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A geometrically exact formulation of peridynamics

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Abstract

The main objective of this contribution is to develop a geometrically exact peridynamics (PD) formulation wherein the basic elements of continuum kinematics are preserved. The proposed formulation accounts for large deformations and is variationally consistent. We distinguish between one-, two- and three-neighbour interactions. One-neighbour interactions recover the original (bond-based) PD formalism. Two- and three-neighbour interactions are fundamentally different to state-based PD. We account for material frame indifference and provide a set of appropriate arguments for objective interaction potentials accordingly. This contribution is presented in a manner such that the established theory is immediately suitable for computational implementation. From a computational perspective, the proposed strategy is fully implicit and the quadratic rate of convergence associated with the Newton–Raphson scheme is observed. Finally, we demonstrate the capability of our proposed framework via a series of numerical examples at large deformations.

Keywords: Peridynamics, Continuum kinematics, Geometrically exact, Variationally consistent, Large deformations

1. Introduction

Peridynamics (PD) is an alternative approach to formulate continuum mechanics [1], the roots of which can be, in part, traced back to the pioneering works of Piola [2]. PD is a non-local continuum formulation but differs from the well-known extended continuum formulations of Eringen [3] in that the concepts of stress and strain are absent. As a non-local theory, the behaviour of each material point is dictated by its interactions with other material points in its vicinity. In contrast to classical continuum mechanics, the governing equations of PD are appropriate for problems involving discontinuities such as cracks and interfaces. Since PD inherently accounts for geometrical discontinuities, it is readily employed in fracture mechanics and related problems [4–15]. However, the range of

PD applications is broad and not limited to fracture mechanics. Various applications and extensions of PD other than those dealing exclusively with material failure include quasi-static problems [16–20], coupled problems [21–23], multiscale modeling [24–30], structural mechanics [31–35], constitutive models [36–44], plasticity [45, 46], biomechanics [47, 48] and wave dispersion [49–55]. For an extensive study of the balance laws, applications, and implementations, see [56], and for a brief description of PD together with a review of its applications and related studies in different fields to date, see the review [57]. Fundamental works on PD include [58, 59]. For further connections between PD theory, continuum mechanics and particle systems see [60–63], among others.

The original PD theory of Silling [1] was restricted to bond-based interactions. The bond-based assumption of PD limited

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its applicability for material modelling, including the inability to account for Poisson's ratio other than 1/4 for isotropic materials. This shortcoming was addressed in various contributions and rectified in [64] via the introduction of the notion of *state* and categorising interactions as bond-based and state-based. Alternatively, motivated by multi-body interactions in molecular dynamics [65], the bond-based PD could be enriched by bond rotations such that the interactions between material points within the horizon not only depend on the stretches of the bonds, but also depend on the change of the angles between bond pairs [66, 67]. The goal here is to elaborate on the geometrically exact formulation of continuum-kinematics-inspired peridynamics (CPD) proposed recently by the authors [68]. CPD provides an alternative PD formulation whose underlying concepts are analogous to classical continuum mechanics.

Our contribution on the topic [68] establishes a variational theory for CPD that is discretized for computational implementation in our subsequent contribution [69]. By contrast, here we discretize the energy first and then impose the variational formulation. That is, the key purpose of this contribution is to reformulate CPD with a discretized energy from the onset in the spirit of discrete mechanics as advocated by Marsden and Ortiz [see 70, among others]. By doing so, we are able to establish a theory that is immediately suitable for computational implementation. Thus, this manuscript provides a more streamlined and accessible version of CPD compared to our original formulation [68].

