearizing the strains of the energy densities, and then carrying out the integrals; or (ii) finding the analytical solutions of the integrals in the large deformation framework, and afterwards evaluating the energy densities at the reference configuration. For the harmonic energies, we opt for option (i), simply because the analytical solutions of the integrals proved impossible for us to calculate. To this end, one-neighbor and two-neighbor strain measures are

linearized for a generic, affine deformation in 2D, in Section 4.1. Section 4.2 repeats the process in 3D, accounting for three-neighbor interactions. Next, in Sections 4.3 and 4.4, the total (point-wise) energy densities of harmonic CPD are integrated in 2D and 3D, respectively. Finally, in Sections 4.5.1 and 4.5.2 the 2D and 3D energy densities of harmonic CPD are equated to that of CCM, and the relationships between the material parameters of the two formulations are derived.

Remark on the linearization of the linear strains *The linear strains ε are linear in terms of their arguments, the stretches l/L, a/A and v/V, unlike the non-linear strains E that have their arguments squared. However, the stretches themselves are intrinsically nonlinear and must be projected to and evaluated at the reference configuration. This is what is meant by linearization of the strains in the following sections. Henceforth, the term* linearization *consistently refers to linearizing a functional at the reference configuration in the sense of a Taylor expansion.*

4.1 Linearization of strains in 2D

Throughout this section, $\boldsymbol{\mathcal{F}}$ and $\boldsymbol{\mathcal{I}}$ stand for $\boldsymbol{\mathcal{F}}_{\text{2D}}$ and $\boldsymbol{\mathcal{I}}_{\text{2D}}$, but the subscripts are omitted for the sake of brevity.

4.1.1 Length strain ε_l

In order to linearize the length strain $\varepsilon_l := \lambda_l - 1$, we begin with the equation

$$\mathcal{L}in\, \varepsilon_l = \mathcal{L}in\, [\lambda_l - 1] = \mathcal{L}in\, l/L - 1 = \mathcal{L}in\, \frac{\xi^{|}}{\Xi^{|}} - 1\,, \tag{4.2}$$

that is

$$\mathit{Lin}\ \frac{\xi^{|}}{\Xi^{|}} - 1 := \frac{\xi^{|}}{\Xi^{|}}\bigg|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} + \frac{\partial}{\partial \boldsymbol{\mathcal{F}}}\left(\frac{\xi^{|}}{\Xi^{|}}\right)\bigg|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} : \left[\boldsymbol{\mathcal{F}} - \boldsymbol{\mathcal{I}}\right] - 1\,. \tag{4.3}$$

The first term reduces to 1 as

$$\frac{\xi^{|}}{\Xi^{|}}\bigg|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} = \frac{\|\boldsymbol{\mathcal{F}}\cdot\boldsymbol{\Xi}^{|}\|}{\Xi^{|}}\bigg|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} = \frac{\|\boldsymbol{\mathcal{I}}\cdot\boldsymbol{\Xi}^{|}\|}{\Xi^{|}} = \frac{\Xi^{|}}{\Xi^{|}} = 1\,. \tag{4.4}$$

Next, the derivative of $\xi^{|}/\Xi^{|}$ with respect to $\boldsymbol{\mathcal{F}}$ is evaluated as

$$\frac{\partial}{\partial \boldsymbol{\mathcal{F}}}\left(\frac{\xi^{|}}{\Xi^{|}}\right) = \frac{1}{\Xi^{|}}\frac{\partial \xi^{|}}{\partial \boldsymbol{\mathcal{F}}} = \frac{1}{\Xi^{|}}\frac{\partial \xi^{|}}{\partial \boldsymbol{\xi}^{|}}\cdot\frac{\partial \boldsymbol{\xi}^{|}}{\partial \boldsymbol{\mathcal{F}}}\,, \tag{4.5}$$

with

$$\frac{\partial \boldsymbol{\xi}^{|}}{\partial \boldsymbol{\mathcal{F}}} = \boldsymbol{\mathcal{I}}\otimes\boldsymbol{\Xi}^{|}\,, \tag{4.6}$$

or in index notation

$$\begin{aligned}\left[\frac{\partial \boldsymbol{\xi}^{|}}{\partial \boldsymbol{\mathcal{F}}}\right]_{ikl} &= \frac{\partial\left[\boldsymbol{\xi}^{|}\right]_i}{\partial\left[\boldsymbol{\mathcal{F}}\right]_{kl}} = \frac{\partial}{\partial\left[\boldsymbol{\mathcal{F}}\right]_{kl}}\left(\left[\boldsymbol{\mathcal{F}}\right]_{ij}\left[\boldsymbol{\Xi}^{|}\right]_j\right)\\ &= \left[\boldsymbol{\delta}\right]_{ik}\left[\boldsymbol{\delta}\right]_{jl}\left[\boldsymbol{\Xi}^{|}\right]_j = \left[\boldsymbol{\delta}\right]_{ik}\left[\boldsymbol{\Xi}^{|}\right]_l = \boldsymbol{\mathcal{I}}\otimes\boldsymbol{\Xi}^{|}\,.\end{aligned} \tag{4.7}$$

Thus

$$\frac{\partial}{\partial \boldsymbol{\mathcal{F}}}\left(\frac{\xi^{|}}{\Xi^{|}}\right) = \frac{1}{\Xi^{|}}\frac{\partial \xi^{|}}{\partial \boldsymbol{\xi}^{|}}\cdot\left[\boldsymbol{\mathcal{I}}\otimes\boldsymbol{\Xi}^{|}\right] = \frac{1}{\Xi^{|}}\frac{\boldsymbol{\xi}^{|}}{\xi^{|}}\cdot\left[\boldsymbol{\mathcal{I}}\otimes\boldsymbol{\Xi}^{|}\right]. \tag{4.8}$$

This expression, evaluated at $\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}$ returns

$$\frac{\partial}{\partial \boldsymbol{\mathcal{F}}}\left(\frac{\xi^{|}}{\Xi^{|}}\right)\bigg|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} = \frac{1}{\Xi^{|}}\frac{\partial \Xi^{|}}{\partial \boldsymbol{\Xi}^{|}}\cdot\left[\boldsymbol{\mathcal{I}}\otimes\boldsymbol{\Xi}^{|}\right] = \frac{1}{{\Xi^{|}}^2}\boldsymbol{\Xi}^{|}\otimes\boldsymbol{\Xi}^{|}\,. \tag{4.9}$$

Finally, plugging this and Eq. (4.4) in the initial expression yields

$$\boxed{\mathit{Lin}\,\varepsilon_l = \frac{1}{{\Xi^{|}}^2}\left[\boldsymbol{\Xi}^{|}\otimes\boldsymbol{\Xi}^{|}\right] : \left[\boldsymbol{\mathcal{F}}-\boldsymbol{\mathcal{I}}\right].} \tag{4.10}$$

Another approach to this problem can be defining the mapping between the vectors $\boldsymbol{\Xi}^{|}$ and $\boldsymbol{\xi}^{|}$ as

$$\boldsymbol{\xi}^{|} = \boldsymbol{\mathcal{F}}^{|}\cdot\boldsymbol{\Xi}^{|}, \qquad \text{with} \qquad \boldsymbol{\mathcal{F}}^{|} = \boldsymbol{\mathcal{F}}\cdot\boldsymbol{\mathcal{I}}^{|}, \tag{4.11}$$

where $\boldsymbol{\mathcal{I}}^{|} = \hat{\boldsymbol{\Xi}}^{|}\otimes\hat{\boldsymbol{\Xi}}^{|}$ is a rank-deficient identity with $\hat{\boldsymbol{\Xi}}^{|}$ the unit vector along the direction of $\boldsymbol{\Xi}^{|}$. Next, the *Jacobian* $J^{|}$, corresponding to the mapping between the scalars $\Xi^{|}$ and $\xi^{|}$, is defined as

$$J^{|} := \frac{\xi^{|}}{\Xi^{|}} \qquad \Rightarrow \qquad J^{|} = \mathrm{Det}^{|}\,\boldsymbol{\mathcal{F}}^{|}, \tag{4.12}$$

where $\mathrm{Det}^{|}\{\bullet\}$ is a non-standard operation that is defined as
$\mathrm{Det}^{|}\,\boldsymbol{\mathcal{F}}^{|} := |\boldsymbol{\mathcal{F}}^{|}\cdot\boldsymbol{\Xi}^{|}|/|\boldsymbol{\Xi}^{|}| = \xi^{|}/\Xi^{|}$. Inserting this expression into Eq. (4.2) yields

$$\mathit{Lin}\,\frac{\xi^{|}}{\Xi^{|}} - 1 = \mathit{Lin}\;J^{|} - 1 = \left.\frac{\partial J^{|}}{\partial\boldsymbol{\mathcal{F}}}\right|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} : \left[\boldsymbol{\mathcal{F}}-\boldsymbol{\mathcal{I}}\right]. \tag{4.13}$$

Where

$$\begin{aligned}\frac{\partial J^{|}}{\partial\boldsymbol{\mathcal{F}}} &= \frac{\partial J^{|}}{\partial\boldsymbol{\mathcal{F}}^{|}} : \frac{\partial\boldsymbol{\mathcal{F}}^{|}}{\partial\boldsymbol{\mathcal{F}}}\\ &= J^{|}\,\boldsymbol{\mathcal{F}}^{|\text{-T}} : \mathbb{I}^{|} \qquad \text{with} \qquad \mathbb{I}^{|} = \boldsymbol{\mathcal{I}}\,\overline{\otimes}\,\boldsymbol{\mathcal{I}}^{|},\\ &= J^{|}\,\boldsymbol{\mathcal{I}}\cdot\boldsymbol{\mathcal{F}}^{|\text{-T}}\cdot\boldsymbol{\mathcal{I}}^{|} = J^{|}\,\boldsymbol{\mathcal{F}}^{|\text{-T}}.\end{aligned} \tag{4.14}$$

Since at $\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}$, $J^{|}=1$ and $\boldsymbol{\mathcal{F}}^{|\text{-T}}=\boldsymbol{\mathcal{I}}^{|}$, we are left with

$$\left.\frac{\partial J^{|}}{\partial\boldsymbol{\mathcal{F}}}\right|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} = \boldsymbol{\mathcal{I}}^{|}, \tag{4.15}$$

such that

$$\mathit{Lin}\ \varepsilon_l = \boldsymbol{\mathcal{I}}^{|} : \left[\boldsymbol{\mathcal{F}} - \boldsymbol{\mathcal{I}}\right]. \tag{4.16}$$

Finally, utilizing the relation

$$\boldsymbol{\mathcal{I}}^{|} : \boldsymbol{\mathcal{I}} = \left[\hat{\boldsymbol{\Xi}}^{|} \otimes \hat{\boldsymbol{\Xi}}^{|}\right] : \boldsymbol{\mathcal{I}} = \hat{\boldsymbol{\Xi}} \cdot \boldsymbol{\mathcal{I}} \cdot \hat{\boldsymbol{\Xi}} = 1\,, \tag{4.17}$$

gives

$$\boxed{\mathit{Lin}\ \varepsilon_l = \boldsymbol{\mathcal{I}}^{|} : \boldsymbol{\mathcal{F}} - 1} \tag{4.18}$$

which is an alternate form of the previously derived expression in Eq. (4.10). *The significance of this alternate solution method comes from its similarity to the upcoming derivations in the following sections, showing that the linearization procedures for the different strains are suitable for unification.*

4.1.2 Area strain ε_a

To linearize the area strain, we begin with the equation

$$\mathit{Lin}\,\varepsilon_a = \mathit{Lin}\ [\lambda_a - 1] = \mathit{Lin}\ a/A - 1 = \mathit{Lin}\ \frac{a^{|/||}}{A^{|/||}} - 1\,, \tag{4.19}$$

that is

$$\mathit{Lin}\ \frac{a^{|/||}}{A^{|/||}} - 1 = \left.\frac{a^{|/||}}{A^{|/||}}\right|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} + \left.\frac{\partial}{\partial \boldsymbol{\mathcal{F}}}\left(\frac{a^{|/||}}{A^{|/||}}\right)\right|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} : [\boldsymbol{\mathcal{F}} - \boldsymbol{\mathcal{I}}] - 1\,. \tag{4.20}$$

Since the problem is confined to a purely two-dimensional space, it follows that the area stretch is identical to the *Jacobian* of $\boldsymbol{\mathcal{F}}$, defined as $J = \mathrm{Det}\,\boldsymbol{\mathcal{F}}$, with

$J = \dfrac{a^{\mathrm{I}/\mathrm{II}}}{A^{\mathrm{I}/\mathrm{II}}}$. Inserting this expression into Eq. (4.20) yields

$$\begin{aligned} \mathit{Lin}\ \frac{a^{\mathrm{I}/\mathrm{II}}}{A^{\mathrm{I}/\mathrm{II}}} - 1 &= \mathit{Lin}\ J - 1 \\ &= \frac{a^{\mathrm{I}/\mathrm{II}}}{A^{\mathrm{I}/\mathrm{II}}}\bigg|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} + \frac{\partial J}{\partial \boldsymbol{\mathcal{F}}}\bigg|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} : \left[\boldsymbol{\mathcal{F}} - \boldsymbol{\mathcal{I}}\right] - 1\,, \end{aligned} \tag{4.21}$$

with the first term reducing to 1 as

$$\begin{aligned} \frac{a^{\mathrm{I}/\mathrm{II}}}{A^{\mathrm{I}/\mathrm{II}}}\bigg|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} &= \frac{\left\| \left[\boldsymbol{\mathcal{F}} \cdot \boldsymbol{\Xi}^{\mathrm{I}}\right] \times \left[\boldsymbol{\mathcal{F}} \cdot \boldsymbol{\Xi}^{\mathrm{II}}\right] \right\|}{\|\boldsymbol{\Xi}^{\mathrm{I}} \times \boldsymbol{\Xi}^{\mathrm{II}}\|}\bigg|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} \\ &= \frac{\left\| \left[\boldsymbol{\mathcal{I}} \cdot \boldsymbol{\Xi}^{\mathrm{I}}\right] \times \left[\boldsymbol{\mathcal{I}} \cdot \boldsymbol{\Xi}^{\mathrm{II}}\right] \right\|}{\|\boldsymbol{\Xi}^{\mathrm{I}} \times \boldsymbol{\Xi}^{\mathrm{II}}\|} = \frac{A^{\mathrm{I}/\mathrm{II}}}{A^{\mathrm{I}/\mathrm{II}}} = 1\,. \end{aligned} \tag{4.22}$$

It follows that

$$\frac{\partial J}{\partial \boldsymbol{\mathcal{F}}} = J \boldsymbol{\mathcal{F}}^{-\mathrm{T}} \qquad \Rightarrow \qquad \frac{\partial J}{\partial \boldsymbol{\mathcal{F}}}\bigg|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} = \boldsymbol{\mathcal{I}}. \tag{4.23}$$

Thus we are left with

$$\mathit{Lin}\, \varepsilon_a = \boldsymbol{\mathcal{I}} : \left[\boldsymbol{\mathcal{F}} - \boldsymbol{\mathcal{I}}\right] \qquad \text{with} \qquad \boldsymbol{\mathcal{I}} : \boldsymbol{\mathcal{I}} = 2\,, \tag{4.24}$$

that is

$$\boxed{\mathit{Lin}\, \varepsilon_a = \boldsymbol{\mathcal{I}} : \boldsymbol{\mathcal{F}} - 2} \tag{4.25}$$

4.2 Linearization of strains in 3D

In this section, $\boldsymbol{\mathcal{F}}$ and $\boldsymbol{\mathcal{I}}$ stand for $\boldsymbol{\mathcal{F}}_{\mathrm{3D}}$ and $\boldsymbol{\mathcal{I}}_{\mathrm{3D}}$, but the subscripts are ommited for the sake of brevity.

4.2.1 Length strain ε_l

In order to linearize the length strain, we begin with the equation

$$\mathcal{L}in\ \varepsilon_l = \mathcal{L}in\ \frac{l}{L} - 1 = \frac{l}{L}\bigg|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} + \frac{\partial}{\partial \boldsymbol{\mathcal{F}}}\left(\frac{l}{L}\right)\bigg|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} : \left[\boldsymbol{\mathcal{F}} - \boldsymbol{\mathcal{I}}\right] - 1\,. \tag{4.26}$$

The first term reduces to 1 as

$$\frac{l}{L}\bigg|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} = \frac{\xi^{|}}{\Xi^{|}}\bigg|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} = \frac{|\boldsymbol{\mathcal{F}}\cdot\boldsymbol{\Xi}^{|}|}{\Xi^{|}}\bigg|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} = \frac{|\boldsymbol{\mathcal{I}}\cdot\boldsymbol{\Xi}^{|}|}{\Xi^{|}} = \frac{\Xi^{|}}{\Xi^{|}} = 1\,. \tag{4.27}$$

Moving on to the second term, we define the mapping between the vectors $\boldsymbol{\Xi}^{|}$ and $\boldsymbol{\xi}^{|}$ as $\boldsymbol{\xi}^{|} = \boldsymbol{\mathcal{F}}^{|}\cdot\boldsymbol{\Xi}^{|}$, with $\boldsymbol{\mathcal{F}}^{|} = \boldsymbol{\mathcal{F}}\cdot\boldsymbol{\mathcal{I}}^{|}$, where $\boldsymbol{\mathcal{I}}^{|} = \hat{\boldsymbol{\Xi}}^{|}\otimes\hat{\boldsymbol{\Xi}}^{|}$ is a rank-deficient identity with $\hat{\boldsymbol{\Xi}}^{|}$ the unit vector along the direction of $\boldsymbol{\Xi}^{|}$. *Note, the identity $\boldsymbol{\mathcal{I}}^{|}$ is different from the one introduced in Section 4.1, as the previous one was in 2D, and the current one is in 3D. They are however denoted with the same notation as they are conceptually identical, they both project their respective $\boldsymbol{\mathcal{F}}$'s onto the bond direction, producing an $\boldsymbol{\mathcal{F}}^{|}$ that maps lengths.* Next, the *Jacobian* $J^{|}$ is defined as $J^{|} := \mathrm{Det}^{|}\,\boldsymbol{\mathcal{F}}^{|}$. Note that $\boldsymbol{\mathcal{F}}^{|}$ is a rank-deficient tensor and therefore its determinant operator is not a standard one and requires a special treatment. In this particular case we define $\mathrm{Det}^{|}\,\boldsymbol{\mathcal{F}}^{|} := |\boldsymbol{\mathcal{F}}^{|}\cdot\boldsymbol{\Xi}^{|}|/|\boldsymbol{\Xi}^{|}| = \xi^{|}/\Xi^{|}$. Inserting this expression into Eq. (4.26) yields

$$\mathcal{L}in\ \frac{l}{L} - 1 = \mathcal{L}in\ \frac{\xi^{|}}{\Xi^{|}} - 1 = \mathcal{L}in\ J^{|} - 1 = \frac{\partial J^{|}}{\partial \boldsymbol{\mathcal{F}}}\bigg|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} : \left[\boldsymbol{\mathcal{F}} - \boldsymbol{\mathcal{I}}\right], \tag{4.28}$$

where

$$\frac{\partial J^{|}}{\partial \boldsymbol{\mathcal{F}}} = \frac{\partial J^{|}}{\partial \boldsymbol{\mathcal{F}}^{|}} : \frac{\partial \boldsymbol{\mathcal{F}}^{|}}{\partial \boldsymbol{\mathcal{F}}} = J^{|}\,\boldsymbol{\mathcal{F}}^{|\text{-T}} : \mathbb{I}^{|} = J^{|}\,\boldsymbol{\mathcal{F}}^{|\text{-T}}, \tag{4.29}$$

with $\mathbb{I}^{|} = \boldsymbol{\mathcal{I}}\,\overline{\otimes}\,\boldsymbol{\mathcal{I}}^{|}$. Again, we emphasize that $\boldsymbol{\mathcal{F}}^{|}$ is rank-deficient and its inverse $\boldsymbol{\mathcal{F}}^{|\text{-1}}$ is obtained in a non-standard manner [33] such that $\boldsymbol{\mathcal{F}}^{|\text{-1}}\cdot\boldsymbol{\mathcal{F}}^{|} = \boldsymbol{\mathcal{I}}^{|}$ holds.

Since at $\boldsymbol{\mathcal{F}} = \boldsymbol{\mathcal{I}}$, $J^{|} = 1$ and $\boldsymbol{\mathcal{F}}^{|\text{-T}} = \boldsymbol{\mathcal{I}}^{|}$, we are left with

$$\left.\frac{\partial J^{|}}{\partial \boldsymbol{\mathcal{F}}}\right|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} = \boldsymbol{\mathcal{I}}^{|}\,, \tag{4.30}$$

and therefore

$$\mathit{Lin}\ \varepsilon_l = \boldsymbol{\mathcal{I}}^{|} : \left[\boldsymbol{\mathcal{F}} - \boldsymbol{\mathcal{I}}\right]. \tag{4.31}$$

Lastly, inserting the relation

$$\boldsymbol{\mathcal{I}}^{|} : \boldsymbol{\mathcal{I}} = \left[\hat{\boldsymbol{\Xi}}^{|} \otimes \hat{\boldsymbol{\Xi}}^{|}\right] : \boldsymbol{\mathcal{I}} = \hat{\boldsymbol{\Xi}} \cdot \boldsymbol{\mathcal{I}} \cdot \hat{\boldsymbol{\Xi}} = 1\,, \tag{4.32}$$

yields

$$\boxed{\mathit{Lin}\ \varepsilon_l = \boldsymbol{\mathcal{I}}^{|} : \boldsymbol{\mathcal{F}} - 1} \tag{4.33}$$

which shall be compared with Eq. (4.18), its counterpart in 2D.

4.2.2 Area strain ε_a

To linearize the area strain, we begin with the equation

$$\mathit{Lin}\ \varepsilon_a = \mathit{Lin}\ \frac{a}{A} - 1 = \left.\frac{a}{A}\right|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} + \left.\frac{\partial}{\partial \boldsymbol{\mathcal{F}}}\left(\frac{a}{A}\right)\right|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} : \left[\boldsymbol{\mathcal{F}} - \boldsymbol{\mathcal{I}}\right] - 1\,. \tag{4.34}$$

Similar to the linearization of the length strain, we define the mapping between $a^{|/|\!|}$ and $A^{|/|\!|}$. To do so, we introduce the rank-deficient identity $\boldsymbol{\mathcal{I}}^{|/|\!|}$ defined as

$$\boldsymbol{\mathcal{I}}^{|/|\!|} = \boldsymbol{\mathcal{I}} - \hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}} \qquad , \qquad \hat{\boldsymbol{N}} = \frac{\boldsymbol{\Xi}^{|} \times \boldsymbol{\Xi}^{|\!|}}{\left|\boldsymbol{\Xi}^{|} \times \boldsymbol{\Xi}^{|\!|}\right|} = \frac{\hat{\boldsymbol{\Xi}}^{|} \times \hat{\boldsymbol{\Xi}}^{|\!|}}{\left|\hat{\boldsymbol{\Xi}}^{|} \times \hat{\boldsymbol{\Xi}}^{|\!|}\right|}\,. \tag{4.35}$$

The *surface Jacobian* $J^{|/||} := \mathrm{Det}^{|/||}\,\boldsymbol{\mathcal{F}}^{|/||}$ is defined as the determinant of $\boldsymbol{\mathcal{F}}^{|/||} = \boldsymbol{\mathcal{F}} \cdot \boldsymbol{\mathcal{I}}^{|/||}$. Again, the determinant is not standard but can be defined by

$$\mathrm{Det}^{|/||}\,\boldsymbol{\mathcal{F}}^{|/||} := \frac{|[\boldsymbol{\mathcal{F}}^{|/||} \cdot \boldsymbol{\Xi}^{|}] \times [\boldsymbol{\mathcal{F}}^{|/||} \cdot \boldsymbol{\Xi}^{||}]|}{|\boldsymbol{\Xi}^{|} \times \boldsymbol{\Xi}^{||}|} = \frac{a^{|/||}}{A^{|/||}}\,, \tag{4.36}$$

which is indeed a mapping between $a^{|/||}$ and $A^{|/||}$. Inserting this expression into Eq. (4.34) yields

$$\begin{aligned} \mathit{Lin}\ \varepsilon_a &= \mathit{Lin}\ J^{|/||} - 1 \\ &= \left.\frac{a^{|/||}}{A^{|/||}}\right|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} + \left.\frac{\partial J^{|/||}}{\partial \boldsymbol{\mathcal{F}}}\right|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} : \left[\boldsymbol{\mathcal{F}} - \boldsymbol{\mathcal{I}}\right] - 1\,, \end{aligned} \tag{4.37}$$

which, since $a^{|/||}|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} = A^{|/||}$, can be immediately expressed as

$$\mathit{Lin}\,\varepsilon_a = \left.\frac{\partial J^{|/||}}{\partial \boldsymbol{\mathcal{F}}}\right|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} : \left[\boldsymbol{\mathcal{F}} - \boldsymbol{\mathcal{I}}\right]. \tag{4.38}$$

Using the properties of superficial rank-deficient tensors [33], we have

$$\frac{\partial J^{|/||}}{\partial \boldsymbol{\mathcal{F}}} = J^{|/||}\,\boldsymbol{\mathcal{F}}^{|/||\text{-T}} \qquad \Rightarrow \qquad \left.\frac{\partial J^{|/||}}{\partial \boldsymbol{\mathcal{F}}}\right|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} = \boldsymbol{\mathcal{I}}^{|/||}\,. \tag{4.39}$$

Thus we are left with

$$\mathit{Lin}\,\varepsilon_a = \boldsymbol{\mathcal{I}}^{|/||} : \left[\boldsymbol{\mathcal{F}} - \boldsymbol{\mathcal{I}}\right], \tag{4.40}$$

wherein employing the relation

$$\boldsymbol{\mathcal{I}}^{|/||} : \boldsymbol{\mathcal{I}} = \boldsymbol{\mathcal{I}} : \boldsymbol{\mathcal{I}} - \boldsymbol{\mathcal{I}} : \left[\hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}}\right] = 3 - \hat{\boldsymbol{N}} \cdot \boldsymbol{\mathcal{I}} \cdot \hat{\boldsymbol{N}} = 2\,, \tag{4.41}$$

results in

$$\boxed{\mathit{Lin}\,\varepsilon_a = \boldsymbol{\mathcal{I}}^{|/||} : \boldsymbol{\mathcal{F}} - 2} \tag{4.42}$$

4.2.3 Volume strain ε_v

To linearize the volume strain, we begin with the equation

$$\mathit{Lin}\ \varepsilon_v = \mathit{Lin}\ \frac{v}{V} - 1 = \frac{v}{V}\bigg|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} + \frac{\partial}{\partial \boldsymbol{\mathcal{F}}}\left(\frac{v}{V}\right)\bigg|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} : [\boldsymbol{\mathcal{F}} - \boldsymbol{\mathcal{I}}] - 1\,. \tag{4.43}$$

It follows that the volume stretch is identical to the *Jacobian* of $\boldsymbol{\mathcal{F}}$.

$$J = \frac{v}{V} \qquad \Rightarrow \qquad J := \mathrm{Det}\,\boldsymbol{\mathcal{F}}\,. \tag{4.44}$$

Inserting this expression into Eq. (4.43) yields

$$\mathit{Lin}\ \frac{v}{V} - 1 = \mathit{Lin}\ J - 1 = \frac{v}{V}\bigg|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} + \frac{\partial J}{\partial \boldsymbol{\mathcal{F}}}\bigg|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} : \big[\boldsymbol{\mathcal{F}} - \boldsymbol{\mathcal{I}}\big] - 1\,, \tag{4.45}$$

with the first term reducing to 1 as

$$\frac{v}{V}\bigg|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} = \frac{\Big|\big[\boldsymbol{\mathcal{F}}\cdot\boldsymbol{\Xi}^{\mathrm{I}}\big]\cdot\Big[\big[\boldsymbol{\mathcal{F}}\cdot\boldsymbol{\Xi}^{\mathrm{II}}\big]\times\big[\boldsymbol{\mathcal{F}}\cdot\boldsymbol{\Xi}^{\mathrm{III}}\big]\Big]\Big|}{\big|\boldsymbol{\Xi}^{\mathrm{I}}\cdot[\boldsymbol{\Xi}^{\mathrm{II}}\times\boldsymbol{\Xi}^{\mathrm{III}}]\big|}\bigg|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} = \frac{V}{V} = 1\,. \tag{4.46}$$

It follows that

$$\frac{\partial J}{\partial \boldsymbol{\mathcal{F}}} = J\boldsymbol{\mathcal{F}}^{-\mathrm{T}} \qquad \Rightarrow \qquad \frac{\partial J}{\partial \boldsymbol{\mathcal{F}}}\bigg|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} = \boldsymbol{\mathcal{I}}. \tag{4.47}$$

Thus we are left with

$$\mathit{Lin}\ \varepsilon_v = \boldsymbol{\mathcal{I}} : \big[\boldsymbol{\mathcal{F}} - \boldsymbol{\mathcal{I}}\big] \qquad \text{with} \qquad \boldsymbol{\mathcal{I}} : \boldsymbol{\mathcal{I}} = 3\,, \tag{4.48}$$

or

$$\boxed{\mathit{Lin}\ \varepsilon_v = \boldsymbol{\mathcal{I}} : \boldsymbol{\mathcal{F}} - 3} \tag{4.49}$$

Table 4.1: The unification of the linearized strains of CPD.