The manuscript is organized as follows. Section 2 introduces the notation and elaborates on the kinematics of the problem. Multi-neighbour interactions are presented in accordance with CPD and thus the basic elements of classical continuum kinematics are preserved. Thereafter, we derive the governing equations in a variationally consistent manner in Section 3 via a

minimization of the total energy functional, for the special case of a quasi-static conservative problems. Central to the derivations are internal energy densities of multi-neighbour interactions that fulfil material frame indifference via the choice of objective arguments. The governing equations of Section 3 are a set of discretized residuals that must vanish. Section 4 elaborates on the linearization of the residuals such that an implicit computational framework is formed. Using the family of interaction potentials given in Section 5, the numerical examples in Section 6 demonstrate the theory. The examples are devised such that the key features of the framework are captured clearly. Section 8 concludes this work.

2. Kinematics

Central to our formulation is the geometrically exact description of kinematics inspired by classical continuum mechanics. Consider a continuum body that occupies the material configuration $\mathcal{B}_0 \subset \mathbb{R}^3$ at time $t = 0$ and that is mapped to the spatial configuration $\mathcal{B}_t \subset \mathbb{R}^3$ via the nonlinear deformation map $\mathbf{y}$ as $\mathbf{x} = \mathbf{y}(\mathbf{X}, t) : \mathcal{B}_0 \times \mathbb{R}_+ \rightarrow \mathcal{B}_t$ with $\mathbf{X}$ and $\mathbf{x}$ identifying points in the material and spatial configurations, respectively, as illustrated in Fig. 1. Recall the three key elements of classical continuum mechanics that describe the kinematics, i.e. the *local kinematics measures* of relative deformation:

$$\begin{aligned} \text{deformation gradient:} \quad & \mathbf{F} := \text{Grad } \mathbf{y}, \\ \text{cofactor of } \mathbf{F}: \quad & \mathbf{K} := \text{Cof } \mathbf{F}, \\ \text{determinant of } \mathbf{F}: \quad & J := \text{Det } \mathbf{F}, \end{aligned} \tag{1}$$

mapping differential line elements, area elements and volume elements, respectively. In what follows, inspired by these local measures, we introduce three *non-local kinematic measures* of relative deformation that underpin CPD.

In contrast to standard local continuum mechanics, the non-locality assumption dictates that any point $\mathcal{P}$ in the material

Figure 1: Motion of a continuum body within the CPD formulation. The continuum body that occupies the material configuration $\mathcal{B}_0 \subset \mathbb{R}^3$ at time $t = 0$ is mapped to the spatial configuration $\mathcal{B}_t \subset \mathbb{R}^3$ via the nonlinear deformation map $\mathbf{y}$. The neighbourhood of X is mapped to the neighbourhood of $\mathbf{x}$. From a computational perspective, any point $\mathcal{P}^a$ with coordinates X^a corresponds to a collocation point. The neighbour set $\{\mathcal{N}^i, \mathcal{N}^j, \mathcal{N}^k\}$ of the collocation point $\mathcal{P}^a$ is of particular interest in our formulation.

configuration can interact with other points within its finite neighbourhood $\mathcal{H}_0(X)$. The neighbourhood $\mathcal{H}_0$ is referred to as the material *horizon*. The *measure* of the horizon in the material configuration is denoted δ and is generally the radius of a spherical neighbourhood at X . The spatial horizon $\mathcal{H}_t = \mathbf{y}(\mathcal{H}_0, t)$ is the image of the material horizon $\mathcal{H}_0$ under the deformation map $\mathbf{y}$ and, in general, can be visualised as a distorted ellipsoid. In Fig. 1 the material and spatial horizons $\mathcal{H}_0$ and $\mathcal{H}_t$, respectively, are shown as spheres for simplicity. Note that the horizons $\mathcal{H}_0$ and $\mathcal{H}_t$ coincide with the points X and $\mathbf{x}$ in the limit of an infinitesimal neighbourhood and the kinematics of the local continuum mechanics formalism are recovered. This is another key characteristic of CPD [68].