$\mathcal{L}in\ \varepsilon_l$	$=$	$\left.\dfrac{\partial J^{\mid}}{\partial \boldsymbol{\mathcal{F}}}\right\vert_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} : \left[\boldsymbol{\mathcal{F}}-\boldsymbol{\mathcal{I}}\right]$	$=$	$\boldsymbol{\mathcal{I}}^{\mid} : \left[\boldsymbol{\mathcal{F}}-\boldsymbol{\mathcal{I}}\right]$	$=$	$\boldsymbol{\mathcal{I}}^{\mid} : \boldsymbol{\mathcal{F}} - 1$
$\mathcal{L}in\ \varepsilon_a$	$=$	$\left.\dfrac{\partial J^{\mid/\!/}}{\partial \boldsymbol{\mathcal{F}}}\right\vert_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} : \left[\boldsymbol{\mathcal{F}}-\boldsymbol{\mathcal{I}}\right]$	$=$	$\boldsymbol{\mathcal{I}}^{\mid/\!/} : \left[\boldsymbol{\mathcal{F}}-\boldsymbol{\mathcal{I}}\right]$	$=$	$\boldsymbol{\mathcal{I}}^{\mid/\!/} : \boldsymbol{\mathcal{F}} - 2$
$\mathcal{L}in\ \varepsilon_v$	$=$	$\left.\dfrac{\partial J^{\mid/\!/\,/\!/\!/}}{\partial \boldsymbol{\mathcal{F}}}\right\vert_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} : \left[\boldsymbol{\mathcal{F}}-\boldsymbol{\mathcal{I}}\right]$	$=$	$\boldsymbol{\mathcal{I}}^{\mid/\!/\,/\!/\!/} : \left[\boldsymbol{\mathcal{F}}-\boldsymbol{\mathcal{I}}\right]$	$=$	$\boldsymbol{\mathcal{I}}^{\mid/\!/\,/\!/\!/} : \boldsymbol{\mathcal{F}} - 3$
$\mathcal{L}in\ \varepsilon_{\{\bullet\}}$	$=$	$\left.\dfrac{\partial J^{\{\bullet\}}}{\partial \boldsymbol{\mathcal{F}}}\right\vert_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} : \left[\boldsymbol{\mathcal{F}}-\boldsymbol{\mathcal{I}}\right]$	$=$	$\boldsymbol{\mathcal{I}}^{\{\bullet\}} : \left[\boldsymbol{\mathcal{F}}-\boldsymbol{\mathcal{I}}\right]$	,	$J^{\{\bullet\}} := \mathrm{Det}^{\,\{\bullet\}}\boldsymbol{\mathcal{F}}^{\{\bullet\}}$ $\boldsymbol{\mathcal{F}}^{\{\bullet\}} := \boldsymbol{\mathcal{F}}\cdot\boldsymbol{\mathcal{I}}^{\{\bullet\}}$

Remark on the linearized strain measures of CPD *The linearized strains of CPD, (4.18), (4.25), (4.33), (4.42) and (4.49) can be written in the unified format given in Table 4.1. Here,* $\boldsymbol{\mathcal{I}}^{\mid}$ *and* $\boldsymbol{\mathcal{I}}^{\mid/\!/}$ *are essentially "projection onto bond direction" and "projection onto bonds plane" respectively. Written in 2D and 3D space, they are*

$$\mathcal{L}in\ \varepsilon_l = \boldsymbol{\mathcal{I}}^{\mid} : \left[\boldsymbol{\mathcal{F}}-\boldsymbol{\mathcal{I}}\right] \quad \begin{cases} \text{2D}: \ \boldsymbol{\mathcal{I}}^{\mid} := \hat{\boldsymbol{\Xi}}^{\mid} \otimes \hat{\boldsymbol{\Xi}}^{\mid}, \quad \boldsymbol{\mathcal{F}} = \boldsymbol{\mathcal{F}}_{\text{2D}}, \quad \boldsymbol{\mathcal{I}} = \boldsymbol{\mathcal{I}}_{\text{2D}}, \\ \text{3D}: \ \boldsymbol{\mathcal{I}}^{\mid} := \hat{\boldsymbol{\Xi}}^{\mid} \otimes \hat{\boldsymbol{\Xi}}^{\mid}, \quad \boldsymbol{\mathcal{F}} = \boldsymbol{\mathcal{F}}_{\text{3D}}, \quad \boldsymbol{\mathcal{I}} = \boldsymbol{\mathcal{I}}_{\text{3D}}, \end{cases} \tag{4.50}$$

$$\mathcal{L}in\ \varepsilon_a = \boldsymbol{\mathcal{I}}^{\mid/\!/} : \left[\boldsymbol{\mathcal{F}}-\boldsymbol{\mathcal{I}}\right] \quad \begin{cases} \text{2D}: \ \boldsymbol{\mathcal{I}}^{\mid/\!/} := \boldsymbol{\mathcal{I}}_{\text{2D}}, \quad \boldsymbol{\mathcal{F}} = \boldsymbol{\mathcal{F}}_{\text{2D}}, \quad \boldsymbol{\mathcal{I}} = \boldsymbol{\mathcal{I}}_{\text{2D}}, \\ \text{3D}: \ \boldsymbol{\mathcal{I}}_{\text{3D}} := \boldsymbol{\mathcal{I}}_{\text{3D}} - \hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}}, \quad \boldsymbol{\mathcal{F}} = \boldsymbol{\mathcal{F}}_{\text{3D}}, \quad \boldsymbol{\mathcal{I}} = \boldsymbol{\mathcal{I}}_{\text{3D}}, \end{cases}$$

$$\mathcal{L}in\ \varepsilon_v = \boldsymbol{\mathcal{I}}^{\mid/\!/\,/\!/\!/} : \left[\boldsymbol{\mathcal{F}}-\boldsymbol{\mathcal{I}}\right], \qquad \boldsymbol{\mathcal{I}}^{\mid/\!/\,/\!/\!/} := \boldsymbol{\mathcal{I}}_{\text{3D}}, \qquad \boldsymbol{\mathcal{F}} = \boldsymbol{\mathcal{F}}_{\text{3D}}, \qquad \boldsymbol{\mathcal{I}} = \boldsymbol{\mathcal{I}}_{\text{3D}}.$$

In this unifying sense one can think of the identity tensor $\boldsymbol{\mathcal{I}}^{\mid/\!/\,/\!/\!/} := \boldsymbol{\mathcal{I}}$ *as a volume projection. This unification has two crucial consequences. Firstly, due to the symmetric projections* $\boldsymbol{\mathcal{I}}^{\mid}$, $\boldsymbol{\mathcal{I}}^{\mid/\!/}$ *and* $\boldsymbol{\mathcal{I}}^{\mid/\!/\,/\!/\!/}$, *and trace-like operators, only the symmetric part of* $\boldsymbol{\mathcal{F}}$ *enters the energy of CPD in this linearized framework, which is expected to have a meaningful comparison to classical small-strain linear elasticity. This first consequence is an outcome of choosing objective deformation measures for the arguments of CPD energy densities. Secondly, the unifying*

relationships clearly demonstrate that, after integration, the resulting energy density of isotropic, harmonic CPD will depend on the trace-like functions of $\boldsymbol{\mathcal{F}}$, for an affine deformation. This conclusion is unlike what one may guess intuitively, that each interaction type corresponds to an entirely independent function of $\boldsymbol{\mathcal{F}}$ that maps either length, area or volume change. Admittedly, this intuition would indeed hold for (i) non-affine deformations, and (ii) before the integration of the energy densities over the horizon. Nonetheless, in the framework of linear-elastic and isotropic CPD, the strain energy becomes a function of only two linearly independent functions of $\boldsymbol{\mathcal{F}}$, as we will see later in Sections 4.5.1 and 4.5.2. □

4.3 Integration of the energy densities in 2D

Equipped with the linearized strains, the next goal is to integrate them over their horizons to arrive at the point-wise energy densities. We begin the analysis for the 2D case with one-neighbor interactions.

Remark on the operations on $\boldsymbol{\mathcal{F}}_{2D}$ and $\boldsymbol{\mathcal{F}}_{3D}$ *In this section, and in Section 4.4, due to the linearization of the strains in the previous steps, the deformation gradients $\boldsymbol{\mathcal{F}}_{2D}$ and $\boldsymbol{\mathcal{F}}_{3D}$ reside in the linear setting, where the distinction between the material and the spatial configuration disappears. Therefore any operations on $\boldsymbol{\mathcal{F}}$ are admissible, regardless of the configurations of the partaking tensors. For instance, the operation $\boldsymbol{\mathcal{F}} : [\hat{\boldsymbol{\Xi}} \otimes \hat{\boldsymbol{\Xi}}]$ would normally be prohibited in the large deformation setting, as $\boldsymbol{\mathcal{F}}$ is a two-point tensor, while $\hat{\boldsymbol{\Xi}} \otimes \hat{\boldsymbol{\Xi}}$ lives purely in the material configuration. However, in the linear framework any similar operation is perfectly valid.*

4.3.1 One-neighbor interactions

To get the point-wise energy density due to one-neighbor interactions Ψ_1, we integrate the harmonic potential ψ_1 over the horizon,

$$\Psi_1 = \int_{\mathcal{H}_0} \psi_1 \, \mathrm{d}A^{\shortmid} \qquad \text{where} \qquad \psi_1 := \frac{1}{2} C_1 \, L \, [\mathcal{L}in \, \varepsilon_l]^2 \, . \tag{4.51}$$

Inserting the linearized length strain $\mathcal{L}in \, \varepsilon_l$ previously derived in Eq. (4.18) gives

$$\begin{aligned} \Psi_1 &= \int_{\mathcal{H}_0} \frac{1}{2} C_1 \, L \left[\boldsymbol{\mathcal{I}}^{\shortmid} : \boldsymbol{\mathcal{F}} - 1 \right]^2 \mathrm{d}A^{\shortmid} \, , \\ &= \int_{\hat{\mathcal{H}}_0{}^{\shortmid}} \int_{\Xi^{\shortmid}=0}^{\Xi^{\shortmid}=\delta} \frac{1}{2} C_1 \, L \left[\boldsymbol{\mathcal{I}}^{\shortmid} : \boldsymbol{\mathcal{F}} - 1 \right]^2 \Xi^{\shortmid} \, \mathrm{d}\Xi^{\shortmid} \, \mathrm{d}\hat{A}^{\shortmid} \, . \end{aligned} \tag{4.52}$$

Since $L := |\boldsymbol{\Xi}^{\shortmid}| = \Xi^{\shortmid}$, and $\boldsymbol{\mathcal{I}}^{\shortmid}$ is only a function of $\hat{\boldsymbol{\Xi}}^{\shortmid}$, the nested integrals can be separated into two as follows

$$\Psi_1 = \frac{1}{2} C_1 \int_{\Xi^{\shortmid}=0}^{\Xi^{\shortmid}=\delta} {\Xi^{\shortmid}}^2 \, \mathrm{d}\Xi^{\shortmid} \int_{\hat{\mathcal{H}}_0{}^{\shortmid}} \left[\boldsymbol{\mathcal{I}}^{\shortmid} : \boldsymbol{\mathcal{F}} - 1 \right]^2 \mathrm{d}\hat{A}^{\shortmid} \, , \tag{4.53}$$

and integrating over $\Xi^{\shortmid}$ yields

$$\Psi_1 = \frac{1}{6} C_1 \, \delta^3 \int_{\hat{\mathcal{H}}_0{}^{\shortmid}} \left[\boldsymbol{\mathcal{I}}^{\shortmid} : \boldsymbol{\mathcal{F}} - 1 \right]^2 \mathrm{d}\hat{A}^{\shortmid} \, . \tag{4.54}$$

Next, we expand the integral over $\hat{\mathcal{H}}_0{}^{\shortmid}$,

$$\int_{\hat{\mathcal{H}}_0{}^{\shortmid}} \left[\boldsymbol{\mathcal{I}}^{\shortmid} : \boldsymbol{\mathcal{F}} - 1 \right]^2 \mathrm{d}\hat{A}^{\shortmid} = \alpha + \beta + \gamma \, , \tag{4.55}$$

where

$$\alpha := \int_{\hat{\mathcal{H}}_0{}^{\shortmid}} \left[\boldsymbol{\mathcal{I}}^{\shortmid} : \boldsymbol{\mathcal{F}} \right]^2 \mathrm{d}\hat{A}^{\shortmid} \, , \quad \beta := -2 \int_{\hat{\mathcal{H}}_0{}^{\shortmid}} \boldsymbol{\mathcal{I}}^{\shortmid} : \boldsymbol{\mathcal{F}} \, \mathrm{d}\hat{A}^{\shortmid} \, , \quad \gamma := \int_{\hat{\mathcal{H}}_0{}^{\shortmid}} 1 \, \mathrm{d}\hat{A}^{\shortmid} \, . \tag{4.56}$$

To be able to evaluate α, $\boldsymbol{\mathcal{F}}$ should be extracted from the integral by utilizing the relation

$$\left[\boldsymbol{\mathcal{I}}^{|} : \boldsymbol{\mathcal{F}}\right]^2 = [\boldsymbol{\mathcal{F}} \otimes \boldsymbol{\mathcal{F}}] :: \left[\boldsymbol{\mathcal{I}}^{|} \otimes \boldsymbol{\mathcal{I}}^{|}\right] = [\boldsymbol{\mathcal{F}} \otimes \boldsymbol{\mathcal{F}}] :: \left[\hat{\boldsymbol{\Xi}} \otimes \hat{\boldsymbol{\Xi}} \otimes \hat{\boldsymbol{\Xi}} \otimes \hat{\boldsymbol{\Xi}}\right] , \quad (4.57)$$

such that

$$\alpha = [\boldsymbol{\mathcal{F}} \otimes \boldsymbol{\mathcal{F}}] :: \int_{\hat{\mathcal{H}}_0{}^{|}} \left[\hat{\boldsymbol{\Xi}} \otimes \hat{\boldsymbol{\Xi}} \otimes \hat{\boldsymbol{\Xi}} \otimes \hat{\boldsymbol{\Xi}}\right] \mathrm{d}\hat{A}^{|} . \quad (4.58)$$

Lastly, invoking Lemma 7 yields

$$\alpha = \frac{1}{4}\pi \, [\boldsymbol{\mathcal{F}} \otimes \boldsymbol{\mathcal{F}}] :: \mathbb{I} = \frac{1}{4}\pi \left[\boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{F}} + \boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{F}}^{\mathrm{T}} + [\boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{I}}]^2\right] . \quad (4.59)$$

Moving onto β, taking $\boldsymbol{\mathcal{F}}$ outside

$$\beta = -2\,\boldsymbol{\mathcal{F}} : \int_{\hat{\mathcal{H}}_0{}^{|}} \hat{\boldsymbol{\Xi}} \otimes \hat{\boldsymbol{\Xi}} \, \mathrm{d}\hat{A}^{|} , \quad (4.60)$$

and invoking Lemma 5 yields

$$\beta = -2\pi\, \boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{I}} . \quad (4.61)$$

Finally, by using Lemma 1, we are left with

$$\gamma := \int_{\hat{\mathcal{H}}_0{}^{|}} 1 \, \mathrm{d}\hat{A}^{|} = 2\pi . \quad (4.62)$$

Equipped with α, β and γ, after some mathematical steps, we can write Ψ_1 as

$$\boxed{\Psi_1 = \frac{1}{24}\pi\, C_1\, \delta^3 \Big[\boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{F}} + \boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{F}}^{\mathrm{T}} + [\boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{I}}]^2 - 8\,\boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{I}} + 8\Big]} \quad (4.63)$$

4.3.2 Two-neighbor interactions

The point-wise energy density due to two-neighbor interactions Ψ_2 is the double integral the harmonic potential ψ_2 over the horizon,

$$\Psi_2 = \int_{\mathcal{H}_0}\int_{\mathcal{H}_0} \psi_2 \, \mathrm{d}A^{\mathrm{I}} \, \mathrm{d}A^{\mathrm{II}} \qquad \text{where} \qquad \psi_2 := \frac{1}{2} C_2 \, A \, [\mathit{Lin}\, \varepsilon_a]^2 \, . \tag{4.64}$$

Inserting the linearized area strain $\mathit{Lin}\, \varepsilon_a$ previously derived in Eq. (4.25) gives

$$\begin{aligned} \Psi_2 &= \int_{\mathcal{H}_0}\int_{\mathcal{H}_0} \frac{1}{2} C_2 \, A \, [\boldsymbol{\mathcal{I}} : \boldsymbol{\mathcal{F}} - 2]^2 \, \mathrm{d}A^{\mathrm{I}} \, \mathrm{d}A^{\mathrm{II}} \, , \\ &= \int_{\hat{\mathcal{H}}_0{}^{\mathrm{II}}} \int_{\Xi^{\mathrm{II}}=0}^{\Xi^{\mathrm{II}}=\delta} \int_{\hat{\mathcal{H}}_0{}^{\mathrm{I}}} \int_{\Xi^{\mathrm{I}}=0}^{\Xi^{\mathrm{I}}=\delta} \frac{1}{2} C_2 \, A \, [\boldsymbol{\mathcal{I}} : \boldsymbol{\mathcal{F}} - 2]^2 \, \Xi^{\mathrm{I}} \, \Xi^{\mathrm{II}} \, \mathrm{d}\Xi^{\mathrm{I}} \, \mathrm{d}\hat{A}^{\mathrm{I}} \, \mathrm{d}\Xi^{\mathrm{II}} \, \mathrm{d}\hat{A}^{\mathrm{II}} \, . \end{aligned} \tag{4.65}$$

Here, $A := |\boldsymbol{\Xi}^{\mathrm{I}} \times \boldsymbol{\Xi}^{\mathrm{II}}|$, which can also be written as $A = |\boldsymbol{\Xi}^{\mathrm{I}}||\boldsymbol{\Xi}^{\mathrm{II}}||\hat{\boldsymbol{\Xi}}^{\mathrm{I}} \times \hat{\boldsymbol{\Xi}}^{\mathrm{II}}|$, allowing us to isolate the integrals as follows

$$\begin{aligned} \Psi_2 = \frac{1}{2} C_2 \, [\boldsymbol{\mathcal{I}} : \boldsymbol{\mathcal{F}} - 2]^2 \int_{\Xi^{\mathrm{II}}=0}^{\Xi^{\mathrm{II}}=\delta} {\Xi^{\mathrm{II}}}^2 \, \mathrm{d}\Xi^{\mathrm{II}} \\ \times \int_{\Xi^{\mathrm{I}}=0}^{\Xi^{\mathrm{I}}=\delta} {\Xi^{\mathrm{I}}}^2 \, \mathrm{d}\Xi^{\mathrm{I}} \int_{\hat{\mathcal{H}}_0{}^{\mathrm{II}}} \int_{\hat{\mathcal{H}}_0{}^{\mathrm{I}}} |\hat{\boldsymbol{\Xi}}^{\mathrm{I}} \times \hat{\boldsymbol{\Xi}}^{\mathrm{II}}| \, \mathrm{d}\hat{A}^{\mathrm{I}} \, \mathrm{d}\hat{A}^{\mathrm{II}} \, , \end{aligned} \tag{4.66}$$

and integrating over Ξ^{I} and Ξ^{II} yields

$$\Psi_2 = \frac{1}{18} C_2 \, \delta^6 \, [\boldsymbol{\mathcal{I}} : \boldsymbol{\mathcal{F}} - 2]^2 \int_{\hat{\mathcal{H}}_0{}^{\mathrm{II}}} \int_{\hat{\mathcal{H}}_0{}^{\mathrm{I}}} |\hat{\boldsymbol{\Xi}}^{\mathrm{I}} \times \hat{\boldsymbol{\Xi}}^{\mathrm{II}}| \, \mathrm{d}\hat{A}^{\mathrm{I}} \, \mathrm{d}\hat{A}^{\mathrm{II}} \, . \tag{4.67}$$

Lastly, invoking Lemma 3 gives

$$\boxed{\Psi_2 = \frac{4}{9} \pi \, C_2 \, \delta^6 \, [\boldsymbol{\mathcal{I}} : \boldsymbol{\mathcal{F}} - 2]^2} \tag{4.68}$$

4.3.3 Total point-wise energy density

Recalling from Eq.(2.24) that the total energy density of harmonic CPD in 2D is

$$\Psi_{\mathrm{H}}^{\mathrm{2D}} := \frac{1}{2}\,\Psi_1 + \frac{1}{3}\,\Psi_2\,, \tag{4.69}$$

and using the results of Eq.(4.63) and Eq.(4.68) renders

$$\boxed{\begin{aligned}\Psi_{\mathrm{H}}^{\mathrm{2D}} = \frac{\pi}{48}C_1\delta^3\Big[\boldsymbol{\mathcal{F}} : \big[\boldsymbol{\mathcal{F}} + \boldsymbol{\mathcal{F}}^{\mathrm{T}}\big]\Big] + \left[\frac{\pi}{48}C_1\delta^3 + \frac{4\pi}{27}C_2\delta^6\right]\big[\boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{I}}\big]^2 \\ + \left[\frac{\pi}{6}C_1\delta^3 + \frac{16\pi}{27}C_2\delta^6\right]\big[1 - \boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{I}}\big]\end{aligned}} \tag{4.70}$$

4.4 Integration of the energy densities in 3D

In this section, we will repeat the integration process of 2D, now in the 3D setting, accounting for three-neighbor interactions.

4.4.1 One-neighbor interactions

The point-wise energy density due to one-neighbor interactions Ψ_1, is the integral the harmonic potential ψ_1 over the spherical horizon,

$$\Psi_1 = \int_{\mathcal{H}_0} \psi_1 \,\mathrm{d}V^{\shortmid} \qquad \text{where} \qquad \psi_1 := \frac{1}{2}\,C_1\,L\,[\mathit{Lin}\,\varepsilon_l]^2\,. \tag{4.71}$$

Inserting the linearized length strain $\mathit{Lin}\,\varepsilon_l$ previously derived in Eq. (4.33) gives

$$\begin{aligned}\Psi_1 &= \int_{\mathcal{H}_0} \frac{1}{2}\,C_1\,L\left[\boldsymbol{\mathcal{I}}^{\shortmid} : \boldsymbol{\mathcal{F}} - 1\right]^2 \mathrm{d}V^{\shortmid}\,, \\ &= \int_{\hat{\mathcal{H}}_0{}^{\shortmid}} \int_{\Xi^{\shortmid}=0}^{\Xi^{\shortmid}=\delta} \frac{1}{2}\,C_1\,L\left[\boldsymbol{\mathcal{I}}^{\shortmid} : \boldsymbol{\mathcal{F}} - 1\right]^2 \Xi^{\shortmid 2}\mathrm{d}\Xi^{\shortmid}\,\mathrm{d}\hat{V}^{\shortmid}\,.\end{aligned} \tag{4.72}$$

As $\boldsymbol{\mathcal{I}}^{|}$ is only a function of $\hat{\boldsymbol{\Xi}}^{|}$, and $L := |\boldsymbol{\Xi}^{|}| = \Xi^{|}$, the integrals can be separated as follows

$$\Psi_1 = \frac{1}{2}\, C_1 \int_{\Xi^{|}=0}^{\Xi^{|}=\delta} {\Xi^{|}}^3 \, \mathrm{d}\Xi^{|} \int_{\hat{\mathcal{H}}_0{}^{|}} \left[\boldsymbol{\mathcal{I}}^{|} : \boldsymbol{\mathcal{F}} - 1\right]^2 \mathrm{d}\hat{V}^{|} \,, \tag{4.73}$$

and integrating over $\Xi^{|}$ yields

$$\Psi_1 = \frac{1}{8}\, C_1\, \delta^4 \int_{\hat{\mathcal{H}}_0{}^{|}} \left[\boldsymbol{\mathcal{I}}^{|} : \boldsymbol{\mathcal{F}} - 1\right]^2 \mathrm{d}\hat{V}^{|} \,. \tag{4.74}$$

Next, we expand the integral,

$$\int_{\hat{\mathcal{H}}_0{}^{|}} \left[\boldsymbol{\mathcal{I}}^{|} : \boldsymbol{\mathcal{F}} - 1\right]^2 \mathrm{d}\hat{V}^{|} = \alpha + \beta + \gamma \,, \tag{4.75}$$

where

$$\alpha := \int_{\hat{\mathcal{H}}_0{}^{|}} \left[\boldsymbol{\mathcal{I}}^{|} : \boldsymbol{\mathcal{F}}\right]^2 \mathrm{d}\hat{V}^{|} \,, \quad \beta := -2 \int_{\hat{\mathcal{H}}_0{}^{|}} \boldsymbol{\mathcal{I}}^{|} : \boldsymbol{\mathcal{F}} \, \mathrm{d}\hat{V}^{|} \,, \quad \gamma := \int_{\hat{\mathcal{H}}_0{}^{|}} \mathrm{d}\hat{V}^{|} \,. \tag{4.76}$$

To evaluate α, $\boldsymbol{\mathcal{F}}$ is extracted from the integral by utilizing the relation

$$\begin{aligned} \left[\boldsymbol{\mathcal{I}}^{|} : \boldsymbol{\mathcal{F}}\right]^2 &= [\boldsymbol{\mathcal{F}} \otimes \boldsymbol{\mathcal{F}}] :: \left[\boldsymbol{\mathcal{I}}^{|} \otimes \boldsymbol{\mathcal{I}}^{|}\right] \\ &= [\boldsymbol{\mathcal{F}} \otimes \boldsymbol{\mathcal{F}}] :: \left[\hat{\boldsymbol{\Xi}} \otimes \hat{\boldsymbol{\Xi}} \otimes \hat{\boldsymbol{\Xi}} \otimes \hat{\boldsymbol{\Xi}}\right] \,, \end{aligned} \tag{4.77}$$

such that

$$\alpha = [\boldsymbol{\mathcal{F}} \otimes \boldsymbol{\mathcal{F}}] :: \int_{\hat{\mathcal{H}}_0{}^{|}} \left[\hat{\boldsymbol{\Xi}} \otimes \hat{\boldsymbol{\Xi}} \otimes \hat{\boldsymbol{\Xi}} \otimes \hat{\boldsymbol{\Xi}}\right] \mathrm{d}\hat{V}^{|} \,. \tag{4.78}$$

Lastly, invoking Lemma 8 yields

$$\alpha = \frac{4}{15}\pi \, [\boldsymbol{\mathcal{F}} \otimes \boldsymbol{\mathcal{F}}] :: \mathbb{I} = \frac{4}{15}\pi \Big[\boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{F}} + \boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{F}}^{\mathrm{T}} + [\boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{I}}]^2\Big] \,. \tag{4.79}$$

Next, moving onto β and taking $\boldsymbol{\mathcal{F}}$ out of the integral yields

$$\beta = -2\, \boldsymbol{\mathcal{F}} : \int_{\hat{\mathcal{H}}_0{}^{|}} \hat{\boldsymbol{\Xi}} \otimes \hat{\boldsymbol{\Xi}} \, \mathrm{d}\hat{V}^{|} \,, \tag{4.80}$$

which by invoking Lemma 6 becomes

$$\beta = -\frac{8}{3}\pi\, \boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{I}}\,. \tag{4.81}$$

Finally for γ, we use Lemma 2 to get

$$\gamma := \int_{\hat{\mathcal{H}}_0{}^{|}} 1\, \mathrm{d}\hat{V}^{|} = 4\pi\,. \tag{4.82}$$

Now, using equations (4.74), (4.75) and (4.82), we can write Ψ_1 as

$$\Psi_1 = \frac{1}{8}\, C_1\, \delta^4 \left[\alpha + \beta + \gamma\right]\,, \tag{4.83}$$

which is

$$\boxed{\Psi_1 = \frac{1}{30}\pi\, C_1\, \delta^4 \left[\boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{F}} + \boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{F}}^{\mathrm{T}} + [\boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{I}}]^2 - 10\, \boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{I}} + 15\right]} \tag{4.84}$$

4.4.2 Two-neighbor interactions

To derive Ψ_2, we integrate ψ_2 over the horizon twice,

$$\Psi_2 = \int_{\mathcal{H}_0}\int_{\mathcal{H}_0} \psi_2\, \mathrm{d}V^{|}\, \mathrm{d}V^{||} \qquad \text{where} \qquad \psi_2 := \frac{1}{2}\, C_2\, A\, [\mathit{\mathcal{L}in}\, \varepsilon_a]^2\,. \tag{4.85}$$

Plugging in the linearized area strain $\mathit{\mathcal{L}in}\, \varepsilon_a$ from Eq. (4.42), and the relation $A = |\boldsymbol{\Xi}^{|}||\boldsymbol{\Xi}^{||}||\hat{\boldsymbol{\Xi}}^{|} \times \hat{\boldsymbol{\Xi}}^{||}|$ gives

$$\Psi_2 = \int_{\mathcal{H}_0}\int_{\mathcal{H}_0} \frac{1}{2}\, C_2\, |\boldsymbol{\Xi}^{|}||\boldsymbol{\Xi}^{||}||\hat{\boldsymbol{\Xi}}^{|} \times \hat{\boldsymbol{\Xi}}^{||}| \left[\boldsymbol{\mathcal{I}}^{|/||} : \boldsymbol{\mathcal{F}} - 2\right]^2 \mathrm{d}V^{|}\, \mathrm{d}V^{||}\,. \tag{4.86}$$

As $\boldsymbol{\mathcal{I}}^{|/||}$ is only a function of $\hat{\boldsymbol{\Xi}}^{|}$ and $\hat{\boldsymbol{\Xi}}^{||}$, we can separate the integrals as

$$\begin{aligned}\Psi_2 = \frac{1}{2}\, C_2 &\int_{\Xi^{||}=0}^{\Xi^{||}=\delta} {\Xi^{||}}^3\, \mathrm{d}\Xi^{||} \int_{\Xi^{|}=0}^{\Xi^{|}=\delta} {\Xi^{|}}^3\, \mathrm{d}\Xi^{|} \\ &\times \int_{\hat{\mathcal{H}}_0{}^{||}}\int_{\hat{\mathcal{H}}_0{}^{|}} |\hat{\boldsymbol{\Xi}}^{|} \times \hat{\boldsymbol{\Xi}}^{||}| \left[\boldsymbol{\mathcal{I}}^{|/||} : \boldsymbol{\mathcal{F}} - 2\right]^2 \mathrm{d}\hat{V}^{|}\, \mathrm{d}\hat{V}^{||}\,.\end{aligned} \tag{4.87}$$

Integrating over $\Xi^{\mid}$ and $\Xi^{\mid\mid}$ yields

$$\Psi_2 = \frac{1}{32}\, C_2\, \delta^8 \int_{\hat{\mathcal{H}}_0{}^{\mid\mid}} \int_{\hat{\mathcal{H}}_0{}^{\mid}} |\hat{\boldsymbol{\Xi}}^{\mid} \times \hat{\boldsymbol{\Xi}}^{\mid\mid}| \left[\boldsymbol{\mathcal{I}}^{\prime\mid\mid} : \boldsymbol{\mathcal{F}} - 2\right]^2 \mathrm{d}\hat{V}^{\mid}\, \mathrm{d}\hat{V}^{\mid\mid}\,. \tag{4.88}$$

Recall from Eq. (4.35) that $\boldsymbol{\mathcal{I}}^{\prime\mid\mid} := \boldsymbol{\mathcal{I}} - \hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}}$, rendering the energy density

$$\Psi_2 = \frac{1}{32}\, C_2\, \delta^8 \int_{\hat{\mathcal{H}}_0{}^{\mid\mid}} \int_{\hat{\mathcal{H}}_0{}^{\mid}} |\hat{\boldsymbol{\Xi}}^{\mid} \times \hat{\boldsymbol{\Xi}}^{\mid\mid}| \Big[\boldsymbol{\mathcal{I}} : \boldsymbol{\mathcal{F}} - \left[\hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}}\right] : \boldsymbol{\mathcal{F}} - 2\Big]^2 \mathrm{d}\hat{V}^{\mid}\, \mathrm{d}\hat{V}^{\mid\mid}\,. \tag{4.89}$$

Now we expand the integrand such that

$$\Psi_2 = \frac{1}{32}\, C_2\, \delta^8 \left[\left[\boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{I}} - 2\right]^2 \alpha - \Big[2\left[\boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{I}} - 2\right]\Big]\, \beta + \gamma\right], \tag{4.90}$$

where

$$\begin{aligned}
\alpha &:= \int_{\hat{\mathcal{H}}_0{}^{\mid\mid}} \int_{\hat{\mathcal{H}}_0{}^{\mid}} |\hat{\boldsymbol{\Xi}}^{\mid} \times \hat{\boldsymbol{\Xi}}^{\mid\mid}|\, \mathrm{d}\hat{V}^{\mid}\, \mathrm{d}\hat{V}^{\mid\mid}\,, \\
\beta &:= \int_{\hat{\mathcal{H}}_0{}^{\mid\mid}} \int_{\hat{\mathcal{H}}_0{}^{\mid}} |\hat{\boldsymbol{\Xi}}^{\mid} \times \hat{\boldsymbol{\Xi}}^{\mid\mid}|\, \boldsymbol{\mathcal{F}} \colon \left[\hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}}\right] \mathrm{d}\hat{V}^{\mid}\, \mathrm{d}\hat{V}^{\mid\mid}\,, \\
\gamma &:= \int_{\hat{\mathcal{H}}_0{}^{\mid\mid}} \int_{\hat{\mathcal{H}}_0{}^{\mid}} |\hat{\boldsymbol{\Xi}}^{\mid} \times \hat{\boldsymbol{\Xi}}^{\mid\mid}| \Big[\boldsymbol{\mathcal{F}} \colon \left[\hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}}\right]\Big]^2 \mathrm{d}\hat{V}^{\mid}\, \mathrm{d}\hat{V}^{\mid\mid}\,.
\end{aligned} \tag{4.91}$$

Firstly, recalling Lemma 4, renders

$$\alpha = 4\pi^3\,. \tag{4.92}$$

Next, taking $\boldsymbol{\mathcal{F}}$ out of the integrals and invoking Lemma 10 yields

$$\beta = \frac{4}{3}\pi^3\, \boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{I}}\,. \tag{4.93}$$

Like before, the relation

$$\Big[\boldsymbol{\mathcal{F}} \colon \left[\hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}}\right]\Big]^2 = \left[\boldsymbol{\mathcal{F}} \otimes \boldsymbol{\mathcal{F}}\right] :: \left[\hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}}\right], \tag{4.94}$$

allows us to rewrite the last term γ as

$$\gamma = \left[\boldsymbol{\mathcal{F}} \otimes \boldsymbol{\mathcal{F}}\right] :: \int_{\hat{\mathcal{H}}_0{}^{\text{II}}} \int_{\hat{\mathcal{H}}_0{}^{\text{I}}} |\hat{\boldsymbol{\Xi}}^{\text{I}} \times \hat{\boldsymbol{\Xi}}^{\text{II}}| \left[\hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}}\right] \mathrm{d}\hat{V}^{\text{I}} \, \mathrm{d}\hat{V}^{\text{II}} \,, \tag{4.95}$$

which, by the use of Lemma 11, reduces to

$$\begin{aligned} \gamma &= \frac{4}{15}\pi^3 \left[\boldsymbol{\mathcal{F}} \otimes \boldsymbol{\mathcal{F}}\right] :: \mathbb{I} \,, \\ &= \frac{4}{15}\pi^3 \Big[\boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{F}} + \boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{F}}^{\text{T}} + [\boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{I}}]^2\Big] \,. \end{aligned} \tag{4.96}$$

Equipped with α, β and γ, we return to Eq. (4.90), which finally yields

$$\boxed{\Psi_2 = \frac{1}{120}\pi^3 \, C_2 \, \delta^8 \left[\boldsymbol{\mathcal{F}} : [\boldsymbol{\mathcal{F}} + \boldsymbol{\mathcal{F}}^{\text{T}}] + 6\,[\boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{I}}]^2 - 40\,\boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{I}} + 60\right]} \tag{4.97}$$

4.4.3 Three-neighbor interactions

The energy density due to three-neighbor interactions Ψ_3 is defined as

$$\Psi_3 = \int_{\mathcal{H}_0} \int_{\mathcal{H}_0} \int_{\mathcal{H}_0} \psi_3 \, \mathrm{d}V^{\text{I}} \, \mathrm{d}V^{\text{II}} \, \mathrm{d}V^{\text{III}} \qquad \text{where} \qquad \psi_3 := \frac{1}{2} \, C_3 \, V \, [\mathit{Lin}\, \varepsilon_v]^2 \,. \tag{4.98}$$

Inserting the linearized volume strain $\mathit{Lin}\, \varepsilon_v$ from Eq. (4.49), and the relation $V = |\boldsymbol{\Xi}^{\text{I}}||\boldsymbol{\Xi}^{\text{II}}||\boldsymbol{\Xi}^{\text{II}}||\hat{\boldsymbol{\Xi}}^{\text{I}} \cdot [\hat{\boldsymbol{\Xi}}^{\text{II}} \times \hat{\boldsymbol{\Xi}}^{\text{III}}]|$ gives

$$\Psi_3 = \int_{\mathcal{H}_0} \int_{\mathcal{H}_0} \int_{\mathcal{H}_0} \frac{1}{2} \, C_3 \, |\boldsymbol{\Xi}^{\text{I}}||\boldsymbol{\Xi}^{\text{II}}||\boldsymbol{\Xi}^{\text{III}}| \big|\hat{\boldsymbol{\Xi}}^{\text{I}} \cdot [\hat{\boldsymbol{\Xi}}^{\text{II}} \times \hat{\boldsymbol{\Xi}}^{\text{III}}]\big| \, [\boldsymbol{\mathcal{I}} : \boldsymbol{\mathcal{F}} - 3]^2 \, \mathrm{d}V^{\text{I}} \, \mathrm{d}V^{\text{II}} \, \mathrm{d}V^{\text{III}} \,. \tag{4.99}$$

Next, we rewrite the integrals

$$\begin{aligned}\Psi_3 = \frac{1}{2}\, C_3\, [\boldsymbol{\mathcal{I}} : \boldsymbol{\mathcal{F}} - 3]^2 \int_{\Xi^{\mathrm{III}}=0}^{\Xi^{\mathrm{III}}=\delta} {\Xi^{\mathrm{III}}}^3 \,\mathrm{d}\Xi^{\mathrm{III}} \int_{\Xi^{\mathrm{II}}=0}^{\Xi^{\mathrm{II}}=\delta} {\Xi^{\mathrm{II}}}^3 \,\mathrm{d}\Xi^{\mathrm{II}} \int_{\Xi^{\mathrm{I}}=0}^{\Xi^{\mathrm{I}}=\delta} {\Xi^{\mathrm{I}}}^3 \,\mathrm{d}\Xi^{\mathrm{I}} \\ \times \int_{\hat{\mathcal{H}}_0{}^{\mathrm{III}}} \int_{\hat{\mathcal{H}}_0{}^{\mathrm{II}}} \int_{\hat{\mathcal{H}}_0{}^{\mathrm{I}}} \left| \hat{\boldsymbol{\Xi}}^{\mathrm{I}} \cdot [\hat{\boldsymbol{\Xi}}^{\mathrm{II}} \times \hat{\boldsymbol{\Xi}}^{\mathrm{III}}] \right| \mathrm{d}\hat{V}^{\mathrm{I}}\, \mathrm{d}\hat{V}^{\mathrm{II}}\, \mathrm{d}\hat{V}^{\mathrm{III}}\,,\end{aligned} \tag{4.100}$$

and carrying out the integrals over Ξ^{I}, Ξ^{II} and Ξ^{III} yields

$$\Psi_3 = \frac{1}{128}\, C_3\, \delta^{12}\, [\boldsymbol{\mathcal{I}} : \boldsymbol{\mathcal{F}} - 3]^2 \int_{\hat{\mathcal{H}}_0{}^{\mathrm{III}}} \int_{\hat{\mathcal{H}}_0{}^{\mathrm{II}}} \int_{\hat{\mathcal{H}}_0{}^{\mathrm{I}}} \left| \hat{\boldsymbol{\Xi}}^{\mathrm{I}} \cdot [\hat{\boldsymbol{\Xi}}^{\mathrm{II}} \times \hat{\boldsymbol{\Xi}}^{\mathrm{III}}] \right| \mathrm{d}\hat{V}^{\mathrm{I}}\, \mathrm{d}\hat{V}^{\mathrm{II}}\, \mathrm{d}\hat{V}^{\mathrm{III}}\,. \tag{4.101}$$

Lastly, invoking Lemma 9 gives

$$\Psi_3 = \frac{1}{16}\pi^4\, C_3\, \delta^{12}\, [\boldsymbol{\mathcal{I}} : \boldsymbol{\mathcal{F}} - 3]^2\,, \tag{4.102}$$

or

$$\boxed{\Psi_3 = \frac{1}{16}\pi^4\, C_3\, \delta^{12} \Big[[\boldsymbol{\mathcal{I}} : \boldsymbol{\mathcal{F}}]^2 - 6\, \boldsymbol{\mathcal{I}} : \boldsymbol{\mathcal{F}} + 9 \Big]} \tag{4.103}$$

4.4.4 Total point-wise energy density

Recalling from Eq.(2.24) that the total energy density of harmonic CPD in 3D is

$$\Psi_{\mathrm{H}}^{\mathrm{3D}} := \frac{1}{2}\, \Psi_1 + \frac{1}{3}\, \Psi_2 + \frac{1}{4}\, \Psi_3\,, \tag{4.104}$$

and using the results of Eq.(4.84), (4.97) and (4.103) renders

$$\begin{aligned}\Psi_{\mathrm{H}}^{\mathrm{3D}} = &\left[\frac{\pi}{60}\,C_1\,\delta^4 + \frac{\pi^3}{360}\,C_2\,\delta^8\right]\left[\boldsymbol{\mathcal{F}} : \left[\boldsymbol{\mathcal{F}} + \boldsymbol{\mathcal{F}}^{\mathrm{T}}\right]\right] \\ &+ \left[\frac{\pi}{60}\,C_1\,\delta^4 + \frac{\pi^3}{60}\,C_2\,\delta^8 + \frac{\pi^4}{64}\,C_3\,\delta^{12}\right]\left[\boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{I}}\right]^2 \\ &- \left[\frac{\pi}{6}\,C_1\,\delta^4 + \frac{\pi^3}{9}\,C_2\,\delta^8 + \frac{3\pi^4}{32}\,C_3\,\delta^{12}\right]\left[\boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{I}}\right] \\ &+ \frac{\pi}{4}\,C_1\,\delta^4 + \frac{\pi^3}{6}\,C_2\,\delta^8 + \frac{9\pi^4}{64}\,C_3\,\delta^{12}\end{aligned} \tag{4.105}$$

4.5 Material parameter relations

To obtain the relationship between the material parameters of harmonic CPD and CCM, we proceed to equate their respective energy densities, Ψ_{H} and Ψ_{CCM}. To do so, we first have to write Ψ_{H} as a function of $\boldsymbol{\varepsilon}$ such that both energy densities are functions of the same variable. Note that this is a special case, which the symmetric nature of the energy densities (4.70) and (4.105), $\Psi_{\mathrm{H}}^{\mathrm{2D}}(\boldsymbol{\mathcal{F}}) = \Psi_{\mathrm{H}}^{\mathrm{2D}}(\boldsymbol{\mathcal{F}}^{\mathrm{T}})$ and $\Psi_{\mathrm{H}}^{\mathrm{3D}}(\boldsymbol{\mathcal{F}}) = \Psi_{\mathrm{H}}^{\mathrm{3D}}(\boldsymbol{\mathcal{F}}^{\mathrm{T}})$ allows for. More specifically, the symmetric nature of the terms $\boldsymbol{\mathcal{F}} : \left[\boldsymbol{\mathcal{F}} + \boldsymbol{\mathcal{F}}^{\mathrm{T}}\right]$ and $\boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{I}}$ in the energy densities enables us to rewrite them as a function of $\boldsymbol{\varepsilon}$. To do so, we utilize the relations

$$\boldsymbol{\mathcal{F}} = \boldsymbol{\mathcal{I}} + \mathrm{Grad}\,\boldsymbol{u} \quad , \quad \boldsymbol{\varepsilon} = \mathrm{Grad}^{\mathrm{sym}}\,\boldsymbol{u} \quad , \quad \boldsymbol{\mathcal{F}} + \boldsymbol{\mathcal{F}}^{\mathrm{T}} = 2\left[\boldsymbol{\varepsilon} + \boldsymbol{\mathcal{I}}\right], \tag{4.106}$$

and the identities

$$\boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{I}} = \boldsymbol{\mathcal{F}}^{\mathrm{T}} : \boldsymbol{\mathcal{I}} \qquad \text{and} \qquad \boldsymbol{\mathcal{F}} : \left[\boldsymbol{\mathcal{F}} + \boldsymbol{\mathcal{F}}^{\mathrm{T}}\right] = \boldsymbol{\mathcal{F}}^{\mathrm{T}} : \left[\boldsymbol{\mathcal{F}} + \boldsymbol{\mathcal{F}}^{\mathrm{T}}\right], \tag{4.107}$$

we replace $\boldsymbol{\mathcal{F}}$ with $\frac{1}{2}\left[\boldsymbol{\mathcal{F}}+\boldsymbol{\mathcal{F}}^{\mathrm{T}}\right]$, in the energy densities (4.70) and (4.105) which immediately leads to

$$\begin{aligned}\boldsymbol{\mathcal{F}}:\boldsymbol{\mathcal{I}}&=\boldsymbol{\varepsilon}:\boldsymbol{\mathcal{I}}+\boldsymbol{\mathcal{I}}:\boldsymbol{\mathcal{I}}\,,\\ \boldsymbol{\mathcal{F}}:\left[\boldsymbol{\mathcal{F}}+\boldsymbol{\mathcal{F}}^{\mathrm{T}}\right]&=2\left[\boldsymbol{\varepsilon}:\boldsymbol{\varepsilon}\right]+4\left[\boldsymbol{\varepsilon}:\boldsymbol{\mathcal{I}}\right]+2\left[\boldsymbol{\mathcal{I}}:\boldsymbol{\mathcal{I}}\right],\end{aligned} \tag{4.108}$$

resulting in the total energy densities of harmonic CPD,

$$\Psi_{\mathrm{H}}^{\mathrm{2D}}=\frac{\pi}{24}C_1\delta^3\left[\boldsymbol{\varepsilon}:\boldsymbol{\varepsilon}\right]+\left[\frac{\pi}{48}C_1\delta^3+\frac{4}{27}\pi\,C_2\,\delta^6\right]\left[\boldsymbol{\varepsilon}:\boldsymbol{\mathcal{I}}\right]^2, \tag{4.109}$$

and

$$\begin{aligned}\Psi_{\mathrm{H}}^{\mathrm{3D}}=&\left[\frac{\pi}{30}C_1\delta^4+\frac{\pi^3}{180}C_2\delta^8\right]\left[\boldsymbol{\varepsilon}:\boldsymbol{\varepsilon}\right]\\&+\left[\frac{\pi}{60}C_1\delta^4+\frac{\pi^3}{60}C_2\delta^8+\frac{\pi^4}{64}C_3\delta^{12}\right]\left[\boldsymbol{\varepsilon}:\boldsymbol{\mathcal{I}}\right]^2.\end{aligned} \tag{4.110}$$

It should be noted that Ψ_{CCM} is a function of $\boldsymbol{\varepsilon}:\boldsymbol{\varepsilon}$ and $\boldsymbol{\varepsilon}:\boldsymbol{I}$, which are linearly independent functions of $\boldsymbol{\varepsilon}$. Thus $\Psi_{\mathrm{H}}^{\mathrm{2D}}$ and $\Psi_{\mathrm{H}}^{\mathrm{3D}}$ should also be functions of these two linearly independent variables, which is evidently satisfied by the results obtained above. Now we can proceed to derive the material parameter relations in 2D and 3D respectively.

4.5.1 Material parameters in 2D

For the rest of this section, any generic term will be in 2D space, such as $\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{F}}_{\mathrm{2D}}$, or $\boldsymbol{\mathcal{I}}=\boldsymbol{\mathcal{I}}_{\mathrm{2D}}$, for the sake of brevity. To derive the material parameter relations, we now equate the coefficients of the identical terms in $\Psi_{\mathrm{H}}^{\mathrm{2D}}$ and Ψ_{CCM} and arrive at two relations

$$\mu\left[\boldsymbol{\varepsilon}:\boldsymbol{\varepsilon}\right]=\frac{\pi}{24}C_1\delta^3\left[\boldsymbol{\varepsilon}:\boldsymbol{\varepsilon}\right]\quad,\quad\frac{1}{2}\lambda\left[\boldsymbol{\varepsilon}:\boldsymbol{\mathcal{I}}\right]^2=\left[\frac{\pi}{48}C_1\delta^3+\frac{4}{27}\pi\,C_2\,\delta^6\right]\left[\boldsymbol{\varepsilon}:\boldsymbol{\mathcal{I}}\right]^2, \tag{4.111}$$

rendering

$$\mu = \frac{\pi}{24} C_1 \delta^3 \qquad \text{and} \qquad \lambda = \frac{\pi}{24} C_1 \delta^3 + \frac{8}{27}\, \pi\, C_2\, \delta^6 \,. \tag{4.112}$$

Equipped with the expressions for μ and λ, we proceed to derive the relations for other commonly employed elastic material parameters. For this purpose, we will utilize the relations established in the literature for the material parameters of an isotropic, linear elastic, two-dimensional domain in two-dimensional space, given in Table 4.2, see [33] for further details. Using the results of Eq. (4.112) and Table (4.2), the relations for the rest of the 2D material parameters E, ν, and κ are derived, and are given in terms of the CPD parameters C_1, C_2 and δ in Table 4.3. Note that C_1 and C_2 are coefficients that correspond to the resistances to length and area change respectively, while δ is the horizon size that affects the span of non-local effects. We also extract the CPD counterparts of these relations in terms of different combinations of CCM material parameters, gathered in Table 4.3.

Table 4.2: Relations between the elastic material parameters for a two-dimensional domain in two-dimensional space, where ζ is defined by $\zeta := E^2+4\lambda^2$. λ and μ are the first and second Lamé parameters, E is the Young's modulus, ν is the Poisson ratio and κ is the bulk modulus. Note the difference to the three-dimensional case. Of particular interest in this section is the Poisson ratio that ranges from -1 to 1 for the two-dimensional problem of interest, unlike its three-dimensional counterpart that ranges from -1 to 0.5. For more details, see the counterpart of this table for three-dimensional isotropic elasticity, Table 4.5.

	λ	μ	E	ν	κ
λ , μ			$\frac{4\mu[\lambda+\mu]}{\lambda+2\mu}$	$\frac{\lambda}{\lambda+2\mu}$	$\lambda+\mu$
λ , E		$\frac{E-2\lambda\pm\sqrt{\zeta}}{4}$		$\frac{2\lambda}{E\pm\sqrt{\zeta}}$	$\frac{E+2\lambda\pm\sqrt{\zeta}}{4}$
λ , ν		$\frac{\lambda[1-\nu]}{2\nu}$	$\frac{\lambda\left[1-\nu^2\right]}{\nu}$		$\frac{\lambda[1+\nu]}{2\nu}$
λ , κ		$\kappa-\lambda$	$\frac{4\kappa[\kappa-\lambda]}{2\kappa-\lambda}$	$\frac{\lambda}{2\kappa-\lambda}$	
μ , E	$\lambda\frac{2\mu[E-2\mu]}{4\mu-E}$			$\frac{E-2\mu}{2\mu}$	$\frac{\mu E}{4\mu-E}$
μ , ν	$\frac{2\mu\nu}{1-\nu}$		$2\mu[1+\nu]$		$\frac{\mu[1+\nu]}{1-\nu}$
μ , κ	$\kappa-\mu$		$\frac{4\mu\kappa}{\mu+\kappa}$	$\frac{\kappa-\mu}{\kappa+\mu}$	
E , ν	$\frac{E\nu}{1-\nu^2}$	$\frac{E}{2[1+\nu]}$			$\frac{E}{2[1-\nu]}$
E , κ	$\frac{2\kappa[2\kappa-E]}{4\kappa-E}$	$\frac{E\kappa}{4\kappa-E}$		$\frac{2\kappa-E}{2\kappa}$	
ν , κ	$\frac{2\kappa\nu}{1+\nu}$	$\frac{\kappa[1-\nu]}{1+\nu}$	$2\kappa[1-\nu]$		

Table 4.3: Material parameter relations between CPD and CCM. λ and μ are the first and second Lamé parameters, E is the Young's modulus, ν is the Poisson ratio and κ is the bulk modulus.