A key feature of this contribution is that from the onset the problem is formulated from the perspective of computational mechanics. To do so, instead of a *continuum point*, we refer to a *collocation point* $\mathcal{P}^a$ with coordinates X^a and $\mathbf{x}^a$ in the material and spatial configurations, respectively, with $\mathbf{x}^a = \mathbf{y}(X^a, t)$. We

derive and satisfy the governing equations at each collocation point. The horizon of the collocation point $\mathcal{P}^a$ is denoted by $\mathcal{H}_0^a$ and $\mathcal{H}_t^a$ in the material and spatial configurations, respectively. Of particular importance in our formulation is the neighbour set $\{\mathcal{N}^i, \mathcal{N}^j, \mathcal{N}^k\}$ of the collocation point $\mathcal{P}^a$ identified as

$$\{\mathcal{N}^i, \mathcal{N}^j, \mathcal{N}^k\} \quad \forall \mathcal{N}^i, \mathcal{N}^j, \mathcal{N}^k \in \mathcal{H}_0^a.$$

All quantities with a superscript follow from discretising the problem in space and are thus immediately applicable for a computational implementation. The neighbours i, j and k are referred to as the first, second and third neighbours of the collocation point a , respectively. The coordinates of the neighbours i, j and k in the material configuration are X^i, X^j and X^k , respectively, and are mapped to their spatial counterparts via the nonlinear deformation map $\mathbf{y}$. That is

$$\mathbf{x}^i = \mathbf{y}(X^i, t) \quad , \quad \mathbf{x}^j = \mathbf{y}(X^j, t) \quad , \quad \mathbf{x}^k = \mathbf{y}(X^k, t).$$

Table 1: Summary of CPD kinematics.

one-neighbour interactions	two-neighbour interactions	three-neighbour interactions
$\Xi^{ai} = X^i - X^a$	$\Xi^{aj} = X^j - X^a$	$\Xi^{ak} = X^k - X^a$
$\xi^{ai} = \mathbf{x}^i - \mathbf{x}^a$	$\xi^{aj} = \mathbf{x}^j - \mathbf{x}^a$	$\xi^{ak} = \mathbf{x}^k - \mathbf{x}^a$
Ξ^{ai}	$A^{aij} = \Xi^{ai} \times \Xi^{aj}$	$V^{aijk} = \Xi^{ai} \cdot [\Xi^{aj} \times \Xi^{ak}]$
ξ^{ai}	$\mathbf{a}^{aij} = \xi^{ai} \times \xi^{aj}$	$\mathbf{v}^{aijk} = [\xi^{ai} \times \xi^{aj}] \cdot \xi^{ak}$
$L := \Xi^{ai} $, $l := \xi^{ai} $	$A := A^{aij} $, $a := \mathbf{a}^{aij} $	$V := V^{aijk} $, $v := \mathbf{v}^{aijk} $

Ξ^{ai} : relative positions between a collocation point a and its neighbour i in the material configuration with magnitude L

ξ^{ai} : relative positions between a collocation point a and its neighbour i in the spatial configuration with magnitude l

A^{aij} : area vector between a collocation point a and its neighbour pair i and j in the material configuration with magnitude A

$\mathbf{a}^{aij}$: area vector between a collocation point a and its neighbour pair i and j in the spatial configuration with magnitude a

V^{aijk} : volume between a collocation point a and its neighbour triplet i, j and k in the material configuration with magnitude V

$\mathbf{v}^{aijk}$: volume between a collocation point a and its neighbour triplet i, j and k in the spatial configuration with magnitude v

The relative positions between a collocation point a and its neighbours i, j and k are denoted as $\Xi^{(\bullet)}$ and $\xi^{(\bullet)}$ in the material and spatial configurations, respectively, where the superscript $\{\bullet\}$ identifies the pair. That is

$$\begin{aligned} \Xi^{ai} &:= X^i - X^a , & \xi^{ai} &:= \mathbf{x}^i - \mathbf{x}^a , \\ \Xi^{aj} &:= X^j - X^a , & \xi^{aj} &:= \mathbf{x}^j - \mathbf{x}^a , \\ \Xi^{ak} &:= X^k - X^a , & \xi^{ak} &:= \mathbf{x}^k - \mathbf{x}^a . \end{aligned}$$