	C_1	C_2		C_1	C_2
λ , μ	$\frac{24}{\pi\delta^3}\mu$	$\frac{27}{8\pi\delta^6}[\lambda-\mu]$	μ , ν	$\frac{24}{\pi\delta^3}\mu$	$\frac{27}{8\pi\delta^6}\frac{\mu[1-3\nu]}{[\nu-1]}$
λ , E	$\frac{6}{\pi\delta^3}\left[E-2\lambda+\sqrt{\zeta}\right]$	$\frac{27}{32\pi\delta^6}\left[-E+6\lambda-\sqrt{\zeta}\right]$	μ , κ	$\frac{24}{\pi\delta^3}\mu$	$\frac{27}{8\pi\delta^6}[\kappa-2\mu]$
λ , ν	$\frac{12}{\pi\delta^3}\frac{\lambda[1-\nu]}{\nu}$	$\frac{27}{16\pi\delta^6}\frac{\lambda[3\nu-1]}{\nu}$	E , ν	$\frac{12}{\pi\delta^3}\frac{E}{[\nu+1]}$	$\frac{27}{16\pi\delta^6}\frac{E[1-3\nu]}{[\nu^2-1]}$
λ , κ	$\frac{24}{\pi\delta^3}[\kappa-\lambda]$	$\frac{27}{8\pi\delta^6}[2\lambda-\kappa]$	E , κ	$\frac{24}{\pi\delta^3}\frac{\kappa E}{[4\kappa-E]}$	$\frac{27}{8\pi\delta^6}\frac{\kappa[3E-4\kappa]}{[E-4\kappa]}$
μ , E	$\frac{24}{\pi\delta^3}\mu$	$\frac{27}{8\pi\delta^6}\frac{\mu[8\mu-3E]}{[E-4\mu]}$	ν , κ	$\frac{24}{\pi\delta^3}\frac{\kappa[1-\nu]}{[\nu+1]}$	$\frac{27}{8\pi\delta^6}\frac{\kappa[3\nu-1]}{[\nu+1]}$

$\lambda=\frac{C_1\pi\delta^3}{24}+\frac{8\,C_2\pi\delta^6}{27}$	$\mu=\frac{C_1\pi\delta^3}{24}$	$\nu=\frac{9\,C_1+64\,C_2\delta^3}{27\,C_1+64\,C_2\delta^3}$	$E=\frac{C_1\pi\delta^3\left[9\,C_1+32\,C_2\delta^3\right]}{81\,C_1+192\,C_2\delta^3}$	$\kappa=\frac{C_1\pi\delta^3}{12}+\frac{8\,C_2\pi\delta^6}{27}$

Remark on the horizon size δ *In view of the relationships between the material parameters of CPD and CCM in Table 4.3, at first glance it may seem counter-intuitive to have the horizon size δ, or rather its powers, in the denominator. This is particularly relevant to the discussion here since we expect the energy of CPD to converge to that of CCM as the horizon size approaches zero, i.e. if $\delta\to 0$. We argue that despite having δ^3 and δ^6 in the denominators of C_1 and C_2, respectively, the point-wise energy of CPD assumes a finite value under finite deformations. To explain that, it should be emphasized again that the point-wise energy of CPD is a non-local quantity and is calculated via integrations over the horizon as*

$$\Psi_1=\frac{1}{2}\int_{\mathcal{H}_0}\frac{1}{2}\,C_1\,L\left[\frac{l}{L}-1\right]^2 dA^{\shortmid}=\int_{\mathcal{H}_0}\frac{6\,\mu}{\pi\,\delta^3}\,L\left[\frac{l}{L}-1\right]^2 dA^{\shortmid}\,,$$

$$\Psi_2=\frac{1}{3}\int_{\mathcal{H}_0}\int_{\mathcal{H}_0}\frac{1}{2}\,C_2\,A\left[\frac{a}{A}-1\right]^2 dA^{\shortmid}\,dA^{\shortparallel}=\int_{\mathcal{H}_0}\int_{\mathcal{H}_0}\frac{9\,[\lambda-\mu]}{16\,\pi\,\delta^6}\,A\left[\frac{a}{A}-1\right]^2 dA^{\shortmid}\,dA^{\shortparallel},$$

that clearly show that both Ψ_1 and Ψ_2 will be of finite value even if $\delta\to 0$ since $dA^{\shortmid}$ and $dA^{\shortparallel}$ are proportional to δ^2; and L and A are each proportional to δ and δ^2, respectively. □

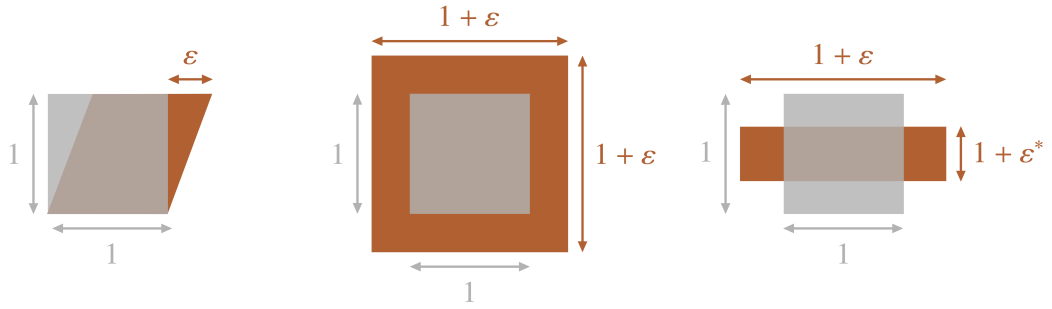

Figure 4.1: The three canonical deformation types of simple shear (left), uniform expansion (center) and uni-axial tension (right) in 2D. In simple shear, a unit square undergoes a shear deformation of ε with the top and bottom sides constrained vertically. In uniform expansion, the unit square is uniformly expanded an amount of ε in all directions. In uni-axial tension, the unit square is extended by an amount of ε along the horizontal direction and is allowed to relax on the vertical direction to reach equilibrium, resulting in a deformation by an amount of $\varepsilon^* = -\nu\,\varepsilon$, with ν being the Poisson ratio.

Examples

To verify the material parameter relations, we prescribe affine deformations for three canonical deformation types of (i) simple shear, (ii) uniform expansion and (iii) uni-axial tension shown in Fig. 4.1. For shear and expansion, $\Psi_{\mathrm{H}}^{\mathrm{2D}}$ and Ψ_{CPD} are calculated and equated to extract the material parameter relations. For the uni-axial tension test, we impose equilibrium to the CPD energy to arrive at the Poisson ratio ν.

Simple Shear *For the prescribed $\boldsymbol{\mathcal{F}}$ below, the energy densities of CCM and CPD are*

$$[\boldsymbol{\mathcal{F}}] = \begin{bmatrix} 1 & \varepsilon \\ 0 & 1 \end{bmatrix} \qquad \Rightarrow \qquad [\boldsymbol{\varepsilon}] = \begin{bmatrix} 0 & \frac{\varepsilon}{2} \\ \frac{\varepsilon}{2} & 0 \end{bmatrix}, \tag{4.113}$$

such that

$$\Psi_{\mathrm{CCM}} = \mu\frac{\varepsilon^2}{2} \qquad \text{and} \qquad \Psi_{\mathrm{H}}^{\mathrm{2D}} = \frac{\pi}{48}C_1\delta^3\varepsilon^2\,. \tag{4.114}$$

Equating the energy densities yields $\mu = \dfrac{\pi}{24}C_1\delta^3$. This resulting expression for μ

verifies the previous relation (4.112) derived for a generic, affine deformation. □

Expansion *For the prescribed $\boldsymbol{\mathcal{F}}$ below, the energy densities of CCM and CPD are*

$$[\boldsymbol{\mathcal{F}}] = \begin{bmatrix} 1+\varepsilon & 0 \\ 0 & 1+\varepsilon \end{bmatrix} \qquad \Rightarrow \qquad [\boldsymbol{\varepsilon}] = \begin{bmatrix} \varepsilon & 0 \\ 0 & \varepsilon \end{bmatrix}, \tag{4.115}$$

such that

$$\Psi_{\mathrm{CCM}} = 2\kappa\varepsilon^2 \qquad \text{and} \qquad \Psi_{\mathrm{H}}^{\mathrm{2D}} = \left[\frac{\pi}{6}C_1\delta^3 + \frac{16\pi}{27}C_1\delta^6\right]\varepsilon^2 . \tag{4.116}$$

Equating the energy densities yields $\kappa = \dfrac{\pi}{12}C_1\delta^3 + \dfrac{8\pi}{27}C_2\delta^6$. This newly derived κ is equal to the one given in Table 4.3, valid for any generic, affine deformation. Note that in the absence of two-neighbor interactions, i.e. $C_2 = 0$, the bulk modulus reads $\kappa = \dfrac{\pi}{12}C_1\delta^3$, which is well established in bond-based PD [34]. □

Uni-Axial Tension *For the uni-axial tension test, the domain is extended laterally and relaxed vertically, to impose a traction-free condition along the vertical direction, according to*

$$[\boldsymbol{\mathcal{F}}] = \begin{bmatrix} 1+\varepsilon & 0 \\ 0 & 1+\varepsilon^* \end{bmatrix} \quad \text{with} \quad \varepsilon^* = -\nu\varepsilon \quad \Rightarrow \quad [\boldsymbol{\varepsilon}] = \begin{bmatrix} \varepsilon & 0 \\ 0 & -\nu\varepsilon \end{bmatrix}, \tag{4.117}$$

rendering the following energy density

$$\Psi_{\mathrm{H}}^{\mathrm{2D}} = \left[\frac{\pi}{16}C_1\delta^3 + \frac{4\pi}{27}C_2\delta^6\right]\left[1+\nu^2\right]\varepsilon^2 - \left[\frac{\pi}{24}C_1\delta^3 + \frac{8\pi}{27}C_2\delta^6\right]\nu\,\varepsilon^2 . \tag{4.118}$$

To impose equilibrium, we set the variation of Ψ_{H} to zero as follows

$$\delta\Psi_{\mathrm{H}}^{\mathrm{2D}} \doteq 0 \qquad \Leftrightarrow \qquad \frac{\partial\Psi_{\mathrm{H}}^{\mathrm{2D}}}{\partial\varepsilon}\delta\varepsilon + \frac{\partial\Psi_{\mathrm{H}}^{\mathrm{2D}}}{\partial\nu}\delta\nu \quad \doteq 0 , \tag{4.119}$$

where $\delta\varepsilon = 0$, as ε is a prescribed variable. However the variation of ν is not

necessarily zero, and thus the variation of $\Psi_{\mathrm{H}}^{\mathrm{2D}}$ *with respect to* ν *should be zero to satisfy equilibrium. Imposing this condition gives*

$$\frac{\partial \Psi_{\mathrm{H}}^{\mathrm{2D}}}{\partial \nu} = \left[\left[\frac{\pi}{8} C_1 \delta^3 + \frac{8\pi}{27} C_2 \delta^6 \right] \nu - \frac{\pi}{24} C_1 \delta^3 - \frac{8\pi}{27} C_2 \delta^6 \right] \varepsilon^2 \doteq 0 \,, \tag{4.120}$$

rendering

$$\nu = \frac{9\, C_1 + 64\, C_2 \delta^3}{27\, C_1 + 64\, C_2 \delta^3} \,, \tag{4.121}$$

which is in agreement with the ν *previously derived as a function* λ *and* μ*, for a generic, affine deformation, given in Table 4.3.* □

To better illustrate the relationship between the Poisson ratio and the material parameters of CPD, we rewrite the relation as

$$\nu = \frac{9 + 64\, [C_2/C_1] \delta^3}{27 + 64\, [C_2/C_1] \delta^3} \,, \tag{4.122}$$

and plot the variation of ν with changing C_2/C_1 and δ, and with changing $\delta^3\, C_2/C_1$, as seen in Fig. 4.2. The grey surface is generated using the previously derived relation (4.122), with isolines drawn for different values of C_2/C_1. The first thing to notice is the tendency of the Poisson ratio to reach the upper bound $\nu = 1$ (in a two dimensional setting), or incompressibility, for extremely large values of C_2/C_1, which is valid for any value of $\delta > 0$. This brings us to our next observation, the case in which $\nu = 1/3$. For sufficiently small values of $|C_2/C_1|$, the formulation effectively recovers bond-based PD, where the Poisson ratio is constant with $\nu = 1/3$. This is expected as in this particular region, the effect of C_2, or two-neighbor interactions, are negligible in comparison to one-neighbor interactions. Decreasing C_2/C_1 further for different values of δ results in an auxetic behavior, where $\nu < 0$. The values of ν continue to decrease with decreasing C_2/C_1, until the lower bound $\nu = -1$ is reached. The inadmissible region, where $\nu \leq -1$, is highlighted in Fig. 4.2, along with the equation of the lower bound, $\frac{C_2}{C_1}\delta^3 = -\frac{9}{32}$.

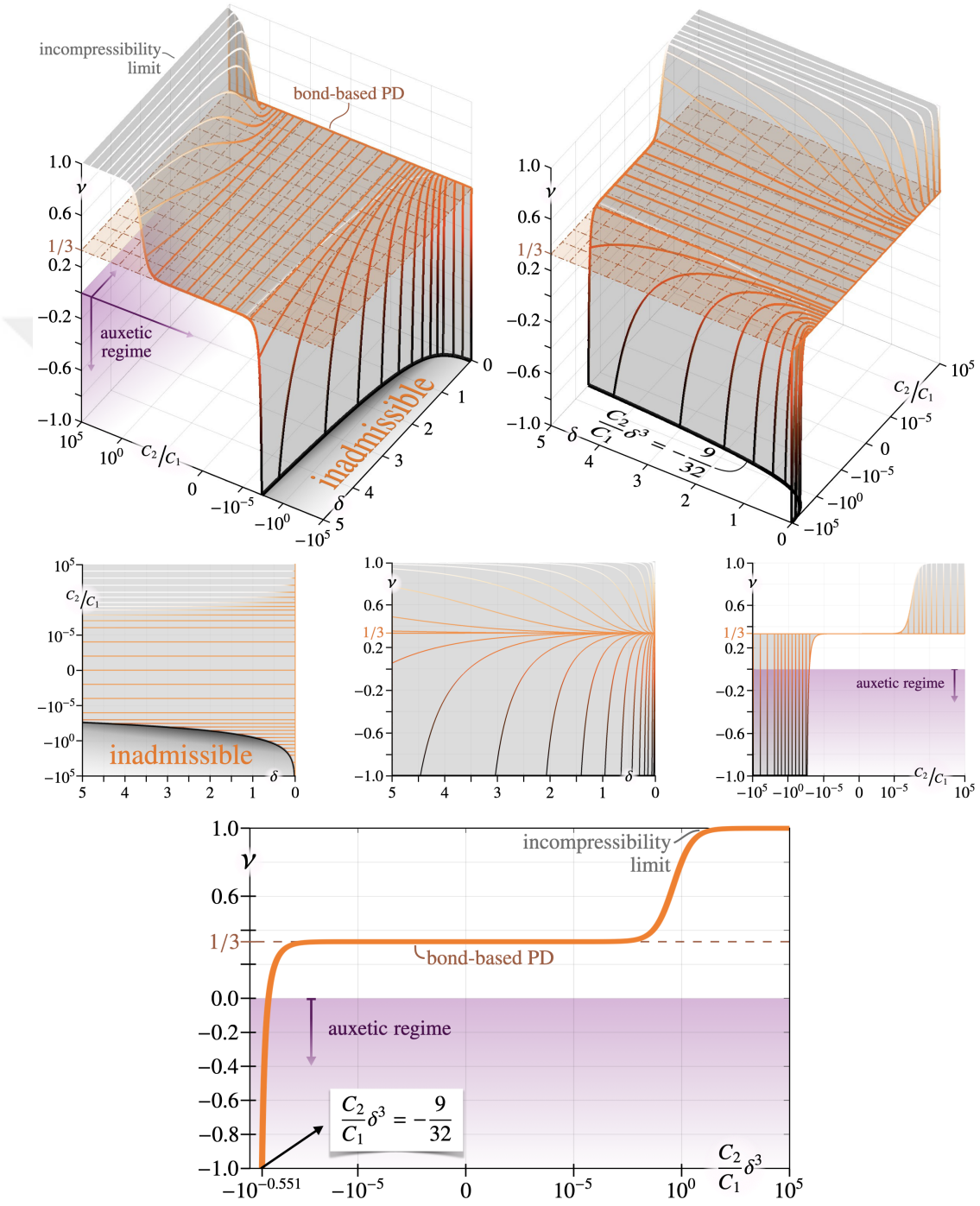

Figure 4.2: The variation of the Poisson ratio ν with the material parameters of CPD, the ratio $\frac{C_2}{C_1}$, δ and $\frac{C_2}{C_1}\delta^3$.

The bounds for the CPD parameters can be expressed vis-à-vis the bounds of

the CCM material parameters, as we are now equipped with the relations between the parameters of the two formulations. The resulting bounds are collected in Table 4.4.

Table 4.4: Admissible ranges for CPD and CCM parameters in 2D.

	CCM	
	$\kappa \geq 0$	$\mu \geq 0$
CPD	$C_2 > -\frac{9}{32\,\delta^3} C_1$	$C_1 > 0$

4.5.2 Material parameters in 3D

In this section, we follow the same procedure as we did in 2D, this time for the 3D energy densities. For the rest of this section, any generic term will be in 3D space, such as $\boldsymbol{\mathcal{F}} = \boldsymbol{\mathcal{F}}_{\text{3D}}$, or $\boldsymbol{\mathcal{I}} = \boldsymbol{\mathcal{I}}_{\text{3D}}$, for the sake of brevity. By equating the coefficients of the terms $\boldsymbol{\varepsilon} : \boldsymbol{\varepsilon}$ and $\boldsymbol{\varepsilon} : \boldsymbol{\mathcal{I}}$ in (4.1) and (4.110), we arrive at the first two relations between the material parameters of 3D, harmonic CPD and CCM

$$\begin{aligned} \mu \left[\boldsymbol{\varepsilon} : \boldsymbol{\varepsilon}\right] &= \left[\frac{\pi}{30} C_1 \delta^4 + \frac{\pi^3}{180} C_2 \delta^8\right] \left[\boldsymbol{\varepsilon} : \boldsymbol{\varepsilon}\right], \\ \frac{1}{2}\lambda \left[\boldsymbol{\varepsilon} : \boldsymbol{\mathcal{I}}\right]^2 &= \left[\frac{\pi}{60} C_1 \delta^4 + \frac{\pi^3}{60} C_2 \delta^8 + \frac{\pi^4}{64} C_3 \delta^{12}\right] \left[\boldsymbol{\varepsilon} : \boldsymbol{\mathcal{I}}\right]^2, \end{aligned} \tag{4.123}$$

rendering

$$\mu = \frac{\pi}{30} C_1 \delta^4 + \frac{\pi^3}{180} C_2 \delta^8 \quad , \quad \lambda = \frac{\pi}{30} C_1 \delta^4 + \frac{\pi^3}{30} C_2 \delta^8 + \frac{\pi^4}{32} C_3 \delta^{12}, \tag{4.124}$$

where λ and μ are the first and second Lamé parameters, respectively. To derive the relations with the remaining material parameters of CCM, we utilize Table 4.5, and in turn obtain the relations in Table 4.6.

Remark on the horizon size δ *In view of the relationships between the material parameters of CPD and CCM in Table 4.6, the horizon size δ appears with*

Table 4.5: Relations between the elastic material parameters for three-dimensional isotropic elasticity, where ζ is defined by $\zeta := E^2 + 9\lambda^2 + 2E\lambda$. λ and μ are the first and second Lamé parameters, E is the Young's modulus, ν is the Poisson ratio and κ is the bulk modulus.

	λ	μ	E	ν	κ
λ , μ			$\frac{\mu[3\lambda+2\mu]}{\lambda+\mu}$	$\frac{\lambda}{2[\lambda+\mu]}$	$\lambda+\frac{2}{3}\mu$
λ , E		$\frac{E-3\lambda+\sqrt{\zeta}}{4}$		$\frac{2\lambda}{E+\lambda+\sqrt{\zeta}}$	$\frac{E+3\lambda+\sqrt{\zeta}}{6}$
λ , ν		$\frac{\lambda[1-2\nu]}{2\nu}$	$\frac{\lambda[1+\nu][1-2\nu]}{\nu}$		$\frac{\lambda[1+\nu]}{3\nu}$
λ , κ		$\frac{3}{2}[\kappa-\lambda]$	$\frac{9\kappa[\kappa-\lambda]}{3\kappa-\lambda}$	$\frac{\lambda}{3\kappa-\lambda}$	
μ , E	$\frac{\mu[E-2\mu]}{3\mu-E}$			$\frac{E-2\mu}{2\mu}$	$\frac{\mu E}{3(3\mu-E)}$
μ , ν	$\frac{2\mu\nu}{1-2\nu}$		$2\mu[1+\nu]$		$\frac{2\mu[1+\nu]}{3[1-2\nu]}$
μ , κ	$\kappa-\frac{2}{3}\mu$		$\frac{9\mu\kappa}{\mu+3\kappa}$	$\frac{3\kappa-2\mu}{6\kappa+2\mu}$	
E , ν	$\frac{E\nu}{[1+\nu][1-2\nu]}$	$\frac{E}{2[1+\nu]}$			$\frac{E}{3[1-2\nu]}$
E , κ	$\frac{3\kappa[3\kappa-E]}{9\kappa-E}$	$\frac{3E\kappa}{9\kappa-E}$		$\frac{3\kappa-E}{6\kappa}$	
ν , κ	$\frac{3\kappa\nu}{1+\nu}$	$\frac{3\kappa[1-2\nu]}{2[1+\nu]}$	$3\kappa[1-2\nu]$		

different powers which ensures dimensional consistency, although at first glance this may seem counter-intuitive. Having δ, or rather its powers, multiplied by the elastic parameters of CPD is particularly relevant to the discussion here since we expect the energy of CPD to converge to that of CCM as the horizon size approaches zero, i.e. if $\delta \to 0$. We argue that despite having δ^4, δ^8 and δ^{12} multiplied to C_1, C_2 and C_3, respectively, the point-wise energy of CPD assumes a finite value under finite deformations, comparable to CCM, when $\delta \to 0$. To explain that, it should be emphasized again that the point-wise energy of CPD is

Table 4.6: λ, μ, E, ν, and κ, and in terms of C_1, C_2, C_3 and δ.

λ	$\frac{\pi}{30}C_1\delta^4 + \frac{\pi^3}{30}C_2\delta^8 + \frac{\pi^4}{32}C_3\delta^{12}$
μ	$\frac{\pi}{30}C_1\delta^4 + \frac{\pi^3}{180}C_2\delta^8$
E	$\frac{\pi\delta^4\left[6C_1+\pi^2C_2\delta^4\right]\left[48C_1+32\pi^2C_2\delta^4+27\pi^3C_3\delta^8\right]}{36\left[96C_1+56\pi^2C_2\delta^4+45\pi^3C_3\delta^8\right]}$
ν	$\frac{48C_1+48\pi^2C_2\delta^4+45\pi^3C_3\delta^8}{2\left[96C_1+56\pi^2C_2\delta^4+45\pi^3C_3\delta^8\right]}$
κ	$\frac{\pi}{18}C_1\delta^4 + \frac{\pi^3}{27}C_2\delta^8 + \frac{\pi^4}{32}C_3\delta^{12}$

a non-local quantity and is calculated via integrations over the horizon as

$$\Psi_1 = \int_{\mathcal{H}_0} \frac{1}{2}\, C_1\, L \left[\frac{l}{L} - 1\right]^2 \mathrm{d}V^{\mathrm{I}} \quad \Rightarrow \quad \left[\, C_1 \,\right] = \frac{\left[\, \Psi_1 \,\right]}{\mathrm{m}^4}\,,$$

$$\Psi_2 = \int_{\mathcal{H}_0}\int_{\mathcal{H}_0} \frac{1}{2}\, C_2\, A \left[\frac{a}{A} - 1\right]^2 \mathrm{d}V^{\mathrm{I}}\, \mathrm{d}V^{\mathrm{II}} \quad \Rightarrow \quad \left[\, C_2 \,\right] = \frac{\left[\, \Psi_2 \,\right]}{\mathrm{m}^8}\,,$$

$$\Psi_3 = \int_{\mathcal{H}_0}\int_{\mathcal{H}_0}\int_{\mathcal{H}_0} \frac{1}{2}\, C_3\, V \left[\frac{v}{V} - 1\right]^2 \mathrm{d}V^{\mathrm{I}}\, \mathrm{d}V^{\mathrm{II}}\, \mathrm{d}V^{\mathrm{III}} \quad \Rightarrow \quad \left[\, C_3 \,\right] = \frac{\left[\, \Psi_3 \,\right]}{\mathrm{m}^{12}}\,,$$

that clearly show when $\delta \to 0$, the energy densities Ψ_1, Ψ_2 and Ψ_3 will be of finite value only if the elastic constants of CPD could become infinitely large. This discussion motivates the idea of introducing a different set of parameters D_1 and D_2 as follows.

The three material parameters of the CPD formulation C_1, C_2 and C_3 correspond to different physical phenomena, namely the resistances to length, area and volume change, respectively, while the fourth parameter δ measures the degree of non-local effects. It proves useful to define two coefficients that will serve as the CPD counterpart of the material parameter pairs prevalent in CCM. In that spirit we define the coefficients D_1 and D_2, with the same dimensions as μ and

λ, as

$$\begin{aligned} D_1 &= \frac{\pi}{30} C_1 \delta^4 + \frac{\pi^3}{180} C_2 \delta^8 \qquad \Rightarrow \qquad D_1 = \mu\,, \\ D_2 &= \frac{\pi^3}{36} C_2 \delta^8 + \frac{\pi^4}{32} C_3 \delta^{12} \qquad \Rightarrow \qquad D_2 = \lambda - \mu\,. \end{aligned} \tag{4.125}$$

It is now possible to write the CPD parameters D_1 and D_2 in terms of CCM parameters. The unification of the relations between D_1, D_2 and the material parameters of CCM, as well as the expressions of D_1 and D_2 in terms of C_1, C_2, C_3 and δ are given in Table 4.7.

Remark on the physical relevance of D_1 and D_2 *The choice of D_1 and D_2, for now, is based purely on the mathematical elegance they present, motivated by the insight given in Table 4.6. Their physical relevance, on the other hand, remains to be discussed. The first CPD parameter D_1, being equal to μ, corresponds to shear (or isochoric) deformations, whereas a physical deformation mode cannot be immediately attributed to exclusively D_2, similar to the first Lamé parameter λ. More specifically, looking at the point-wise strain energy density of isotropic linear elasticity (4.1), it can be seen that for the contribution of μ to vanish, $\boldsymbol{\varepsilon} : \boldsymbol{\varepsilon}$ should be equal to zero. This holds only if every element of $\boldsymbol{\varepsilon}$ is equal to zero, making the term $\boldsymbol{\varepsilon} : \boldsymbol{\mathcal{I}}$ also zero. In fact, this is exactly what the second Lamé parameter λ suffers from. It has no physical meaning as one cannot propose a deformation mode that renders the contribution of μ zero while keeping the contribution of λ non-zero. As we will see shortly, equipped with the insight obtained from CPD, we will be able to provide a physical explanation of the first Lamé parameter λ.* □

To validate our findings, and also to provide a more accessible and familiar procedure, we re-derive the relations for μ, κ and ν by prescribing affine (i) shear, (ii) expansion and (iii) uni-axial tension deformations as shown in Fig.4.3. To find μ and κ, Ψ_{CCM} and $\Psi_{\text{H}}^{\text{3D}}$ are equated and the material parameter relations are extracted. For ν, the variation of the resulting $\Psi_{\text{H}}^{\text{3D}}$ from the uni-axial tension test is set to zero to impose equilibrium.

Table 4.7: D_1 and D_2 in terms of λ, μ, E, ν, and κ. The parameter ζ is defined as $\zeta := E^2 + 9\lambda^2 + 2E\lambda$.