Next, in the spirit of the local measures (1), we introduce three *non-local kinematic measures* of relative deformation. *The first relative deformation measure* ξ^{ai} mimics the linear map $\mathbf{F}$ of the infinitesimal line element $d\mathbf{X}$ in the material configuration to its spatial counterpart $d\mathbf{x}$. In view of our proposed for-

malism, the relative measure

$$\xi^{ai} = \mathbf{x}^i - \mathbf{x}^a , \quad (2)$$

is the main ingredient to describe *one-neighbour interactions*.

It can be shown [68] that in the infinitesimal limit the relation $\xi^{ai} = \mathbf{F} \cdot \Xi^{ai}$ holds. *The second relative deformation measure* $\mathbf{a}^{aij}$ is reminiscent of the linear map $\mathbf{K}$ from the infinitesimal vectorial area element $d\mathbf{A}$ in the material configuration to its spatial counterpart $d\mathbf{a}$. This is essentially Nanson's formula. In our proposed framework, the relative (area) measure

$$\mathbf{a}^{aij} = [\mathbf{x}^i - \mathbf{x}^a] \times [\mathbf{x}^j - \mathbf{x}^a] , \quad (3)$$

is the main ingredient to describe *two-neighbour interactions*.

In the infinitesimal limit, the relation $\mathbf{a}^{aij} = \mathbf{K} \cdot A^{aij}$ is ob-

tained [68], see Table 2. *The third relative deformation measure* v^{aijk} mimics the linear map J of the infinitesimal volume element dV in the material configuration to its spatial counterpart dv . The relative (volume) measure

$$v^{aijk} = [[\mathbf{x}^i - \mathbf{x}^a] \times [\mathbf{x}^j - \mathbf{x}^a]] \cdot [\mathbf{x}^k - \mathbf{x}^a], \quad (4)$$

is the main ingredient to describe *three-neighbour interactions*. Similarly, the relation $v^{aijk} = J V^{aijk}$ is obtained in the infinitesimal limit [68]. Table 2 summarizes the kinematics and provides useful definitions that are frequently used throughout the manuscript. As will be seen shortly, appropriate norms of the kinematics measures are suitable arguments to define physically meaningful interaction potentials.

3. Governing equations

In order to obtain the governing equations, the total potential energy functional is minimized. This is done by setting the first variation of the total potential energy functional to zero. The total potential energy functional Π that we seek to minimize with respect to all admissible (spatial) variations $\delta \mathbf{y}$ at a fixed material placement is composed of internal and external contributions Ψ and Υ , respectively. That is

$$\Pi = \Psi + \Upsilon \quad \Rightarrow \quad \delta \Pi = 0 \quad \forall \delta \mathbf{y}, \quad (5)$$

We emphasise that the current discussion on the variational setting is for non-dissipative processes.

3.1. Internal potential energy

The internal potential energy functional Ψ itself is composed of the internal potential energy due to one-neighbour interactions Ψ_1 , two-neighbour interactions Ψ_2 and three-neighbour

interactions Ψ_3 . That is

$$\Psi = \Psi_1 + \Psi_2 + \Psi_3,$$

where the number in the subscript indicates the type of interaction. Furthermore, we define the point-wise internal energy densities per volume in the material configuration ψ_1^a , ψ_2^a and ψ_3^a associated with one-neighbour, two-neighbour and three-neighbour interactions, respectively. That is

$$\Psi_1 = \sum_{a=1}^{\#\mathcal{P}} \psi_1^a \mathcal{V}^a, \quad \Psi_2 = \sum_{a=1}^{\#\mathcal{P}} \psi_2^a \mathcal{V}^a, \quad \Psi_3 = \sum_{a=1}^{\#\mathcal{P}} \psi_3^a \mathcal{V}^a, \quad (6)$$