	D_1	D_2		D_1	D_2
λ , μ	μ	$\lambda - \mu$	μ , ν	μ	$\frac{\mu\,[1-4\nu]}{2\nu-1}$
λ , E	$\frac{E-3\lambda+\sqrt{\zeta}}{4}$	$\frac{7\lambda-E-\sqrt{\zeta}}{4}$	μ , κ	μ	$\kappa - \frac{5}{3}\mu$
λ , ν	$\frac{\lambda\,[1-2\nu]}{2\nu}$	$\frac{\lambda\,[4\nu-1]}{2\nu}$	E , ν	$\frac{E}{2\,[\nu+1]}$	$\frac{E\,[1-4\nu]}{2\,[\nu+1]\,[2\nu-1]}$
λ , κ	$\frac{3\,[\kappa-\lambda]}{2}$	$\frac{5\lambda-3\kappa}{2}$	E , κ	$\frac{3\kappa\,E}{9\kappa-E}$	$\frac{3\kappa\,[2E-3\kappa]}{[E-9\kappa]}$
μ , E	μ	$\frac{\mu\,[5\mu-2E]}{E-3\mu}$	ν , κ	$\frac{3\kappa\,[1-2\nu]}{2\,[\nu+1]}$	$\frac{3\kappa\,[4\nu-1]}{2\,[\nu+1]}$

$\lambda = D_1 + D_2$	$\mu = D_1$	$\nu = \frac{D_1+D_2}{2\,[2D_1+D_2]}$	$E = \frac{D_1\,[5D_1+3D_2]}{2D_1+D_2}$	$\kappa = \frac{5}{3}D_1 + D_2$

$D_1 = \frac{\pi}{30}C_1\delta^4 + \frac{\pi^3}{180}C_2\delta^8$	$D_2 = \frac{\pi^3}{36}C_2\delta^8 + \frac{\pi^4}{32}C_3\delta^{12}$

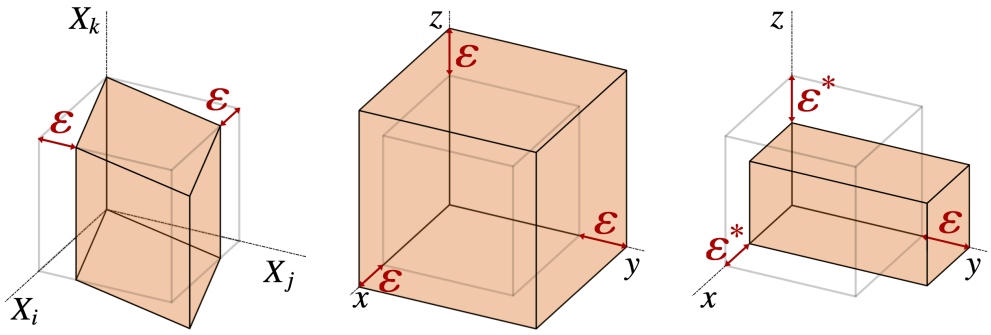

Figure 4.3: The three canonical deformation types of shear (left), uniform expansion (center) and uni-axial tension (right) in 3D. In shear, a unit cube undergoes a shear deformation of ε on all axes. In uniform expansion, the unit cube is uniformly expanded an amount of ε in all directions. In uni-axial tension, the unit cube is extended by an amount of ε along direction y and is allowed to relax on the directions x and z to reach equilibrium, resulting in a deformation by an amount of $\varepsilon^* = -\nu\,\varepsilon$, with ν being the Poisson ratio.

Shear *Prescribing a shear deformation with the* $\boldsymbol{\mathcal{F}}$ *below yields the energy densities* Ψ_H^{3D} *and* Ψ_{CCM}

$$[\boldsymbol{\mathcal{F}}] = \begin{bmatrix} 1 & \varepsilon & \varepsilon \\ \varepsilon & 1 & \varepsilon \\ \varepsilon & \varepsilon & 1 \end{bmatrix} \qquad \Rightarrow \qquad [\boldsymbol{\varepsilon}] = \begin{bmatrix} 0 & \varepsilon & \varepsilon \\ \varepsilon & 0 & \varepsilon \\ \varepsilon & \varepsilon & 0 \end{bmatrix}, \tag{4.126}$$

and therefore

$$\Psi_{\mathrm{CCM}} = 6\mu\varepsilon^2 \qquad \text{and} \qquad \Psi_{\mathrm{H}}^{\mathrm{3D}} = \left[\frac{\pi}{30}C_1\delta^4 + \frac{\pi^3}{180}C_2\delta^8\right]\varepsilon^2 . \tag{4.127}$$

Imposing $\Psi_H^{3D} = \Psi_{CCM}$ *results in the relation*

$$\mu = \frac{\pi}{30}C_1\delta^4 + \frac{\pi^3}{180}C_2\delta^8 , \tag{4.128}$$

in agreement with Eq. (4.124)$_1$.

Expansion *Prescribing an expansion deformation with the* $\boldsymbol{\mathcal{F}}$ *below yields*

$$[\boldsymbol{\mathcal{F}}] = \begin{bmatrix} 1+\varepsilon & 0 & 0 \\ 0 & 1+\varepsilon & 0 \\ 0 & 0 & 1+\varepsilon \end{bmatrix} \qquad \Rightarrow \qquad [\boldsymbol{\varepsilon}] = \begin{bmatrix} \varepsilon & 0 & 0 \\ 0 & \varepsilon & 0 \\ 0 & 0 & \varepsilon \end{bmatrix}, \tag{4.129}$$

which renders the energy densities

$$\Psi_{\mathrm{CCM}} = \frac{9}{2}\kappa\varepsilon^2 \quad \text{and} \quad \Psi_{\mathrm{H}}^{\mathrm{3D}} = \left[\frac{\pi}{4}C_1\delta^4 + \frac{\pi^3}{6}C_2\delta^8 + \frac{9\pi^4}{64}C_3\delta^{12}\right]\varepsilon^2 , \tag{4.130}$$

that result in the relation

$$\kappa = \frac{\pi}{18}C_1\delta^4 + \frac{\pi^3}{27}C_2\delta^8 + \frac{\pi^4}{32}C_3\delta^{12} \tag{4.131}$$

when equated, validating the previously derived relation in Table 4.6.

Uni-Axial Tension *In the uni-axial tension test, the domain is extended along*

y and relaxed along x and z, imposing a traction-free condition along x and z as

$$[\boldsymbol{\mathcal{F}}] = \begin{bmatrix} 1+\varepsilon^* & 0 & 0 \\ 0 & 1+\varepsilon & 0 \\ 0 & 0 & 1+\varepsilon^* \end{bmatrix} \qquad \text{with} \qquad \varepsilon^* = -\nu\varepsilon\,, \tag{4.132}$$

rendering the following energy density

$$\begin{aligned} \Psi_{\mathrm{H}}^{3\mathrm{D}} = &\left[\frac{\pi}{20}C_1\delta^4 + \frac{\pi^3}{45}C_2\delta^8 + \frac{\pi^4}{64}C_3\delta^{12}\right]\varepsilon^2 \\ &- \left[\Big[2\nu-1\Big]\frac{\pi}{15}C_1\delta^4 + \Big[7\nu-6\Big]\frac{\pi^3}{90}C_2\delta^8 + \Big[\nu-1\Big]\frac{\pi^4}{16}C_3\delta^{12}\right]\nu\,\varepsilon^2\,. \end{aligned} \tag{4.133}$$

To impose equilibrium, we set the variation of $\Psi_{\mathrm{H}}^{3\mathrm{D}}$ *to zero*

$$\delta\Psi_{\mathrm{H}}^{3\mathrm{D}} \doteq 0\,, \tag{4.134}$$

which can be expressed as

$$\frac{\partial\Psi_{\mathrm{H}}^{3\mathrm{D}}}{\partial\varepsilon}\delta\varepsilon + \frac{\partial\Psi_{\mathrm{H}}^{3\mathrm{D}}}{\partial\nu}\delta\nu \doteq 0\,. \tag{4.135}$$

Here the variation of ε *is zero, as* ε *is a prescribed variable, unlike the variation of* ν*, which is not necessarily zero. Thus to satisfy equilibrium, the variation of* $\Psi_{\mathrm{H}}^{3\mathrm{D}}$ *with respect to* ν *should yield zero. Imposing this condition gives*

$$\begin{aligned} &\frac{\partial\Psi_{\mathrm{H}}^{3\mathrm{D}}}{\partial\nu} \doteq 0 \\ &\hookrightarrow \quad \left[\Big[4\nu-1\Big]\frac{\pi}{15}C_1\delta^4 + \Big[7\nu-3\Big]\frac{\pi^3}{45}C_2\delta^8 + \Big[2\nu-1\Big]\frac{\pi^4}{16}C_3\delta^{12}\right]\varepsilon^2 \doteq 0\,, \end{aligned} \tag{4.136}$$

which immediately renders

$$\nu = \frac{48\,C_1 + 48\,\pi^2 C_2\delta^4 + 45\,\pi^3 C_3\delta^8}{2\big[96\,C_1 + 45\,\pi^2 C_2\delta^4 + 45\,\pi^3 C_3\delta^8\big]}\,, \tag{4.137}$$

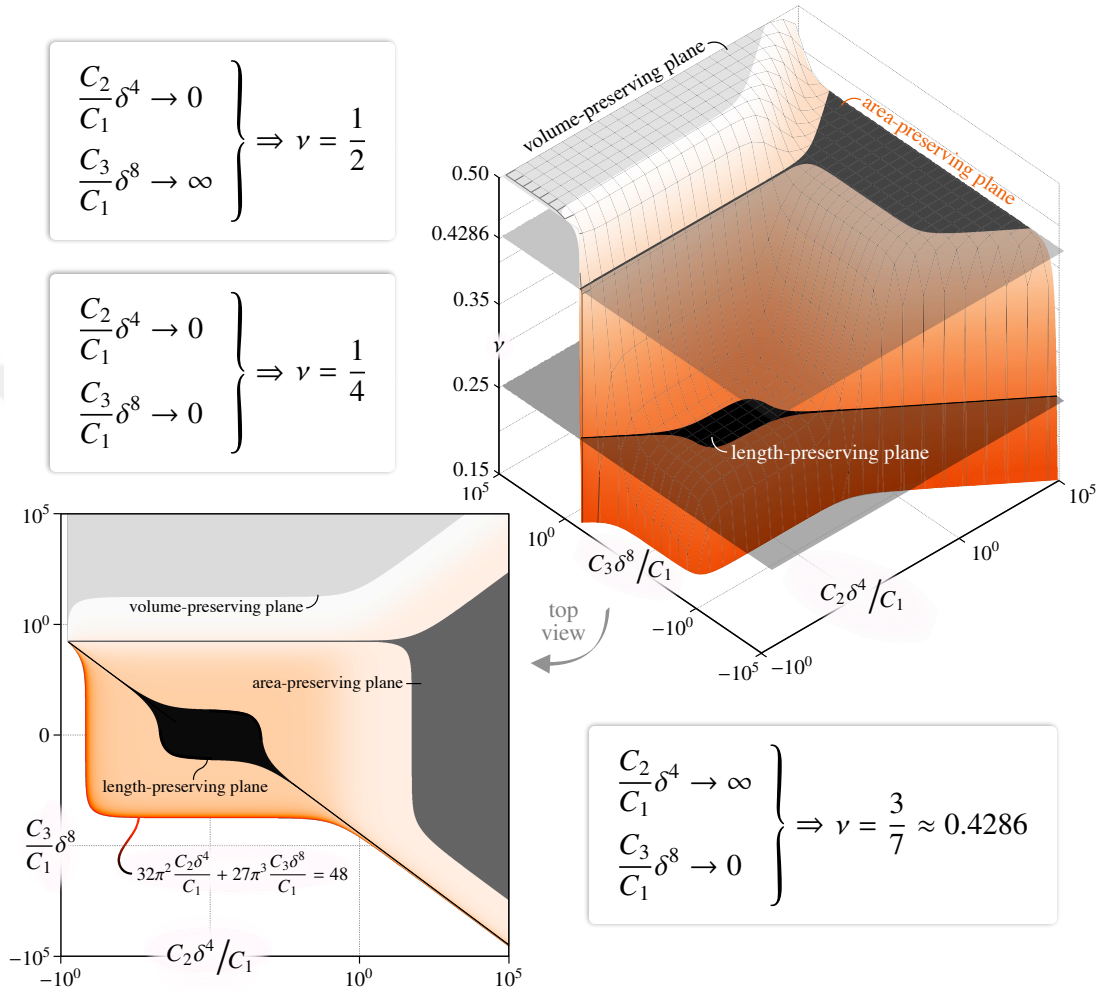

Figure 4.4: Poisson ratio ν versus the material parameters of CPD, the ratio $\frac{C_2}{C_1}\delta^4$ and $\frac{C_3}{C_1}\delta^8$, when $C_1 > 0$.

verifying the ν previously derived for a generic, affine deformation, given in Table 4.6. It can be seen immediately that in the absence of two and three-neighbor interactions, i.e. $C_2 = 0$ and $C_3 = 0$, the Poisson ratio recovers $\frac{1}{4}$, which is well established for bond-based PD. □

Lastly, we look at the behavior of the four CPD parameters combined. Figure 4.4 illustrates the three prevalent values of the Poisson ratio for different CPD parameters. There exists a *length preserving* plane, where C_1 is dominant over the remaining two elastic parameters, resulting in a bond-based response with $\nu = \frac{1}{4}$, as expected. Where C_3 is dominant, we see the *volume preserving* plane,

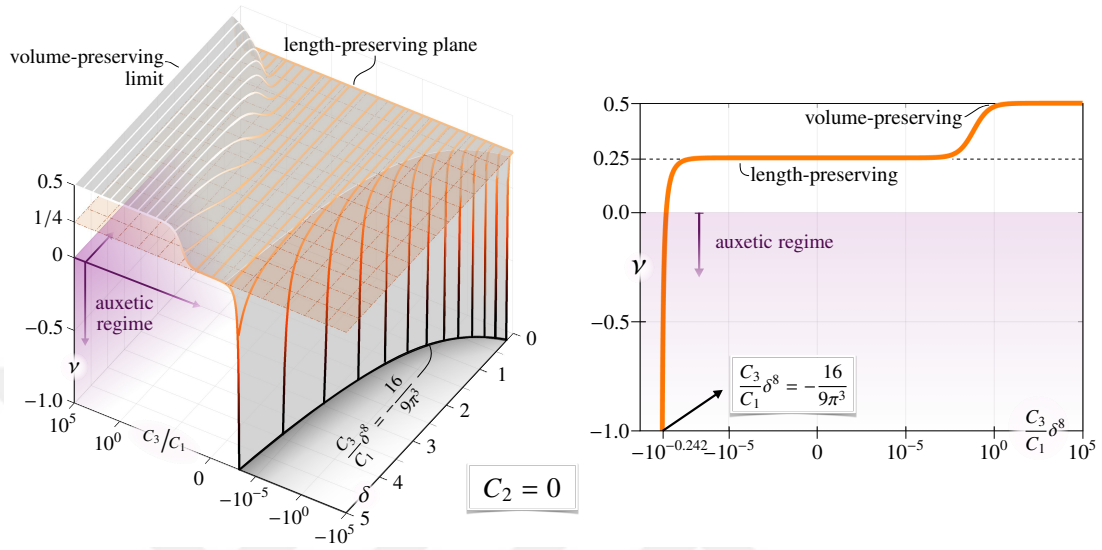

Figure 4.5: The variation of the Poisson ratio ν with the material parameters of CPD, $\frac{C_3}{C_1}$ and δ, for $C_2 = 0$, and $C_1 > 0$.

on which the material is nearly incompressible, with $\nu = \frac{1}{2}$. A rather unexpected observation is the *area preserving* plane that yields a Poisson ratio of $\frac{3}{7}$, where C_2 dominates the material response.

Remark on why $C_2 = 0$ is both physically and mathematically a valid assumption *A key feature of the CPD formulation is its "inheritance" in the sense of downward compatibility. That is, in the absence of two-neighbor and three-neighbor interactions CPD must recover purely bond-based PD. In our framework, this feature is embedded in the additive decomposition of the energy density (2.8) to its contributions from one-, two- and three-neighbor interactions. On the other hand, in order to satisfy the well-established point-wise stability conditions (i) D_1 must be positive as it is equivalent to the shear modulus μ and (ii) $5/3D_1 + D_2$ must be positive as it is equivalent to the bulk modulus κ. Mathematically speaking, these two conditions can allow for $C_1 < 0$ as long as $D_1 > 0$ and $5/3D_1 + D_2 > 0$. Physically speaking, however, we preclude the case of $C_1 < 0$ since it does not allow for $C_2 = 0$ and $C_3 = 0$. Note that $C_2 = 0$ and $C_3 = 0$ must remain a permissible choice since it recovers a purely bond-based PD formulation. This implies, without loss of generality and at small deformations, we can define an admissible range of CPD material parameters that are to be sufficiently, but*

not necessarily, fulfilled. Therefore, we impose $C_2 = 0$ resulting in a CPD constitutive law that has only two material parameters C_1 and C_3. Note that this assumption is not only physically meaningful but also mathematically supported, or even motivated, (i) by the structure of CPD material parameters (4.125) indicating the redundancy of C_2, for small deformations analysis here and (ii) from the unification (4.50) showing that the three linearized deformation measures of CPD are not independent and only two of them are sufficient. Figure 4.5 demonstrates that this assumption does not limit the range of Poisson's ratio that can be captured in CPD and that the range $-1 < \nu \leq 0.5$ is covered. Also, Table 4.8 provides the admissible range of material parameters for CPD and CCM.

Table 4.8: Admissible ranges for CPD and CCM parameters in 3D.

		CPD	
		$C_2 \neq 0$	$C_2 = 0$
CCM	$\mu \geq 0$	$C_1 \geq -\frac{6}{\pi^2\delta^4}C_2$	$C_1 \geq 0$
	$\kappa \geq 0$	$C_3 \geq -\frac{16}{9\pi^3\delta^8}C_1 - \frac{32}{27\pi\delta^4}C_2$	$C_3 \geq -\frac{32}{\pi^3\delta^8}C_1$

Remark on the physical explanation of the first Lamé parameter λ
Although from a mathematical perspective, the necessity of the first Lamé constant λ is well justified, it is commonly stated that λ, unlike other classical elasticity constants, has no physical interpretation and remains somewhat abstract. The analysis here provides a different perspective and sheds new light on the matter. In other words, now that we have established that without loss of generality $C_2 = 0$ can be assumed, the relationships $D_1 = \mu$ and $D_2 = \lambda - \mu$ hold with $D_1 \propto C_1$ and $D_2 \propto C_3$. This clearly indicates that (i) the second Lamé parameter μ is proportional to the resistance against length changes associated with one-neighbor interactions and (ii) the deviation of the first Lamé parameter from the second one, $\lambda - \mu$, is proportional to the resistance against volume changes corresponding to three-neighbor interactions. That is, if $\lambda = \mu$, then $D_2 = 0$ and therefore no additional resistance exists against volume changes due to multi-neighbor interactions, which also results in the Poisson ratio of $\nu = \frac{1}{4}$. This

finding provides a physical explanation for the first Lamé parameter λ but also it shows that (i) in fact not λ but its deviation from μ should be attributed a physical interpretation and (ii) the roots of λ can surprisingly be found in CPD, which is possibly the reason as to why this interpretation has remained elusive to date. □

Chapter 5

Super-Harmonic Model

The essential feature of the proposed super-harmonic energy densities is that the analytical solutions of the integrals can be calculated without needing to linearize the non-linear strain measures. This is a significant property as it allows us to derive the analytical solutions of the energy densities for a generic, affine, and *finite* deformation, not restricting our analysis to the small deformation regime. After arriving at the analytical solutions, we can utilize different methods to derive the material parameters in the linear elastic framework. In this section, we opted to derive the constitutive relations, and evaluate them for small deformations to find the material parameter relations between super-harmonic CPD and CCM. Before we proceed with the integration of the energy densities in the 2D and 3D formulations, we shall first examine the non-linear strains, and simplify them in a generic manner. Continuing with the simplified strains will make the derivations ahead more straightforward to follow.

5.1 Simplified strains

5.1.1 Length strain E_l in 2D and 3D

Starting with the length strain E_l, recall its definition (2.26)

$$E_l = \frac{1}{2}\left[\lambda_l^2 - 1\right] \qquad \text{where} \qquad \lambda_l := l/L\,. \tag{5.1}$$

We can rewrite the length stretch as

$$\lambda_l = \frac{\xi^{|}}{\Xi^{|}} = \frac{|\boldsymbol{\mathcal{F}}\cdot\boldsymbol{\Xi}^{|}|}{|\boldsymbol{\Xi}^{|}|} = \frac{|\boldsymbol{\Xi}^{|}||\boldsymbol{\mathcal{F}}\cdot\hat{\boldsymbol{\Xi}}^{|}|}{|\boldsymbol{\Xi}^{|}|} = |\boldsymbol{\mathcal{F}}\cdot\hat{\boldsymbol{\Xi}}^{|}|\,, \tag{5.2}$$

such that

$$\lambda_l^2 = |\boldsymbol{\mathcal{F}}\cdot\hat{\boldsymbol{\Xi}}^{|}|^2 = \left[\boldsymbol{\mathcal{F}}\cdot\hat{\boldsymbol{\Xi}}^{|}\right]\cdot\left[\boldsymbol{\mathcal{F}}\cdot\hat{\boldsymbol{\Xi}}^{|}\right] = \boldsymbol{\mathcal{C}} : \left[\hat{\boldsymbol{\Xi}}^{|}\otimes\hat{\boldsymbol{\Xi}}^{|}\right], \tag{5.3}$$

where $\boldsymbol{\mathcal{C}} := \boldsymbol{\mathcal{F}}^{\mathrm{T}}\cdot\boldsymbol{\mathcal{F}}$, the right Cauchy-Green deformation tensor. Therefore the length strain reads

$$\boxed{E_l = \frac{1}{2}\left[\boldsymbol{\mathcal{C}} : \left[\hat{\boldsymbol{\Xi}}^{|}\otimes\hat{\boldsymbol{\Xi}}^{|}\right] - 1\right]} \tag{5.4}$$

Note that this relation holds in both 2D and 3D formulations, only the tensor $\boldsymbol{\mathcal{C}}$ *changes to either* $\boldsymbol{\mathcal{C}}_{2D}$ *or* $\boldsymbol{\mathcal{C}}_{3D}$*, depending on the formulation.*

5.1.2 Area strain E_a in 2D

The area strain E_a previously defined in Eq. (2.26) is

$$E_a = \frac{1}{2}\left[\lambda_a^2 - 1\right] \qquad \text{where} \qquad \lambda_a := a/A\,. \tag{5.5}$$

Recall that in Section 4.1, the mapping between the area elements was established (4.44) to be the determinant of $\boldsymbol{\mathcal{F}}$ in 2D, or

$$\lambda_a = \frac{a}{A} = \operatorname{Det} \boldsymbol{\mathcal{F}}\,, \tag{5.6}$$

such that

$$\lambda_a^2 = \big[\operatorname{Det} \boldsymbol{\mathcal{F}}\big]^2 = \operatorname{Det} \boldsymbol{\mathcal{C}}\,. \tag{5.7}$$

Therefore the area strain in 2D reads

$$\boxed{E_a = \frac{1}{2}\big[\operatorname{Det} \boldsymbol{\mathcal{C}} - 1\big]} \tag{5.8}$$

5.1.3 Area strain E_a in 3D

Again, the area strain E_a is

$$E_a = \frac{1}{2}\left[\lambda_a^2 - 1\right] \qquad \text{where} \qquad \lambda_a := a/A\,. \tag{5.9}$$

We can rewrite the area stretch in 3D as

$$\lambda_a = \frac{|\boldsymbol{\xi}^{|} \times \boldsymbol{\xi}^{||}|}{|\boldsymbol{\Xi}^{|} \times \boldsymbol{\Xi}^{||}|} = \frac{|[\boldsymbol{\mathcal{F}} \cdot \hat{\boldsymbol{\Xi}}^{|}] \times [\boldsymbol{\mathcal{F}} \cdot \hat{\boldsymbol{\Xi}}^{||}]|}{|\hat{\boldsymbol{\Xi}}^{|} \times \hat{\boldsymbol{\Xi}}^{||}|} = \frac{|\boldsymbol{\mathcal{F}}^{\#} \cdot [\hat{\boldsymbol{\Xi}}^{|} \times \hat{\boldsymbol{\Xi}}^{||}]|}{|\hat{\boldsymbol{\Xi}}^{|} \times \hat{\boldsymbol{\Xi}}^{||}|}\,, \tag{5.10}$$

where $\boldsymbol{\mathcal{F}}^{\#} := \operatorname{Det} \boldsymbol{\mathcal{F}}\, \boldsymbol{\mathcal{F}}^{-\mathrm{T}}$ is the cofactor of $\boldsymbol{\mathcal{F}}$. This renders

$$\begin{aligned}
\lambda_a^2 &= \frac{|\boldsymbol{\mathcal{F}}^{\#} \cdot [\hat{\boldsymbol{\Xi}}^{|} \times \hat{\boldsymbol{\Xi}}^{||}]|^2}{|\hat{\boldsymbol{\Xi}}^{|} \times \hat{\boldsymbol{\Xi}}^{||}|^2} \\
&= \left[\frac{\boldsymbol{\mathcal{F}}^{\#} \cdot [\hat{\boldsymbol{\Xi}}^{|} \times \hat{\boldsymbol{\Xi}}^{||}]}{|\hat{\boldsymbol{\Xi}}^{|} \times \hat{\boldsymbol{\Xi}}^{||}|}\right] \cdot \left[\frac{\boldsymbol{\mathcal{F}}^{\#} \cdot [\hat{\boldsymbol{\Xi}}^{|} \times \hat{\boldsymbol{\Xi}}^{||}]}{|\hat{\boldsymbol{\Xi}}^{|} \times \hat{\boldsymbol{\Xi}}^{||}|}\right] \\
&= \left[\boldsymbol{\mathcal{F}}^{\#} \cdot \hat{\boldsymbol{N}}\right] \cdot \left[\boldsymbol{\mathcal{F}}^{\#} \cdot \hat{\boldsymbol{N}}\right] \qquad \text{where} \qquad \hat{\boldsymbol{N}} := \frac{\hat{\boldsymbol{\Xi}}^{|} \times \hat{\boldsymbol{\Xi}}^{||}}{|\hat{\boldsymbol{\Xi}}^{|} \times \hat{\boldsymbol{\Xi}}^{||}|}\,, \\
&= \boldsymbol{\mathcal{C}}^{\#} : \left[\hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}}\right],
\end{aligned} \tag{5.11}$$

where $\boldsymbol{\mathcal{C}}^{\#} := \boldsymbol{\mathcal{F}}^{\#\mathrm{T}} \cdot \boldsymbol{\mathcal{F}}^{\#}$, the cofactor of the right Cauchy-Green deformation tensor. Finally the area strain in 3D reads

$$\boxed{E_a = \frac{1}{2}\Big[\boldsymbol{\mathcal{C}}^{\#} : \big[\hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}}\big] - 1\Big]} \tag{5.12}$$

5.1.4 Volume strain E_v in 3D

Lastly, the volume strain E_v, a purely 3D concept, was previously defined in Eq. (2.26) as

$$E_v = \frac{1}{2}\left[\lambda_v^2 - 1\right] \qquad \text{where} \qquad \lambda_v := v/V\,. \tag{5.13}$$

When discussing the volume strain of the harmonic interactions in Section 4.2, it was established (4.44) that the mapping between the volume elements is J, the determinant of $\boldsymbol{\mathcal{F}}$, or

$$\lambda_v = \frac{v}{V} = \mathrm{Det}\,\boldsymbol{\mathcal{F}}\,, \tag{5.14}$$

such that

$$\lambda_v^2 = \big[\mathrm{Det}\,\boldsymbol{\mathcal{F}}\big]^2 = \mathrm{Det}\,\boldsymbol{\mathcal{C}}\,. \tag{5.15}$$

Therefore the volume strain reads

$$\boxed{E_v = \frac{1}{2}\big[\mathrm{Det}\,\boldsymbol{\mathcal{C}} - 1\big]} \tag{5.16}$$

5.2 Integration of the energy densities in 2D

Equipped with the simplified definitions of the non-linear strains, we continue to integrate the energy densities of the different contributions in 2D.

5.2.1 One-neighbor interactions

To get the point-wise energy density due to one-neighbor interactions Ψ_1, we integrate the super-harmonic potential ψ_1 over the horizon,

$$\Psi_1 = \int_{\mathcal{H}_0} \psi_1 \, \mathrm{d}A^{\mid} \qquad \text{where} \qquad \psi_1 := \frac{1}{2} C_1 \, L \, E_l^2 \, . \tag{5.17}$$

It was established in Eq. (5.4) that the length strain E_l is only a function of the direction vector $\hat{\boldsymbol{\Xi}}^{\mid}$ and $\boldsymbol{\mathcal{C}}$. Therefore we can split the integral into two as

$$\begin{aligned} \Psi_1 &= \int_{\mathcal{H}_0} \frac{1}{2} C_1 \, L E_l^2 \, \mathrm{d}A^{\mid} \\ &= \frac{1}{2} C_1 \int_{\Xi^{\mid}=0}^{\Xi^{\mid}=\delta} L \, \Xi^{\mid} \, \mathrm{d}\Xi^{\mid} \int_{\hat{\mathcal{H}}_0{}^{\mid}} E_l^2 \, \mathrm{d}\hat{A}^{\mid} \\ &= \frac{1}{6} C_1 \, \delta^3 \int_{\hat{\mathcal{H}}_0{}^{\mid}} E_l^2 \, \mathrm{d}\hat{A}^{\mid} \, . \end{aligned} \tag{5.18}$$

Inserting the length strain E_l previously defined in Eq. (2.26) gives

$$\begin{aligned} \Psi_1 &= \frac{1}{24} C_1 \, \delta^3 \int_{\hat{\mathcal{H}}_0{}^{\mid}} \left[\lambda_l^4 - 2 \, \lambda_l^2 + 1 \right] \mathrm{d}\hat{A}^{\mid} \\ &= \frac{1}{24} C_1 \, \delta^3 \left[\underbrace{\int_{\hat{\mathcal{H}}_0{}^{\mid}} \lambda_l^4 \, \mathrm{d}\hat{A}^{\mid}}_{\alpha} - 2 \underbrace{\int_{\hat{\mathcal{H}}_0{}^{\mid}} \lambda_l^2 \, \mathrm{d}\hat{A}^{\mid}}_{\beta} + \underbrace{\int_{\hat{\mathcal{H}}_0{}^{\mid}} 1 \, \mathrm{d}\hat{A}^{\mid}}_{\gamma} \right] . \end{aligned} \tag{5.19}$$

We shall proceed to evaluate the integrals α, β and γ separately. Starting with α and recalling the simplified definition of λ_l^2 (5.3) renders,

$$\begin{aligned} \alpha &:= \int_{\hat{\mathcal{H}}_0{}^{\mid}} \lambda_l^4 \, \mathrm{d}\hat{A}^{\mid} = \int_{\hat{\mathcal{H}}_0{}^{\mid}} \left[\boldsymbol{\mathcal{C}} : \left[\hat{\boldsymbol{\Xi}}^{\mid} \otimes \hat{\boldsymbol{\Xi}}^{\mid} \right] \right]^2 \mathrm{d}\hat{A}^{\mid} \\ &= \int_{\hat{\mathcal{H}}_0{}^{\mid}} \left[\left[\boldsymbol{\mathcal{C}} \otimes \boldsymbol{\mathcal{C}} \right] :: \left[\hat{\boldsymbol{\Xi}}^{\mid} \otimes \hat{\boldsymbol{\Xi}}^{\mid} \otimes \hat{\boldsymbol{\Xi}}^{\mid} \otimes \hat{\boldsymbol{\Xi}}^{\mid} \right] \right] \mathrm{d}\hat{A}^{\mid} \\ &= \left[\boldsymbol{\mathcal{C}} \otimes \boldsymbol{\mathcal{C}} \right] :: \int_{\hat{\mathcal{H}}_0{}^{\mid}} \left[\hat{\boldsymbol{\Xi}}^{\mid} \otimes \hat{\boldsymbol{\Xi}}^{\mid} \otimes \hat{\boldsymbol{\Xi}}^{\mid} \otimes \hat{\boldsymbol{\Xi}}^{\mid} \right] \mathrm{d}\hat{A}^{\mid} \, . \end{aligned} \tag{5.20}$$

Lastly, invoking Lemma 7 yields

$$\alpha = \frac{1}{4}\pi\ [\boldsymbol{\mathcal{C}} \otimes \boldsymbol{\mathcal{C}}] :: \mathbb{I} = \frac{1}{4}\pi \left[\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{C}} + \boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{C}}^{\mathrm{T}} + [\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{I}}]^2\right]. \tag{5.21}$$

Since $\boldsymbol{\mathcal{C}}$ is symmetric, $\boldsymbol{\mathcal{C}} = \boldsymbol{\mathcal{C}}^{\mathrm{T}}$, and α further simplifies to

$$\alpha = \frac{1}{4}\pi \left[2\,\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{C}} + [\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{I}}]^2\right]. \tag{5.22}$$

Moving onto β,

$$\begin{aligned} \beta &:= \int_{\hat{\mathcal{H}}_0{}^{\mathrm{I}}} \lambda_I^2 \,\mathrm{d}\hat{A}^{\mathrm{I}} = \int_{\mathcal{H}_0} \left[\boldsymbol{\mathcal{C}} : \left[\hat{\boldsymbol{\Xi}}^{\mathrm{I}} \otimes \hat{\boldsymbol{\Xi}}^{\mathrm{I}}\right]\right] \mathrm{d}\hat{A}^{\mathrm{I}} \\ &= \boldsymbol{\mathcal{C}} : \int_{\hat{\mathcal{H}}_0{}^{\mathrm{I}}} \left[\hat{\boldsymbol{\Xi}}^{\mathrm{I}} \otimes \hat{\boldsymbol{\Xi}}^{\mathrm{I}}\right] \mathrm{d}\hat{A}^{\mathrm{I}}, \end{aligned} \tag{5.23}$$

which, by invoking Lemma 5, becomes

$$\beta = \pi\,\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{I}}. \tag{5.24}$$

Lastly, using Lemma 1 renders γ

$$\gamma := \int_{\hat{\mathcal{H}}_0{}^{\mathrm{I}}} 1 \,\mathrm{d}\hat{A}^{\mathrm{I}} = 2\pi. \tag{5.25}$$

Equipped with α, β and γ, we can write Ψ_1 as

$$\begin{aligned} \Psi_1 &= \frac{1}{24}\, C_1\, \delta^3 \left[\alpha - 2\beta + \gamma\right] \\ &= \frac{1}{24}\, C_1\, \delta^3 \left[\frac{\pi}{4}\left[2\,\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{C}} + [\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{I}}]^2\right] - 2\pi\,\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{I}} + 2\pi\right], \end{aligned} \tag{5.26}$$

which finally reads

$$\boxed{\Psi_1 = \frac{1}{96}\pi\, C_1\, \delta^3 \left[2\,\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{C}} + [\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{I}}]^2 - 8\,\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{I}} + 8\right]} \tag{5.27}$$

5.2.2 Two-neighbor interactions

In 2D, the point-wise energy density due to two-neighbor interactions is the double integral of the super-harmonic potential ψ_2 over the horizon,

$$\Psi_2 = \int_{\mathcal{H}_0}\int_{\mathcal{H}_0} \psi_2 \, \mathrm{d}A^{\shortmid} \, \mathrm{d}A^{\shortmid\shortmid} \qquad \text{where} \qquad \psi_2 := \frac{1}{2} C_2 \, A \, E_a^2 \, . \tag{5.28}$$

Recalling that $A = |\boldsymbol{\Xi}^{\shortmid}||\boldsymbol{\Xi}^{\shortmid\shortmid}||\hat{\boldsymbol{\Xi}}^{\shortmid} \times \hat{\boldsymbol{\Xi}}^{\shortmid\shortmid}|$, and the fact that E_a, in 2D, is only a function of $\boldsymbol{\mathcal{C}}$ (5.8) we can rewrite Ψ_2 as

$$\begin{aligned}
\Psi_2 &= \int_{\mathcal{H}_0}\int_{\mathcal{H}_0} \frac{1}{2} C_2 \, A \, E_a^2 \, \mathrm{d}A^{\shortmid} \, \mathrm{d}A^{\shortmid\shortmid} \\
&= \frac{1}{2} C_2 \int_{\Xi^{\shortmid\shortmid}=0}^{\Xi^{\shortmid\shortmid}=\delta} {\Xi^{\shortmid\shortmid}}^2 \, \mathrm{d}\Xi^{\shortmid\shortmid} \int_{\Xi^{\shortmid}=0}^{\Xi^{\shortmid}=\delta} {\Xi^{\shortmid}}^2 \, \mathrm{d}\Xi^{\shortmid} \int_{\hat{\mathcal{H}}_0{}^{\shortmid\shortmid}} \int_{\hat{\mathcal{H}}_0{}^{\shortmid}} |\hat{\boldsymbol{\Xi}}^{\shortmid} \times \hat{\boldsymbol{\Xi}}^{\shortmid\shortmid}| \, E_a^2 \, \mathrm{d}\hat{A}^{\shortmid} \, \mathrm{d}\hat{A}^{\shortmid\shortmid} \\
&= \frac{1}{18} C_2 \, \delta^6 \int_{\hat{\mathcal{H}}_0{}^{\shortmid\shortmid}} \int_{\hat{\mathcal{H}}_0{}^{\shortmid}} |\hat{\boldsymbol{\Xi}}^{\shortmid} \times \hat{\boldsymbol{\Xi}}^{\shortmid\shortmid}| \, E_a^2 \, \mathrm{d}\hat{A}^{\shortmid} \, \mathrm{d}\hat{A}^{\shortmid\shortmid} \, .
\end{aligned} \tag{5.29}$$

Utilizing the previously derived, simplified form of E_a (5.8) yields

$$\Psi_2 = \frac{1}{72} C_2 \, \delta^6 \big[\mathrm{Det}\, \boldsymbol{\mathcal{C}} - 1\big]^2 \int_{\hat{\mathcal{H}}_0{}^{\shortmid\shortmid}} \int_{\hat{\mathcal{H}}_0{}^{\shortmid}} |\hat{\boldsymbol{\Xi}}^{\shortmid} \times \hat{\boldsymbol{\Xi}}^{\shortmid\shortmid}| \, \mathrm{d}\hat{A}^{\shortmid} \, \mathrm{d}\hat{A}^{\shortmid\shortmid} \, , \tag{5.30}$$

which, by invoking Lemma 3, reduces to

$$\boxed{\Psi_2 = \frac{1}{9} \pi \, C_2 \, \delta^6 \big[\mathrm{Det}\, \boldsymbol{\mathcal{C}} - 1\big]^2} \tag{5.31}$$

5.2.3 Total point-wise energy density

Recalling from Eq.(2.24) that the total energy density of super-harmonic CPD in 2D is

$$\Psi_{\mathrm{S}}^{\mathrm{2D}} := \frac{1}{2} \Psi_1 + \frac{1}{3} \Psi_2 \, , \tag{5.32}$$

and using the results of Eq.(5.27) and Eq.(5.31) renders

$$\Psi_{\rm S}^{\rm 2D} = \frac{1}{192}\pi\, C_1\, \delta^3 \Big[2\,\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{C}} + [\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{I}}]^2 - 8\,\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{I}} + 8 \Big] + \frac{1}{27}\pi\, C_2\, \delta^6 \big[\mathrm{Det}\,\boldsymbol{\mathcal{C}} - 1 \big]^2 , \tag{5.33}$$

or

$$\boxed{\begin{aligned} \Psi_{\rm S}^{\rm 2D} = {} & B_1 \Big[2\,\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{C}} + [\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{I}}]^2 - 8\,\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{I}} + 8 \Big] \\ & + B_2 \big[\mathrm{Det}\,\boldsymbol{\mathcal{C}} - 1 \big]^2 \end{aligned}} \tag{5.34}$$

where

$$B_1 := \frac{1}{192}\pi\, C_1\, \delta^3 \qquad , \qquad B_2 := \frac{1}{27}\pi\, C_2\, \delta^6 \, . \tag{5.35}$$

This total point-wise energy density can also be written in the generalized form

$$\boxed{\begin{aligned} \Psi_{\rm S}^{\rm 2D} = {} & B_1 \Big[2\,\boldsymbol{\mathcal{C}}_1 : \boldsymbol{\mathcal{C}}_1 + [\boldsymbol{\mathcal{C}}_1 : \boldsymbol{\mathcal{I}}]^2 - 8\,\boldsymbol{\mathcal{C}}_1 : \boldsymbol{\mathcal{I}} + 8 \Big] \\ & + \frac{1}{8} B_2 \Big[2\,\boldsymbol{\mathcal{C}}_2 : \boldsymbol{\mathcal{C}}_2 + [\boldsymbol{\mathcal{C}}_2 : \boldsymbol{\mathcal{I}}]^2 - 8\,\boldsymbol{\mathcal{C}}_2 : \boldsymbol{\mathcal{I}} + 8 \Big] \end{aligned}} \tag{5.36}$$

where

$$\boldsymbol{\mathcal{C}}_1 := \boldsymbol{\mathcal{C}} \qquad , \qquad \boldsymbol{\mathcal{C}}_2 := \mathrm{Det}\,\boldsymbol{\mathcal{C}}\,\boldsymbol{\mathcal{I}} \, . \tag{5.37}$$

Here, the energy densities due to the different interactions are essentially unified to have the same form. Alternatively, the total point-wise energy density can also be written in terms of the invariants of $\boldsymbol{\mathcal{C}}$ in 2D, that are $I_1 = \mathrm{Tr}\,\boldsymbol{\mathcal{C}}$ and $I_2 = \mathrm{Det}\,\boldsymbol{\mathcal{C}}$. To do so, we make use of the relation

$$\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{C}} = {I_1}^2 - 2\, I_2 \, , \tag{5.38}$$

and get

$$\boxed{\Psi_{\mathrm{S}}^{\mathrm{2D}} = \quad B_1 \left[3\, {I_1}^2 - 8\, I_1 - 4\, I_2 + 8\right] + B_2 \left[{I_2}^2 - 2\, I_2 + 1\right]} \tag{5.39}$$

5.3 Integration of the energy densities in 3D

Here, we repeat the process in Section 5.2, now in the 3D setting, accounting for three-neighbor interactions.

5.3.1 One-neighbor interactions

To get the point-wise energy density due to one-neighbor interactions Ψ_1, we integrate the super-harmonic potential ψ_1 over the horizon,

$$\Psi_1 = \int_{\mathcal{H}_0} \psi_1 \, \mathrm{d}V^{\shortmid} \qquad \text{where} \qquad \psi_1 := \frac{1}{2}\, C_1\, L\, E_l^2 \,. \tag{5.40}$$

It was established in Eq. (5.4) that the length strain E_l is only a function of the direction vector $\hat{\boldsymbol{\Xi}}^{\shortmid}$ and $\boldsymbol{\mathcal{C}}$. Therefore we can split the integral into two as

$$\begin{aligned}
\Psi_1 &= \int_{\mathcal{H}_0} \frac{1}{2}\, C_1\, L E_l^2 \, \mathrm{d}V^{\shortmid} \\
&= \frac{1}{2}\, C_1 \int_{\Xi^{\shortmid}=0}^{\Xi^{\shortmid}=\delta} L\, {\Xi^{\shortmid}}^2 \, \mathrm{d}\Xi^{\shortmid} \int_{\hat{\mathcal{H}}_0{}^{\shortmid}} E_l^2 \, \mathrm{d}\hat{V}^{\shortmid} \\
&= \frac{1}{8}\, C_1\, \delta^4 \int_{\hat{\mathcal{H}}_0{}^{\shortmid}} E_l^2 \, \mathrm{d}\hat{V}^{\shortmid} \,.
\end{aligned} \tag{5.41}$$

Inserting the length strain E_l previously defined in Eq. (2.26) gives

$$\begin{aligned}\Psi_1 &= \frac{1}{32}\,C_1\,\delta^4 \int_{\hat{\mathcal{H}}_0{}^|} \left[\lambda_l^4 - 2\,\lambda_l^2 + 1\right] \mathrm{d}\hat{V}^| \\ &= \frac{1}{32}\,C_1\,\delta^4 \Bigg[\underbrace{\int_{\hat{\mathcal{H}}_0{}^|} \lambda_l^4 \,\mathrm{d}\hat{V}^|}_{\alpha} - 2 \underbrace{\int_{\hat{\mathcal{H}}_0{}^|} \lambda_l^2 \,\mathrm{d}\hat{V}^|}_{\beta} + \underbrace{\int_{\hat{\mathcal{H}}_0{}^|} 1 \,\mathrm{d}\hat{V}^|}_{\gamma} \Bigg] .\end{aligned} \tag{5.42}$$

We shall proceed to evaluate the integrals α, β and γ separately. Starting with α and recalling the simplified definition of λ_l^2 (5.3) renders,

$$\begin{aligned}\alpha &:= \int_{\hat{\mathcal{H}}_0{}^|} \lambda_l^4 \,\mathrm{d}\hat{V}^| = \int_{\hat{\mathcal{H}}_0{}^|} \Big[\boldsymbol{\mathcal{C}} : \big[\hat{\boldsymbol{\Xi}}^| \otimes \hat{\boldsymbol{\Xi}}^|\big]\Big]^2 \,\mathrm{d}\hat{V}^| \\ &= \int_{\hat{\mathcal{H}}_0{}^|} \Big[\big[\boldsymbol{\mathcal{C}} \otimes \boldsymbol{\mathcal{C}}\big] :: \big[\hat{\boldsymbol{\Xi}}^| \otimes \hat{\boldsymbol{\Xi}}^| \otimes \hat{\boldsymbol{\Xi}}^| \otimes \hat{\boldsymbol{\Xi}}^|\big]\Big] \,\mathrm{d}\hat{V}^| \\ &= \big[\boldsymbol{\mathcal{C}} \otimes \boldsymbol{\mathcal{C}}\big] :: \int_{\hat{\mathcal{H}}_0{}^|} \big[\hat{\boldsymbol{\Xi}}^| \otimes \hat{\boldsymbol{\Xi}}^| \otimes \hat{\boldsymbol{\Xi}}^| \otimes \hat{\boldsymbol{\Xi}}^|\big] \,\mathrm{d}\hat{V}^| .\end{aligned} \tag{5.43}$$

Lastly, invoking Lemma 8 yields

$$\begin{aligned}\alpha &= \frac{4}{15}\pi\, \big[\boldsymbol{\mathcal{C}} \otimes \boldsymbol{\mathcal{C}}\big] :: \mathbb{I} \\ &= \frac{4}{15}\pi \Big[\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{C}} + \boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{C}}^{\mathrm{T}} + [\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{I}}]^2\Big] .\end{aligned} \tag{5.44}$$

Since $\boldsymbol{\mathcal{C}}$ is symmetric, $\boldsymbol{\mathcal{C}} = \boldsymbol{\mathcal{C}}^{\mathrm{T}}$, and α further simplifies to

$$\alpha = \frac{4}{15}\pi \Big[2\,\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{C}} + [\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{I}}]^2\Big] . \tag{5.45}$$

Moving onto β,

$$\begin{aligned}\beta &:= \int_{\hat{\mathcal{H}}_0{}^|} \lambda_l^2 \,\mathrm{d}\hat{V}^| = \int_{\mathcal{H}_0} \Big[\boldsymbol{\mathcal{C}} : \big[\hat{\boldsymbol{\Xi}}^| \otimes \hat{\boldsymbol{\Xi}}^|\big]\Big] \,\mathrm{d}\hat{V}^| \\ &= \boldsymbol{\mathcal{C}} : \int_{\hat{\mathcal{H}}_0{}^|} \big[\hat{\boldsymbol{\Xi}}^| \otimes \hat{\boldsymbol{\Xi}}^|\big] \,\mathrm{d}\hat{V}^| ,\end{aligned} \tag{5.46}$$

which, by invoking Lemma 6, becomes

$$\beta = \frac{4}{3}\pi\, \boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{I}} . \tag{5.47}$$

Lastly, using Lemma 2 renders γ

$$\gamma := \int_{\hat{\mathcal{H}}_0{}^{|}} 1 \, \mathrm{d}\hat{V}^{|} = 4\pi \, . \tag{5.48}$$

Equipped with α, β and γ, we can write Ψ_1 as

$$\begin{aligned} \Psi_1 &= \frac{1}{32} C_1 \, \delta^4 \left[\alpha - 2\beta + \gamma \right] \\ &= \frac{1}{32} C_1 \, \delta^4 \left[\frac{4\pi}{15} \Big[2\, \boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{C}} + [\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{I}}]^2 \Big] - \frac{8}{3} \pi \, \boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{I}} + 4\pi \right] , \end{aligned} \tag{5.49}$$

which finally yields

$$\boxed{\Psi_1 = \frac{1}{120} \pi \, C_1 \, \delta^4 \left[2\, \boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{C}} + [\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{I}}]^2 - 10\, \boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{I}} + 15 \right]} \tag{5.50}$$

5.3.2 Two-neighbor interactions

The point-wise energy density due to two-neighbor interactions Ψ_2, is now the double integral of the super-harmonic potential ψ_2 over the horizon,

$$\Psi_2 = \int_{\mathcal{H}_0} \int_{\mathcal{H}_0} \psi_2 \, \mathrm{d}V^{|} \, \mathrm{d}V^{||} \qquad \text{where} \qquad \psi_2 := \frac{1}{2} C_2 \, A \, E_a^2 \, . \tag{5.51}$$

It was established in Eq. (5.12) that the area strain E_a is only a function of the direction vectors $\hat{\boldsymbol{\Xi}}^{|}$, $\hat{\boldsymbol{\Xi}}^{||}$ and $\boldsymbol{\mathcal{C}}^{\#}$. After recalling that $A = |\boldsymbol{\Xi}^{|}||\boldsymbol{\Xi}^{||}||\hat{\boldsymbol{\Xi}}^{|} \times \hat{\boldsymbol{\Xi}}^{||}|$, we can write Ψ_2 as two independent integrals

$$\begin{aligned} \Psi_2 &= \int_{\mathcal{H}_0} \int_{\mathcal{H}_0} \frac{1}{2} C_2 \, A \, E_a^2 \, \mathrm{d}V^{|} \, \mathrm{d}V^{||} \\ &= \frac{1}{2} C_2 \int_{\Xi^{||}=0}^{\Xi^{||}=\delta} {\Xi^{||}}^3 \, \mathrm{d}\Xi^{||} \int_{\Xi^{|}=0}^{\Xi^{|}=\delta} {\Xi^{|}}^3 \, \mathrm{d}\Xi^{|} \int_{\hat{\mathcal{H}}_0{}^{||}} \int_{\hat{\mathcal{H}}_0{}^{|}} |\hat{\boldsymbol{\Xi}}^{|} \times \hat{\boldsymbol{\Xi}}^{||}| \, E_a^2 \, \mathrm{d}\hat{V}^{|} \, \mathrm{d}\hat{V}^{||} \\ &= \frac{1}{32} C_2 \, \delta^8 \int_{\hat{\mathcal{H}}_0{}^{||}} \int_{\hat{\mathcal{H}}_0{}^{|}} |\hat{\boldsymbol{\Xi}}^{|} \times \hat{\boldsymbol{\Xi}}^{||}| \, E_a^2 \, \mathrm{d}\hat{V}^{|} \, \mathrm{d}\hat{V}^{||} \, . \end{aligned} \tag{5.52}$$

Inserting the previously defined (2.26) area strain E_a gives

$$\begin{aligned}\Psi_2 &= \frac{1}{128}\, C_2\, \delta^8 \int_{\hat{\mathcal{H}}_0{}^{\shortparallel}} \int_{\hat{\mathcal{H}}_0{}^{\shortmid}} |\hat{\boldsymbol{\Xi}}^{\shortmid} \times \hat{\boldsymbol{\Xi}}^{\shortparallel}|\, \left[\lambda_a^4 - 2\,\lambda_a^2 + 1\right] \mathrm{d}\hat{V}^{\shortmid}\, \mathrm{d}\hat{V}^{\shortparallel} \\ &= \frac{1}{128}\, C_2\, \delta^8 \left[\alpha - 2\beta + \gamma\right] ,\end{aligned} \tag{5.53}$$

where

$$\begin{aligned}\alpha &:= \int_{\hat{\mathcal{H}}_0{}^{\shortparallel}} \int_{\hat{\mathcal{H}}_0{}^{\shortmid}} |\hat{\boldsymbol{\Xi}}^{\shortmid} \times \hat{\boldsymbol{\Xi}}^{\shortparallel}|\, \lambda_a^4\, \mathrm{d}\hat{V}^{\shortmid}\, \mathrm{d}\hat{V}^{\shortparallel} , \\ \beta &:= \int_{\hat{\mathcal{H}}_0{}^{\shortparallel}} \int_{\hat{\mathcal{H}}_0{}^{\shortmid}} |\hat{\boldsymbol{\Xi}}^{\shortmid} \times \hat{\boldsymbol{\Xi}}^{\shortparallel}|\, \lambda_a^2\, \mathrm{d}\hat{V}^{\shortmid}\, \mathrm{d}\hat{V}^{\shortparallel} , \\ \gamma &:= \int_{\hat{\mathcal{H}}_0{}^{\shortparallel}} \int_{\hat{\mathcal{H}}_0{}^{\shortmid}} |\hat{\boldsymbol{\Xi}}^{\shortmid} \times \hat{\boldsymbol{\Xi}}^{\shortparallel}|\, \mathrm{d}\hat{V}^{\shortmid}\, \mathrm{d}\hat{V}^{\shortparallel} .\end{aligned} \tag{5.54}$$

Next, we will integrate α, β and γ respectively. Recalling the simplified definition of λ_a^2 (5.11) renders,

$$\begin{aligned}\alpha &:= \int_{\hat{\mathcal{H}}_0{}^{\shortparallel}} \int_{\hat{\mathcal{H}}_0{}^{\shortmid}} |\hat{\boldsymbol{\Xi}}^{\shortmid} \times \hat{\boldsymbol{\Xi}}^{\shortparallel}|\, \lambda_a^4\, \mathrm{d}\hat{V}^{\shortmid} = \int_{\hat{\mathcal{H}}_0{}^{\shortmid}} \left[\boldsymbol{\mathcal{C}}^{\#} : \left[\hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}}\right]\right]^2 \mathrm{d}\hat{V}^{\shortmid}\, \mathrm{d}\hat{V}^{\shortparallel} \\ &= \int_{\hat{\mathcal{H}}_0{}^{\shortparallel}} \int_{\hat{\mathcal{H}}_0{}^{\shortmid}} |\hat{\boldsymbol{\Xi}}^{\shortmid} \times \hat{\boldsymbol{\Xi}}^{\shortparallel}|\, \left[\left[\boldsymbol{\mathcal{C}}^{\#} \otimes \boldsymbol{\mathcal{C}}^{\#}\right] :: \left[\hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}}\right]\right] \mathrm{d}\hat{V}^{\shortmid}\, \mathrm{d}\hat{V}^{\shortparallel} \\ &= \left[\boldsymbol{\mathcal{C}}^{\#} \otimes \boldsymbol{\mathcal{C}}^{\#}\right] :: \int_{\hat{\mathcal{H}}_0{}^{\shortparallel}} \int_{\hat{\mathcal{H}}_0{}^{\shortmid}} |\hat{\boldsymbol{\Xi}}^{\shortmid} \times \hat{\boldsymbol{\Xi}}^{\shortparallel}|\, \left[\hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}}\right] \mathrm{d}\hat{V}^{\shortmid}\, \mathrm{d}\hat{V}^{\shortparallel} .\end{aligned} \tag{5.55}$$

Lastly, invoking Lemma 11 yields

$$\begin{aligned}\alpha &= \frac{4}{15}\pi^3\, \left[\boldsymbol{\mathcal{C}}^{\#} \otimes \boldsymbol{\mathcal{C}}^{\#}\right] :: \mathbb{I} \\ &= \frac{4}{15}\pi^3 \left[\boldsymbol{\mathcal{C}}^{\#} : \boldsymbol{\mathcal{C}}^{\#} + \boldsymbol{\mathcal{C}}^{\#} : \boldsymbol{\mathcal{C}}^{\#\mathrm{T}} + [\boldsymbol{\mathcal{C}}^{\#} : \boldsymbol{\mathcal{I}}]^2\right] .\end{aligned} \tag{5.56}$$

Since $\boldsymbol{\mathcal{C}}$ is symmetric, so is $\boldsymbol{\mathcal{C}}^{\#}$, and thus α further simplifies to

$$\alpha = \frac{4}{15}\pi^3 \left[2\,\boldsymbol{\mathcal{C}}^{\#} : \boldsymbol{\mathcal{C}}^{\#} + [\boldsymbol{\mathcal{C}}^{\#} : \boldsymbol{\mathcal{I}}]^2\right] . \tag{5.57}$$

Moving onto β,

$$\begin{aligned}\beta &:= \int_{\hat{\mathcal{H}}_0{}^{\shortparallel}} \int_{\hat{\mathcal{H}}_0{}^{\shortmid}} |\hat{\boldsymbol{\Xi}}^{\shortmid} \times \hat{\boldsymbol{\Xi}}^{\shortparallel}|\, \lambda_l^2 \, \mathrm{d}\hat{V}^{\shortmid} \, \mathrm{d}\hat{V}^{\shortparallel} \\ &= \int_{\hat{\mathcal{H}}_0{}^{\shortparallel}} \int_{\mathcal{H}_0} |\hat{\boldsymbol{\Xi}}^{\shortmid} \times \hat{\boldsymbol{\Xi}}^{\shortparallel}|\, \Big[\boldsymbol{\mathcal{C}}^{\#} : \big[\hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}}\big]\Big] \, \mathrm{d}\hat{V}^{\shortmid} \, \mathrm{d}\hat{V}^{\shortparallel} \\ &= \boldsymbol{\mathcal{C}}^{\#} : \int_{\hat{\mathcal{H}}_0{}^{\shortparallel}} \int_{\hat{\mathcal{H}}_0{}^{\shortmid}} |\hat{\boldsymbol{\Xi}}^{\shortmid} \times \hat{\boldsymbol{\Xi}}^{\shortparallel}|\, \big[\hat{\boldsymbol{N}} \otimes \hat{\boldsymbol{N}}\big] \, \mathrm{d}\hat{V}^{\shortmid} \, \mathrm{d}\hat{V}^{\shortparallel} \,,\end{aligned} \tag{5.58}$$

which, by invoking Lemma 10, becomes

$$\beta = \frac{4}{3}\pi^3 \, \boldsymbol{\mathcal{C}}^{\#} : \boldsymbol{\mathcal{I}} \,. \tag{5.59}$$

Lastly, using Lemma 3, γ reduces to

$$\gamma := \int_{\hat{\mathcal{H}}_0{}^{\shortparallel}} \int_{\hat{\mathcal{H}}_0{}^{\shortmid}} |\hat{\boldsymbol{\Xi}}^{\shortmid} \times \hat{\boldsymbol{\Xi}}^{\shortparallel}| \, \mathrm{d}\hat{V}^{\shortmid} \, \mathrm{d}\hat{V}^{\shortparallel} = 4\pi^3 \,. \tag{5.60}$$

Equipped with α, β and γ, we can write Ψ_2 as

$$\begin{aligned}\Psi_2 &= \frac{1}{128} \, C_2 \, \delta^8 \, [\alpha - 2\beta + \gamma] \\ &= \frac{1}{128} \, C_1 \, \delta^8 \left[\frac{4\pi^3}{15}\Big[2\,\boldsymbol{\mathcal{C}}^{\#} : \boldsymbol{\mathcal{C}}^{\#} + [\boldsymbol{\mathcal{C}}^{\#} : \boldsymbol{\mathcal{I}}]^2\Big] - \frac{8}{3}\pi^3 \, \boldsymbol{\mathcal{C}}^{\#} : \boldsymbol{\mathcal{I}} + 4\pi^3\right] ,\end{aligned} \tag{5.61}$$

which finally reads

$$\boxed{\Psi_2 = \frac{1}{480}\pi^3 \, C_1 \, \delta^8 \left[2\,\boldsymbol{\mathcal{C}}^{\#} : \boldsymbol{\mathcal{C}}^{\#} + [\boldsymbol{\mathcal{C}}^{\#} : \boldsymbol{\mathcal{I}}]^2 - 10\,\boldsymbol{\mathcal{C}}^{\#} : \boldsymbol{\mathcal{I}} + 15\right]} \tag{5.62}$$

5.3.3 Three-neighbor interactions

For three-neighbor interactions, the point-wise energy density Ψ_3, is the triple integral of the super-harmonic potential ψ_3 over the horizon,

$$\Psi_3 = \int_{\mathcal{H}_0} \int_{\mathcal{H}_0} \int_{\mathcal{H}_0} \psi_3 \, \mathrm{d}V^{\shortmid} \, \mathrm{d}V^{\shortparallel} \, \mathrm{d}V^{\shortparallel\shortmid} \qquad \text{where} \qquad \psi_3 := \frac{1}{2} \, C_3 \, V \, E_v^2 \,. \tag{5.63}$$

Recalling that $V = |\boldsymbol{\Xi}^{\mathrm{I}}||\boldsymbol{\Xi}^{\mathrm{II}}||\boldsymbol{\Xi}^{\mathrm{III}}|\big|\hat{\boldsymbol{\Xi}}^{\mathrm{I}} \cdot [\hat{\boldsymbol{\Xi}}^{\mathrm{II}} \times \hat{\boldsymbol{\Xi}}^{\mathrm{III}}]\big|$, and the fact that E_v is only a function of $\boldsymbol{\mathcal{C}}$ (5.16) we can rewrite Ψ_3 as

$$\begin{aligned}
\Psi_3 &= \int_{\mathcal{H}_0}\int_{\mathcal{H}_0}\int_{\mathcal{H}_0} \frac{1}{2}\, C_3\, V\, E_v^2\, \mathrm{d}V^{\mathrm{I}}\, \mathrm{d}V^{\mathrm{II}}\, \mathrm{d}V^{\mathrm{III}} \\
&= \frac{1}{2}\, C_3 \int_{\Xi^{\mathrm{III}}=0}^{\Xi^{\mathrm{III}}=\delta} {\Xi^{\mathrm{III}}}^3\, \mathrm{d}\Xi^{\mathrm{III}} \int_{\Xi^{\mathrm{II}}=0}^{\Xi^{\mathrm{II}}=\delta} {\Xi^{\mathrm{II}}}^3\, \mathrm{d}\Xi^{\mathrm{II}} \int_{\Xi^{\mathrm{I}}=0}^{\Xi^{\mathrm{I}}=\delta} {\Xi^{\mathrm{I}}}^3\, \mathrm{d}\Xi^{\mathrm{I}} \\
&\qquad \times \int_{\hat{\mathcal{H}}_0{}^{\mathrm{III}}}\int_{\hat{\mathcal{H}}_0{}^{\mathrm{II}}}\int_{\hat{\mathcal{H}}_0{}^{\mathrm{I}}} \big|\hat{\boldsymbol{\Xi}}^{\mathrm{I}} \cdot [\hat{\boldsymbol{\Xi}}^{\mathrm{II}} \times \hat{\boldsymbol{\Xi}}^{\mathrm{III}}]\big|\, E_v^2\, \mathrm{d}\hat{V}^{\mathrm{I}}\, \mathrm{d}\hat{V}^{\mathrm{II}}\, \mathrm{d}\hat{V}^{\mathrm{III}} \\
&= \frac{1}{128}\, C_3\, \delta^{12} \int_{\hat{\mathcal{H}}_0{}^{\mathrm{III}}}\int_{\hat{\mathcal{H}}_0{}^{\mathrm{II}}}\int_{\hat{\mathcal{H}}_0{}^{\mathrm{I}}} \big|\hat{\boldsymbol{\Xi}}^{\mathrm{I}} \cdot [\hat{\boldsymbol{\Xi}}^{\mathrm{II}} \times \hat{\boldsymbol{\Xi}}^{\mathrm{III}}]\big|\, E_v^2\, \mathrm{d}\hat{V}^{\mathrm{I}}\, \mathrm{d}\hat{V}^{\mathrm{II}}\, \mathrm{d}\hat{V}^{\mathrm{III}}\,.
\end{aligned} \tag{5.64}$$

Utilizing the previously derived, simplified form of E_v (5.16) yields

$$\Psi_3 = \frac{1}{512}\, C_3\, \delta^{12} \big[\mathrm{Det}\, \boldsymbol{\mathcal{C}} - 1\big]^2 \int_{\hat{\mathcal{H}}_0{}^{\mathrm{III}}}\int_{\hat{\mathcal{H}}_0{}^{\mathrm{II}}}\int_{\hat{\mathcal{H}}_0{}^{\mathrm{I}}} \big|\hat{\boldsymbol{\Xi}}^{\mathrm{I}} \cdot [\hat{\boldsymbol{\Xi}}^{\mathrm{II}} \times \hat{\boldsymbol{\Xi}}^{\mathrm{III}}]\big| \mathrm{d}\hat{V}^{\mathrm{I}}\, \mathrm{d}\hat{V}^{\mathrm{II}}\, \mathrm{d}\hat{V}^{\mathrm{III}}\,, \tag{5.65}$$

which, by invoking Lemma 9, reduces to

$$\boxed{\Psi_3 = \frac{1}{64}\pi^4\, C_3\, \delta^{12} \big[\mathrm{Det}\, \boldsymbol{\mathcal{C}} - 1\big]^2} \tag{5.66}$$

5.3.4 Total point-wise energy density

Recalling from Eq.(2.24) that the total energy density of super-harmonic CPD in 3D is

$$\Psi_{\mathrm{S}}^{\mathrm{3D}} := \frac{1}{2}\, \Psi_1 + \frac{1}{3}\, \Psi_2 + \frac{1}{4}\, \Psi_3\,, \tag{5.67}$$

and using the results of equations (5.50), (5.62) and (5.66) gives

$$\begin{aligned}\Psi_{\mathrm{S}}^{3\mathrm{D}} = & \frac{1}{240}\pi\, C_1\, \delta^4 \left[2\,\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{C}} + [\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{I}}]^2 - 10\,\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{I}} + 15\right] \\ & + \frac{1}{1440}\pi^3\, C_2\, \delta^8 \left[2\,\boldsymbol{\mathcal{C}}^{\#} : \boldsymbol{\mathcal{C}}^{\#} + [\boldsymbol{\mathcal{C}}^{\#} : \boldsymbol{\mathcal{I}}]^2 - 10\,\boldsymbol{\mathcal{C}}^{\#} : \boldsymbol{\mathcal{I}} + 15\right] \\ & + \frac{1}{256}\pi^4\, C_3\, \delta^{12} \big[\mathrm{Det}\,\boldsymbol{\mathcal{C}} - 1\big]^2 ,\end{aligned} \tag{5.68}$$

or

$$\boxed{\begin{aligned}\Psi_{\mathrm{S}}^{3\mathrm{D}} = & B_1 \left[2\,\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{C}} + [\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{I}}]^2 - 10\,\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{I}} + 15\right] \\ & + B_2 \left[2\,\boldsymbol{\mathcal{C}}^{\#} : \boldsymbol{\mathcal{C}}^{\#} + [\boldsymbol{\mathcal{C}}^{\#} : \boldsymbol{\mathcal{I}}]^2 - 10\,\boldsymbol{\mathcal{C}}^{\#} : \boldsymbol{\mathcal{I}} + 15\right] \\ & + B_3 \left[\mathrm{Det}\,\boldsymbol{\mathcal{C}} - 1\right]^2\end{aligned}} \tag{5.69}$$

where

$$B_1 := \frac{1}{240}\pi\, C_1\, \delta^4 \quad , \quad B_2 := \frac{1}{1440}\pi^3\, C_2\, \delta^8 \quad , \quad B_3 := \frac{1}{256}\pi^4\, C_3\, \delta^{12} . \tag{5.70}$$

This total point-wise energy density can also be written in the generalized form

$$\boxed{\begin{aligned}\Psi_{\mathrm{S}}^{3\mathrm{D}} = & \quad B_1 \quad \Big[2\,\boldsymbol{\mathcal{C}}_1 : \boldsymbol{\mathcal{C}}_1 + [\boldsymbol{\mathcal{C}}_1 : \boldsymbol{\mathcal{I}}]^2 - 10\,\boldsymbol{\mathcal{C}}_1 : \boldsymbol{\mathcal{I}} + 15\Big] \\ & + \; B_2 \quad \Big[2\,\boldsymbol{\mathcal{C}}_2 : \boldsymbol{\mathcal{C}}_2 + [\boldsymbol{\mathcal{C}}_2 : \boldsymbol{\mathcal{I}}]^2 - 10\,\boldsymbol{\mathcal{C}}_2 : \boldsymbol{\mathcal{I}} + 15\Big] \\ & + \frac{1}{15} B_3 \Big[2\,\boldsymbol{\mathcal{C}}_3 : \boldsymbol{\mathcal{C}}_3 + [\boldsymbol{\mathcal{C}}_3 : \boldsymbol{\mathcal{I}}]^2 - 10\,\boldsymbol{\mathcal{C}}_3 : \boldsymbol{\mathcal{I}} + 15\Big]\end{aligned}} \tag{5.71}$$

where

$$\boldsymbol{\mathcal{C}}_1 := \boldsymbol{\mathcal{C}} \quad , \quad \boldsymbol{\mathcal{C}}_2 := \boldsymbol{\mathcal{C}}^{\#} \quad , \quad \boldsymbol{\mathcal{C}}_3 := \boldsymbol{\mathcal{C}}^{\#} \cdot \boldsymbol{\mathcal{C}} = \mathrm{Det}\,\boldsymbol{\mathcal{C}}\,\boldsymbol{\mathcal{I}} . \tag{5.72}$$

Now the energy densities due to the different interactions are unified to have the same form. What changes for each energy density is the effective material parameters, denoted B_1, B_2 and B_3, and the argument of the energy $\boldsymbol{\mathcal{C}}_1$, $\boldsymbol{\mathcal{C}}_2$ and $\boldsymbol{\mathcal{C}}_3$. Another alternate way of expressing the energy densities is in terms of the invariants of $\boldsymbol{\mathcal{C}}$, that are $I_1 := \mathrm{Tr}\,\boldsymbol{\mathcal{C}}$, $I_2 := \mathrm{Tr}\,\mathrm{Cof}\,\boldsymbol{\mathcal{C}}$ and $I_3 := \mathrm{Det}\,\boldsymbol{\mathcal{C}}$. Note that the tensors $\boldsymbol{\mathcal{C}}_1$, $\boldsymbol{\mathcal{C}}_2$ and $\boldsymbol{\mathcal{C}}_3$ essentially contain length, area and volume change

information, respectively. They are tensorial counterparts of the invariants I_1, I_2 and I_3. Utilizing the following relations,

$$\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{C}} = {I_1}^2 - 2\, I_2 \qquad , \qquad \boldsymbol{\mathcal{C}}^{\#} : \boldsymbol{\mathcal{C}}^{\#} = {I_2}^2 - 2\, I_1\, I_3 \,, \tag{5.73}$$

the energy density of super-harmonic CPD in 3D can be expressed as

$$\begin{aligned} \Psi_{\mathrm{S}}^{\mathrm{3D}} = {} & B_1 \left[3\, {I_1}^2 - 10\, I_1 - 4\, I_2 + 15 \right] \\ & + B_2 \left[3\, {I_2}^2 - 10\, I_2 - 4\, I_1\, I_3 + 15 \right] \\ & + B_3 \left[{I_3}^2 - 2\ I_3 + 1 \right] \end{aligned} \tag{5.74}$$

which will prove useful in the upcoming sections, when deriving the material parameter relationships in the linear elastic framework.

5.4 Material parameter relations

For the material parameters of the super-harmonic model, instead of linearizing the strains and comparing the resultant energy densities with the strain energy of CCM, we will use the energy densities of the *finite deformation framework* that were derived in Sections (5.2) and (5.3). In large deformation elasticity, the material behavior is dictated by a constitutive law. Though there are several options to choose from, in our case it is sufficient to focus on the following constitutive relation,

$$\delta \boldsymbol{\mathcal{P}} = \mathbb{A} : \delta \boldsymbol{\mathcal{F}} \,, \tag{5.75}$$

as it is a function of $\boldsymbol{\mathcal{F}}$ rather than other deformation measures that are more commonly used, such as the Green–Lagrange strain tensor $\boldsymbol{E}$. Here, $\boldsymbol{\mathcal{P}}$ is the

Piola Stress[1] and $\mathbb{A}$ is the *constitutive tensor*, which are defined by

$$\boldsymbol{\mathcal{P}} := \frac{\partial \Psi}{\partial \boldsymbol{\mathcal{F}}} \qquad \text{and} \qquad \mathbb{A} := \frac{\partial \boldsymbol{\mathcal{P}}}{\partial \boldsymbol{\mathcal{F}}}\,, \tag{5.76}$$

for any free energy density Ψ. This renders an inherently nonlinear constitutive relation. Although the operation $\mathbb{A} : \delta\boldsymbol{\mathcal{F}}$ is itself linear, as $\mathbb{A}$ is a nonlinear function of $\boldsymbol{\mathcal{F}}$, the constitutive behavior changes with the amount of deformation, which, in other terms, means the material parameters in $\mathbb{A}$ are not constants. Evaluating the constitutive tensor at $\boldsymbol{\mathcal{F}} = \boldsymbol{\mathcal{I}}$ imposes the small deformation assumption necessary to connect the formulation to linear elasticity, and yields a constitutive tensor

$$\mathbb{A}_0 := \frac{\partial}{\partial \boldsymbol{\mathcal{F}}}\left(\frac{\partial \Psi_{\text{CCM}}}{\partial \boldsymbol{\mathcal{F}}}\right)\bigg|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} = \mu\left[\boldsymbol{\mathcal{I}} \overline{\otimes} \boldsymbol{\mathcal{I}} + \boldsymbol{\mathcal{I}} \underline{\otimes} \boldsymbol{\mathcal{I}}\right] + \lambda\, \boldsymbol{\mathcal{I}} \otimes \boldsymbol{\mathcal{I}}\,, \tag{5.77}$$

where, as before, λ and μ denote the first and second Lamé parameters, respectively. In the following sections, we will derive the constitutive tensors of super-harmonic CPD, $\mathbb{A}_{\text{S}}^{\text{2D}}$ and $\mathbb{A}_{\text{S}}^{\text{3D}}$, by differentiating the super-harmonic energy densities with respect to $\boldsymbol{\mathcal{F}}$, twice. Recall that we expressed the super-harmonic energy densities $\Psi_{\text{S}}^{\text{2D}}$ (5.39) and $\Psi_{\text{S}}^{\text{3D}}$ (5.74) in terms of the invariants of $\boldsymbol{\mathcal{C}}$, or I_1, I_2, and I_3. Differentiating these expressions yields

$$\boldsymbol{\mathcal{P}}_{\text{S}} := \frac{\partial \Psi_{\text{S}}(I_i)}{\partial \boldsymbol{\mathcal{F}}} = \frac{\partial \Psi_{\text{S}}}{\partial I_i}\frac{\partial I_i}{\partial \boldsymbol{\mathcal{F}}} \qquad \text{where} \qquad i = \begin{cases} \{1,2\} & \text{in 2D}\,, \\ \{1,2,3\} & \text{in 3D}\,. \end{cases} \tag{5.78}$$

Differentiating with respect to $\boldsymbol{\mathcal{F}}$ for the second time leaves us with

$$\mathbb{A}_{\text{S}} := \frac{\partial \boldsymbol{\mathcal{P}}_{\text{S}}}{\partial \boldsymbol{\mathcal{F}}} = \frac{\partial \Psi_{\text{S}}}{\partial I_i}\frac{\partial}{\partial \boldsymbol{\mathcal{F}}}\left(\frac{\partial I_i}{\partial \boldsymbol{\mathcal{F}}}\right) + \frac{\partial}{\partial I_j}\left(\frac{\partial \Psi_{\text{S}}}{\partial I_i}\right)\left[\frac{\partial I_i}{\partial \boldsymbol{\mathcal{F}}} \otimes \frac{\partial I_j}{\partial \boldsymbol{\mathcal{F}}}\right], \tag{5.79}$$

where $j = \{1,2\}$ in 2D, and $\{1,2,3\}$ in 3D. In the following sections, we will evaluate these terms at $\boldsymbol{\mathcal{F}} = \boldsymbol{\mathcal{I}}$, and compare the resultant constitutive tensors with their CCM counterparts to arrive at the material parameter relations.

[1] or, as it is more commonly called in the literature, the first Piola-Kirchoff Stress.

5.4.1 Constitutive relation in 2D

In this section, we will calculate the terms in Eq. (5.79) for the 2D case, using the energy density given in Eq. (5.39). Starting with the simplest term, $\partial\Psi_{\mathrm{S}}^{\mathrm{2D}}/\partial I_i$, we have

$$\frac{\partial\Psi_{\mathrm{S}}^{\mathrm{2D}}}{\partial I_1} = 6B_1\, I_1 - 8B_1 \qquad , \qquad \frac{\partial\Psi_{\mathrm{S}}^{\mathrm{2D}}}{\partial I_2} = -4B_1 + 2B_2\, I_2 - 2B_2\,, \tag{5.80}$$

which, since at $\boldsymbol{\mathcal{F}} = \boldsymbol{\mathcal{I}}$, $I_1 = 2$ and $I_2 = 1$, yield

$$\frac{\partial\Psi_{\mathrm{S}}^{\mathrm{2D}}}{\partial I_1} = 4B_1 \qquad , \qquad \frac{\partial\Psi_{\mathrm{S}}^{\mathrm{2D}}}{\partial I_2} = -4B_1\,. \tag{5.81}$$

It follows that the derivatives of these terms (5.80) with respect to the invariants are

$$\frac{\partial}{\partial I_1}\left(\frac{\partial\Psi_{\mathrm{S}}^{\mathrm{2D}}}{\partial I_1}\right) = 6B_1 \qquad , \qquad \frac{\partial}{\partial I_2}\left(\frac{\partial\Psi_{\mathrm{S}}^{\mathrm{2D}}}{\partial I_2}\right) = 2B_2\,, \tag{5.82}$$

with the rest of the i, j combinations yielding zero. Next, we have the $\partial I_i/\partial\boldsymbol{\mathcal{F}}$ terms. Invoking the relation $\boldsymbol{\mathcal{I}} : \boldsymbol{\mathcal{C}} = \boldsymbol{\mathcal{I}} : \left[\boldsymbol{\mathcal{F}}^{\mathrm{T}} \cdot \boldsymbol{\mathcal{F}}\right] = \boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{F}}$ renders

$$\frac{\partial I_1}{\partial\boldsymbol{\mathcal{F}}} = \frac{\partial(\boldsymbol{\mathcal{I}} : \boldsymbol{\mathcal{C}})}{\partial\boldsymbol{\mathcal{F}}} = \frac{\partial(\boldsymbol{\mathcal{F}} : \boldsymbol{\mathcal{F}})}{\partial\boldsymbol{\mathcal{F}}} = 2\,\boldsymbol{\mathcal{F}} : \frac{\partial\boldsymbol{\mathcal{F}}}{\partial\boldsymbol{\mathcal{F}}} = 2\,\boldsymbol{\mathcal{F}} : \left[\boldsymbol{\mathcal{I}}\,\overline{\otimes}\,\boldsymbol{\mathcal{I}}\right] = 2\,\boldsymbol{\mathcal{F}}\,. \tag{5.83}$$

Moving onto the next term, we have

$$\frac{\partial I_2}{\partial\boldsymbol{\mathcal{F}}} = \frac{\partial \mathrm{Det}\,\boldsymbol{\mathcal{C}}}{\partial\boldsymbol{\mathcal{F}}} = \frac{\partial[\mathrm{Det}\,\boldsymbol{\mathcal{F}}]^2}{\partial\boldsymbol{\mathcal{F}}} = 2\,[\mathrm{Det}\,\boldsymbol{\mathcal{F}}]^2\,\boldsymbol{\mathcal{F}}^{-\mathrm{T}} = 2\,I_2\,\boldsymbol{\mathcal{F}}^{-\mathrm{T}}\,. \tag{5.84}$$

Evaluating the equations (5.83) and (5.84) at $\boldsymbol{\mathcal{F}} = \boldsymbol{\mathcal{I}}$ results in

$$\left.\frac{\partial I_1}{\partial\boldsymbol{\mathcal{F}}}\right|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} = 2\,\boldsymbol{\mathcal{I}} \qquad , \qquad \left.\frac{\partial I_2}{\partial\boldsymbol{\mathcal{F}}}\right|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} = 2\,\boldsymbol{\mathcal{I}}\,. \tag{5.85}$$

The remaining terms are the second derivatives of the invariants with respect to $\boldsymbol{\mathcal{F}}$. Recalling Eq. (5.83) renders

$$\frac{\partial}{\partial \boldsymbol{\mathcal{F}}}\left(\frac{\partial I_1}{\partial \boldsymbol{\mathcal{F}}}\right) = 2\,\frac{\partial \boldsymbol{\mathcal{F}}}{\partial \boldsymbol{\mathcal{F}}} = 2\,\boldsymbol{\mathcal{I}}\,\overline{\otimes}\,\boldsymbol{\mathcal{I}}\,. \tag{5.86}$$

Next, invoking Eq. (5.84) yields

$$\begin{aligned}\frac{\partial}{\partial \boldsymbol{\mathcal{F}}}\left(\frac{\partial I_2}{\partial \boldsymbol{\mathcal{F}}}\right) &= \frac{\partial}{\partial \boldsymbol{\mathcal{F}}}\left(2\,I_2\,\boldsymbol{\mathcal{F}}^{-\mathrm{T}}\right) = 2\,\boldsymbol{\mathcal{F}}^{-\mathrm{T}} \otimes \frac{\partial I_2}{\partial \boldsymbol{\mathcal{F}}} + 2\,I_2 \frac{\partial \boldsymbol{\mathcal{F}}^{-\mathrm{T}}}{\partial \boldsymbol{\mathcal{F}}} \\ &= 4\,I_2\,\boldsymbol{\mathcal{F}}^{-\mathrm{T}} \otimes \boldsymbol{\mathcal{F}}^{-\mathrm{T}} - 2\,I_2\,\boldsymbol{\mathcal{F}}^{-\mathrm{T}} \underline{\otimes} \boldsymbol{\mathcal{F}}^{-1}\,.\end{aligned} \tag{5.87}$$

The last step before assembling $\mathbb{A}_{\mathrm{S}}^{\mathrm{2D}}$ is to evaluate the second derivatives of the invariants at $\boldsymbol{\mathcal{F}} = \boldsymbol{\mathcal{I}}$. Doing so yields

$$\begin{aligned}\left.\frac{\partial}{\partial \boldsymbol{\mathcal{F}}}\left(\frac{\partial I_1}{\partial \boldsymbol{\mathcal{F}}}\right)\right|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} &= 2\,\boldsymbol{\mathcal{I}}\,\overline{\otimes}\,\boldsymbol{\mathcal{I}}\,, \\ \left.\frac{\partial}{\partial \boldsymbol{\mathcal{F}}}\left(\frac{\partial I_3}{\partial \boldsymbol{\mathcal{F}}}\right)\right|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} &= 4\,\boldsymbol{\mathcal{I}} \otimes \boldsymbol{\mathcal{I}} - 2\,\boldsymbol{\mathcal{I}} \underline{\otimes} \boldsymbol{\mathcal{I}}\,.\end{aligned} \tag{5.88}$$

Now we can assemble the constitutive tensor $\mathbb{A}_{\mathrm{S}}^{\mathrm{2D}}$. Plugging in the results of equations (5.81), (5.82), (5.85) and (5.88) into relation (5.79), after some mathematical steps, reveals

$$\mathbb{A}_{\mathrm{S}}^{\mathrm{2D}} = 8\,B_1\left[\boldsymbol{\mathcal{I}}\,\overline{\otimes}\,\boldsymbol{\mathcal{I}} + \boldsymbol{\mathcal{I}}\,\underline{\otimes}\,\boldsymbol{\mathcal{I}}\right] + 8\big[B_1 + B_2\big]\,\boldsymbol{\mathcal{I}} \otimes \boldsymbol{\mathcal{I}}\,. \tag{5.89}$$

Comparing this result with the constitutive tensor of CCM (5.77) immediately gives the relations

$$\lambda = 8\big[B_1 + B_2\big] \qquad , \qquad \mu = 8\,B_1\,, \tag{5.90}$$

or

$$\lambda = \frac{\pi}{24} C_1 \delta^3 + \frac{8}{27}\,\pi\,C_2\,\delta^6 \qquad , \qquad \mu = \frac{\pi}{24} C_1 \delta^3\,, \tag{5.91}$$

which, as expected, are identical to the relations (4.112) of the harmonic CPD parameters, derived in Section 4.5.1. Naturally, it follows that the remaining material parameter relations, and the overall behavior of the parameters are identical to their counterparts discussed in Section 4.5.1.

5.4.2 Constitutive relation in 3D

In this section, we repeat the procedure of the 2D super-harmonic formulation that was previously followed in Section 5.4.1.

Remark on the invariants in 2D and 3D *Note that I_1, as it is the trace of $\boldsymbol{\mathcal{C}}$ in both 2D and 3D, has identical derivatives with respect to $\boldsymbol{\mathcal{F}}$ in both formulations. Similarly, I_2 of 2D and I_3 of 3D, both determinants of $\boldsymbol{\mathcal{C}}$, should also have identical derivatives with respect to their own $\boldsymbol{\mathcal{F}}$'s (i.e. $\boldsymbol{\mathcal{F}}_{2D}$ and $\boldsymbol{\mathcal{F}}_{3D}$). This simplifies the steps ahead as we can utilize the relations derived in the previous section for I_1 and I_2, for the relations associated with I_1 and I_3 of the 3D formulation, respectively. Though the invariants themselves should be evaluated with care given to the space they reside in, as, for instance, $Tr\boldsymbol{\mathcal{I}} = 2$ in 2D, but $Tr\boldsymbol{\mathcal{I}} = 3$ in 3D.*

We proceed to calculate the terms in Eq. (5.79) separately, using the energy density given in Eq. (5.74). Starting with the terms $\partial\Psi_{\mathrm{S}}^{\mathrm{3D}}/\partial I_i$,

$$\begin{aligned}
\frac{\partial\Psi_{\mathrm{S}}^{\mathrm{3D}}}{\partial I_1} &= 6B_1\, I_1 - 10B_1 - 4B_2\, I_3\,, \\
\frac{\partial\Psi_{\mathrm{S}}^{\mathrm{3D}}}{\partial I_2} &= -4B_1 + 6B_2\, I_2 - 10B_2\,, \\
\frac{\partial\Psi_{\mathrm{S}}^{\mathrm{3D}}}{\partial I_3} &= -4B_2\, I_1 + 2B_3\, I_3 - 2B_3\,,
\end{aligned} \tag{5.92}$$

that become

$$\frac{\partial\Psi_{\mathrm{S}}^{\mathrm{3D}}}{\partial I_1} = 8B_1 - 4B_2\,, \quad \frac{\partial\Psi_{\mathrm{S}}^{\mathrm{3D}}}{\partial I_2} = -4B_1 + 8B_2\,, \quad \frac{\partial\Psi_{\mathrm{S}}^{\mathrm{3D}}}{\partial I_3} = -12B_2\,, \tag{5.93}$$

at $\boldsymbol{\mathcal{F}} = \boldsymbol{\mathcal{I}}$. It follows that the derivatives of these terms with respect to the

invariants are

$$\begin{aligned}
&\frac{\partial}{\partial I_1}\left(\frac{\partial \Psi_{\mathrm{S}}^{3\mathrm{D}}}{\partial I_1}\right) = 6B_1\,, \quad \frac{\partial}{\partial I_2}\left(\frac{\partial \Psi_{\mathrm{S}}^{3\mathrm{D}}}{\partial I_2}\right) = 6B_2\,, \quad \frac{\partial}{\partial I_3}\left(\frac{\partial \Psi_{\mathrm{S}}^{3\mathrm{D}}}{\partial I_3}\right) = 2B_3\,, \\
&\frac{\partial}{\partial I_1}\left(\frac{\partial \Psi_{\mathrm{S}}^{3\mathrm{D}}}{\partial I_3}\right) = -4B_2\,, \quad \frac{\partial}{\partial I_2}\left(\frac{\partial \Psi_{\mathrm{S}}^{3\mathrm{D}}}{\partial I_1}\right) = 0\,, \quad \frac{\partial}{\partial I_3}\left(\frac{\partial \Psi_{\mathrm{S}}^{3\mathrm{D}}}{\partial I_2}\right) = 0\,.
\end{aligned} \tag{5.94}$$

Next, we have the $\partial I_i/\partial \boldsymbol{\mathcal{F}}$ terms. For $\partial I_1/\partial \boldsymbol{\mathcal{F}}$, we simply recall its counterpart in 2D (5.83)

$$\frac{\partial I_1}{\partial \boldsymbol{\mathcal{F}}} = 2\,\boldsymbol{\mathcal{F}}\,. \tag{5.95}$$

To derivate I_2, we utilize the relation $\mathrm{Tr}\,\boldsymbol{\mathcal{C}}^{\#} = \frac{1}{2}\big[[\mathrm{Tr}\,\boldsymbol{\mathcal{C}}]^2 - \boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{C}}\big]$, such that

$$\frac{\partial I_2}{\partial \boldsymbol{\mathcal{F}}} = \frac{1}{2}\frac{\partial \big({I_1}^2\big)}{\partial \boldsymbol{\mathcal{F}}} - \frac{1}{2}\frac{\partial \big(\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{C}}\big)}{\partial \boldsymbol{\mathcal{F}}}\,, \tag{5.96}$$

the first part of which, by invoking the result of Eq. (5.95), becomes

$$\frac{1}{2}\frac{\partial \big({I_1}^2\big)}{\partial \boldsymbol{\mathcal{F}}} = 2\,I_1\,\boldsymbol{\mathcal{F}}\,, \tag{5.97}$$

and the second part reduces to

$$\begin{aligned}
-\frac{1}{2}\frac{\partial \big(\boldsymbol{\mathcal{C}} : \boldsymbol{\mathcal{C}}\big)}{\partial \boldsymbol{\mathcal{F}}} &= -\,\boldsymbol{\mathcal{C}} : \frac{\partial \big(\boldsymbol{\mathcal{F}}^{\mathrm{T}} \cdot \boldsymbol{\mathcal{F}}\big)}{\partial \boldsymbol{\mathcal{F}}} \\
&= -\,\boldsymbol{\mathcal{C}} : \big[\boldsymbol{\mathcal{I}} \underline{\otimes}\, \boldsymbol{\mathcal{F}}^{\mathrm{T}} + \boldsymbol{\mathcal{F}}^{\mathrm{T}} \overline{\otimes}\, \boldsymbol{\mathcal{I}}\big] \\
&= -2\,\boldsymbol{\mathcal{F}} \cdot \boldsymbol{\mathcal{F}}^{\mathrm{T}} \cdot \boldsymbol{\mathcal{F}}\ ,
\end{aligned} \tag{5.98}$$

so that finally the derivative of I_2 reads

$$\frac{\partial I_2}{\partial \boldsymbol{\mathcal{F}}} = 2\,I_1\,\boldsymbol{\mathcal{F}} - 2\,\boldsymbol{\mathcal{F}} \cdot \boldsymbol{\mathcal{F}}^{\mathrm{T}} \cdot \boldsymbol{\mathcal{F}}\,. \tag{5.99}$$

Moving onto the next term, we recall $\partial I_2/\partial \boldsymbol{\mathcal{F}}$ from 2D (5.84),

$$\frac{\partial I_3}{\partial \boldsymbol{\mathcal{F}}} = 2\,I_3\,\boldsymbol{\mathcal{F}}^{-\mathrm{T}}\,. \tag{5.100}$$

Evaluating the Equations (5.95), (5.99) and (5.100) at $\boldsymbol{\mathcal{F}} = \boldsymbol{\mathcal{I}}$ results in

$$\left.\frac{\partial I_1}{\partial \boldsymbol{\mathcal{F}}}\right|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} = 2\,\boldsymbol{\mathcal{I}} \quad , \quad \left.\frac{\partial I_2}{\partial \boldsymbol{\mathcal{F}}}\right|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} = 4\,\boldsymbol{\mathcal{I}} \quad , \quad \left.\frac{\partial I_3}{\partial \boldsymbol{\mathcal{F}}}\right|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} = 2\,\boldsymbol{\mathcal{I}}\,. \tag{5.101}$$

The remaining terms are the second derivatives of the invariants with respect to $\boldsymbol{\mathcal{F}}$. Recalling the result of Eq. (5.86) gives

$$\frac{\partial}{\partial \boldsymbol{\mathcal{F}}}\left(\frac{\partial I_1}{\partial \boldsymbol{\mathcal{F}}}\right) = 2\,\boldsymbol{\mathcal{I}} \,\overline{\otimes}\, \boldsymbol{\mathcal{I}}\,. \tag{5.102}$$

Next, invoking Eq. (5.99) yields

$$\begin{aligned}
\frac{\partial}{\partial \boldsymbol{\mathcal{F}}}\left(\frac{\partial I_2}{\partial \boldsymbol{\mathcal{F}}}\right) &= \frac{\partial}{\partial \boldsymbol{\mathcal{F}}}\left(2\,I_1\,\boldsymbol{\mathcal{F}} - 2\,\boldsymbol{\mathcal{F}}\cdot\boldsymbol{\mathcal{F}}^{\mathrm{T}}\cdot\boldsymbol{\mathcal{F}}\right) \\
&= 2\left[\boldsymbol{\mathcal{F}}\otimes\frac{\partial I_1}{\partial \boldsymbol{\mathcal{F}}} + I_1\frac{\partial \boldsymbol{\mathcal{F}}}{\partial \boldsymbol{\mathcal{F}}} - [\boldsymbol{\mathcal{C}}]_{js}\,\frac{\partial\,[\boldsymbol{\mathcal{F}}]_{ij}}{\partial\,[\boldsymbol{\mathcal{F}}]_{kl}} - [\boldsymbol{\mathcal{F}}]_{ij}\,\frac{\partial\,[\boldsymbol{\mathcal{C}}]_{js}}{\partial\,[\boldsymbol{\mathcal{F}}]_{kl}}\right] \\
&= 2\left[2\,\boldsymbol{\mathcal{F}}\otimes\boldsymbol{\mathcal{F}} + I_1\,\boldsymbol{\mathcal{I}}\,\overline{\otimes}\,\boldsymbol{\mathcal{I}} - \boldsymbol{\mathcal{I}}\,\overline{\otimes}\,\boldsymbol{\mathcal{C}}^{\mathrm{T}} - \boldsymbol{\mathcal{F}}\,\underline{\otimes}\,\boldsymbol{\mathcal{F}}^{\mathrm{T}} - \left[\boldsymbol{\mathcal{F}}\cdot\boldsymbol{\mathcal{F}}^{\mathrm{T}}\right]\overline{\otimes}\,\boldsymbol{\mathcal{I}}\right].
\end{aligned} \tag{5.103}$$

Finally, recalling Eq. (5.87) from 2D, we get

$$\frac{\partial}{\partial \boldsymbol{\mathcal{F}}}\left(\frac{\partial I_3}{\partial \boldsymbol{\mathcal{F}}}\right) = 4\,I_3\,\boldsymbol{\mathcal{F}}^{-\mathrm{T}}\otimes\boldsymbol{\mathcal{F}}^{-\mathrm{T}} - 2\,I_3\,\boldsymbol{\mathcal{F}}^{-\mathrm{T}}\underline{\otimes}\boldsymbol{\mathcal{F}}^{-1}\,. \tag{5.104}$$

The last step before assembling $\mathbb{A}_{\mathrm{S}}^{3\mathrm{D}}$ is evaluating the second derivatives of the invariants at $\boldsymbol{\mathcal{F}} = \boldsymbol{\mathcal{I}}$. Doing so yields

$$\begin{aligned}
\left.\frac{\partial}{\partial \boldsymbol{\mathcal{F}}}\left(\frac{\partial I_1}{\partial \boldsymbol{\mathcal{F}}}\right)\right|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} &= 2\,\boldsymbol{\mathcal{I}}\,\overline{\otimes}\,\boldsymbol{\mathcal{I}}\,, \\
\left.\frac{\partial}{\partial \boldsymbol{\mathcal{F}}}\left(\frac{\partial I_2}{\partial \boldsymbol{\mathcal{F}}}\right)\right|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} &= 2\left[2\,\boldsymbol{\mathcal{I}}\otimes\boldsymbol{\mathcal{I}} + \boldsymbol{\mathcal{I}}\,\overline{\otimes}\,\boldsymbol{\mathcal{I}} - \boldsymbol{\mathcal{I}}\,\underline{\otimes}\,\boldsymbol{\mathcal{I}}\right], \\
\left.\frac{\partial}{\partial \boldsymbol{\mathcal{F}}}\left(\frac{\partial I_3}{\partial \boldsymbol{\mathcal{F}}}\right)\right|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} &= 4\,\boldsymbol{\mathcal{I}}\otimes\boldsymbol{\mathcal{I}} - 2\,\boldsymbol{\mathcal{I}}\underline{\otimes}\boldsymbol{\mathcal{I}}\,.
\end{aligned} \tag{5.105}$$

Now we can assemble the constitutive tensor $\mathbb{A}_{\mathrm{S}}^{3\mathrm{D}}$. Plugging in the results of Equations (5.93), (5.94), (5.101) and (5.105) into relation (5.79), after some mathematical steps, reveals

$$\mathbb{A}_{\mathrm{S}}^{3\mathrm{D}} = 8\big[B_1 + B_2\big]\big[\boldsymbol{\mathcal{I}} \overline{\otimes} \boldsymbol{\mathcal{I}} + \boldsymbol{\mathcal{I}} \underline{\otimes} \boldsymbol{\mathcal{I}}\big] + 8\big[B_1 + 6\,B_2 + B_3\big]\,\boldsymbol{\mathcal{I}} \otimes \boldsymbol{\mathcal{I}}\,. \tag{5.106}$$

Comparing this result with the constitutive tensor of CCM (5.77) immediately gives the relations

$$\lambda = 8\big[B_1 + 6\,B_2 + B_3\big] \qquad , \qquad \mu = 8\big[B_1 + B_2\big]\,, \tag{5.107}$$

or

$$\lambda = \frac{\pi}{30} C_1 \delta^4 + \frac{\pi^3}{30} C_2 \delta^8 + \frac{\pi^4}{32} C_3 \delta^{12} \quad , \quad \mu = \frac{\pi}{30} C_1 \delta^4 + \frac{\pi^3}{180} C_2 \delta^8\,, \tag{5.108}$$

which, as expected, are identical to the relations (4.124) of the harmonic CPD parameters in 3D, derived in Section 4.5.2. Naturally, it follows that the remaining material parameter relations, and the overall behavior of the parameters are identical to their counterparts discussed in Section 4.5.2.

Chapter 6

Conclusion

With an inherent suitability to capture discontinuities, PD has been the subject of various contributions and applications to date. As the recently proposed extension of the PD formulation, CPD adds to the applicability of peridynamics. Despite having been applied to various problems [1, 2, 35–37], the material parameters of CPD, in view of its constitutive modeling at small deformations and their relationship to the well established linear elasticity coefficients of CCM, had yet to be rigorously studied. This contribution presented two methods to relate the material parameters of CPD and CCM, in 2D and 3D, linear elastic, isotropic settings. The harmonic and super-harmonic energy densities, and their linear and non-linear strains have been introduced and analyzed rigorously. The linear strain measures have been presented in a unified format in the small deformation setting. The harmonic energy densities in terms of the linearized strains have been integrated, producing analytical solutions for the linear elastic setting. The non-linear strains have been reformulated for affine deformations, and their super-harmonic energy densities have been analytically integrated, producing solutions for the large-deformation setting. To derive the material parameters (i) the harmonic energy density of CPD has been equated to the energy density of CCM, and (ii) the constitutive tensor for the super-harmonic energy density of CPD have been derived and evaluated at the material configuration, and afterwards equated to that of CCM. The results are validated through prescribed,

affine, canonical deformation tests. Lastly, the admissible ranges for CPD parameters are provided, in line with their CCM counterparts. Four remarkable findings are (i) the unified representations of the linearized measures of deformation; (ii) the observation of CPD material parameter combinations that result in either length-, area- or volume-preserving behavior; (iii) the reduction of the three elastic parameters of CPD into two in the linearized framework, reminiscent of CCM; and (iv) providing a physical interpretation for the first Lamé constant, for the first time.

Intentionally, the focus of the manuscript has purely been theoretical. The analytical solutions provided in this work have been compared with numerical simulations for the purposes of verification, although detailed comparisons are omitted for the sake of brevity. Figures 6.1 and 6.2 provide examples of such comparisons. Nevertheless, it should be noted that computational implementation is a crucial part of PD, and CPD, especially in the non-linear regime where analytical solutions are not available. Equipped with the material parameter relations that allow us to draw comparisons with classical models, computational implementation of CPD remains an open topic of research. An example application of the CPD framework is given in Fig. 6.3, for the simulation of a thermomechanically coupled problem. With the ability to account for discontinuities and non-local effects, this is just one of many possible applications of CPD that we hope to contribute to and see more of in the future.

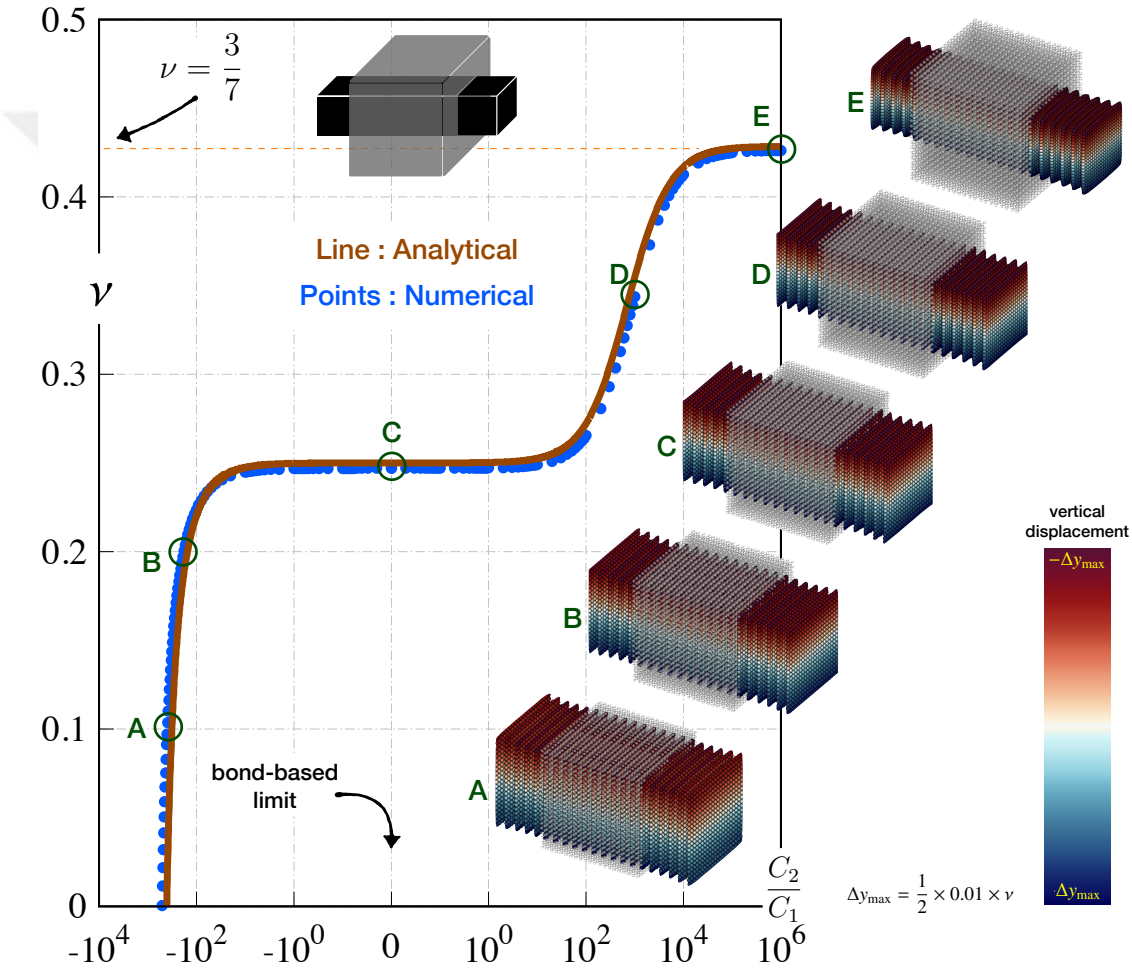

Figure 6.1: Poisson's ratio ν versus C_2/C_1 in a uni-axial tension test under a prescribed stretch of 1% in longitudinal direction for $C_3 = 0$, grid spacing $\Delta = 0.05$, and $\delta = 0.1255$. The deformation is exaggerated by a factor of 100, for the sake of better illustration of the results.

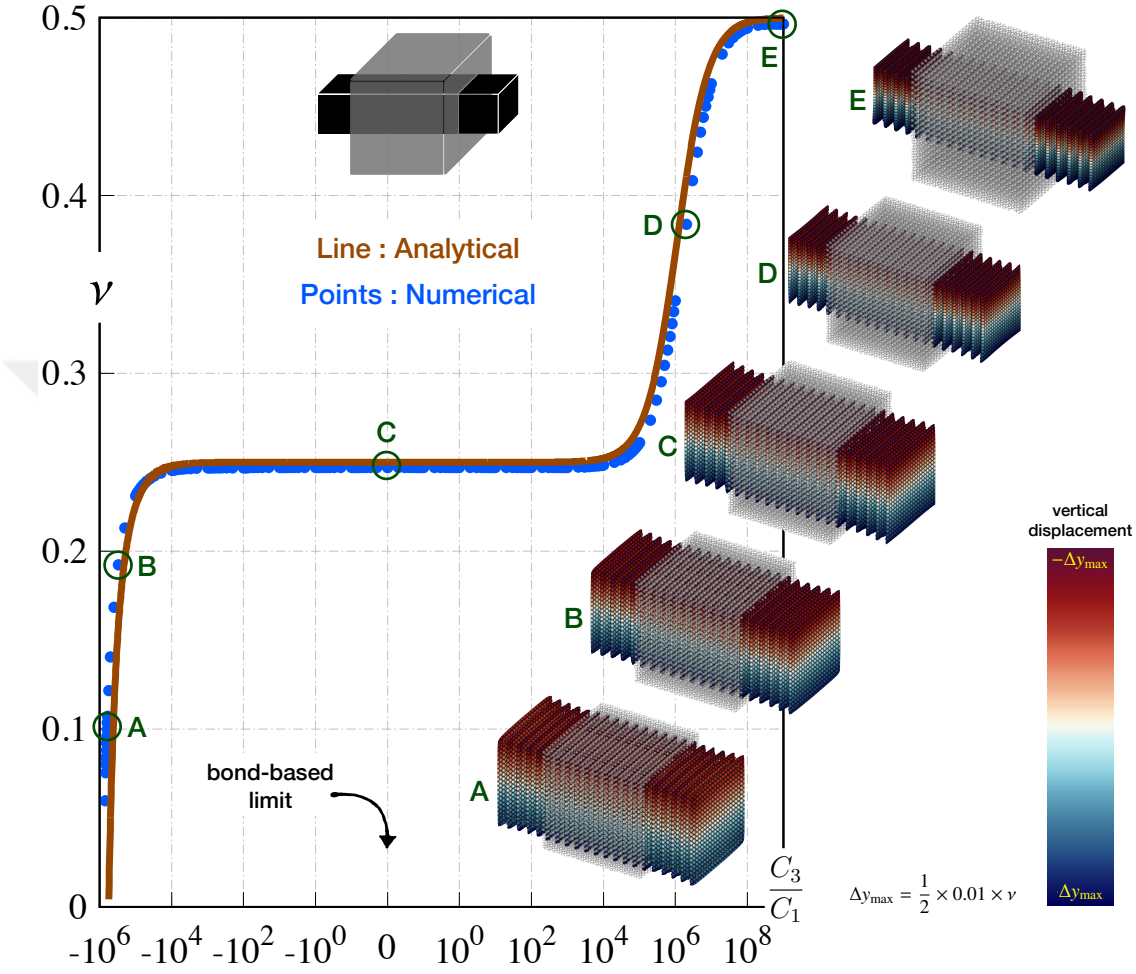

Figure 6.2: Poisson's ratio ν versus C_3/C_1 in a uni-axial tension test under a prescribed stretch of 1% in longitudinal direction for $C_2 = 0$, grid spacing $\Delta = 0.05$, and $\delta = 0.1255$. The deformation is exaggerated by a factor of 100, for the sake of better illustration of the results.

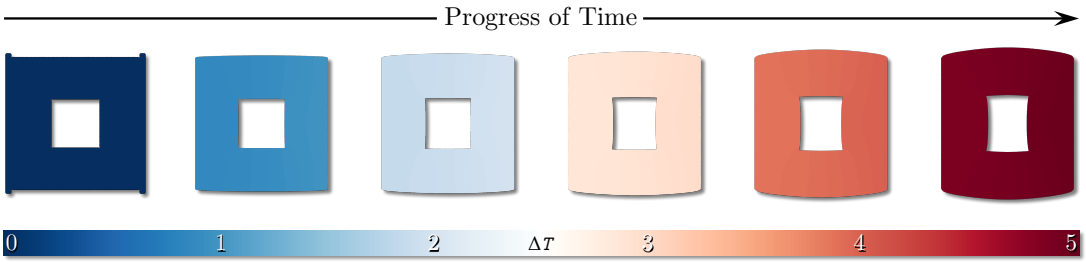

Figure 6.3: An example of a thermo-mechanically coupled problem in 2D. A square domain with a square hole is heated and allowed to expand with time. The theoretical framework presented in [1] is computationally implemented to produce this example.

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