where $\mathcal{V}^a$ is the volume of the support domain of the collocation point $\mathcal{P}^a$ and $\#\mathcal{P}$ is the total number of collocation points. The volume $\mathcal{V}^a$ is computed according to the discretisation strategy employed. For instance, if the points are chosen based on a Voronoi tessellation, the volume of each Voronoi cell can be assigned to the point $\mathcal{P}^a$ at its centre. It is also relatively straightforward to discretise the domain using common discretisation tools of the finite element method and then associate each finite element with the point $\mathcal{P}^a$ at its barycentre with $\mathcal{V}^a$ equal to the volume of the respective element. Equipped with the definitions of the point-wise internal energy densities, their contributions to the internal potential energy, or rather their variations, due to one-, two- and three-neighbour interactions are explored next in Sections 3.1.1, 3.1.2 and 3.1.3, respectively.

3.1.1. One-neighbour interactions

The energy density per volume in the material configuration due to one-neighbour interactions ψ_1^a is a point-wise quantity. That is ψ_1^a is obtained via the summation of neighbour-wise energy densities. Let ψ_1^{ai} denote the one-neighbour interaction energy density per volume squared in the material configuration. Note that while ψ_1^a is an energy density per volume, ψ_1^{ai} is an energy density per volume squared. The number of su-

perscripts identifies the nature of the interaction densities. One superscript corresponds to the familiar energy density per volume and two superscripts are associated with energy density per volume squared. As will be seen in the following sections, this notation avoids possible confusion. Consequently, the one-neighbour interaction energy density per volume ψ_1^a reads

$$\psi_1^a = \frac{1}{2} \sum_{i=1}^{\#\mathcal{N}} \psi_1^{ai} \mathcal{V}^i,$$

where $\#\mathcal{N}$ denotes the number of neighbours within the horizon of the collocation point $\mathcal{P}^a$. The factor one-half prevents double-counting since the combination of $\{a, i\}$ will eventually contribute twice to Ψ_1 , see Eq. (6)₁. The effective volume of the neighbour $\mathcal{N}^i$ is denoted as $\mathcal{V}^i$ and defined by

$$\mathcal{V}^i := \frac{\mathcal{V}_{\mathcal{H}}}{\#\mathcal{N}}, \quad (7)$$

where $\mathcal{V}_{\mathcal{H}}$ is the volume of the horizon of the collocation point $\mathcal{P}^a$. For example if the point $\mathcal{P}^a$ is entirely within the bulk and no part of its horizon outside of $\mathcal{B}_0$, then $\mathcal{V}_{\mathcal{H}} = 4/3 \pi \delta^3$ for 3D and $\mathcal{V}_{\mathcal{H}} = \pi \delta^2$ for 2D. Otherwise, $\mathcal{V}_{\mathcal{H}}$ is modified by a dimensionless correction factor that accounts for the truncated support. In the definition of the effective volume for one-neighbour interactions (7), the denominator corresponds to the total number of *neighbours* within the horizon of $\mathcal{P}^a$ that for one-neighbour interactions is precisely $\#\mathcal{N}$. Next, the variation of Ψ_1 can be expressed as

$$\begin{aligned} \delta\Psi_1 &= \delta \sum_{a=1}^{\#\mathcal{P}} \psi_1^a \mathcal{V}^a \\ &= \delta \sum_{a=1}^{\#\mathcal{P}} \frac{1}{2} \sum_{i=1}^{\#\mathcal{N}} \psi_1^{ai} \mathcal{V}^i \mathcal{V}^a \\ &= \sum_{a=1}^{\#\mathcal{P}} \sum_{i=1}^{\#\mathcal{N}} \delta\psi_1^{ai} \mathcal{V}^i \mathcal{V}^a, \end{aligned} \quad (8)$$

where the factor one-half disappears due to the variation rules on multiple sums.

The one-neighbour interactions energy density ψ_1^{ai} is expressed in terms of the *first relative deformation measure* ξ^{ai} , see Eq. (2). That is

$$\psi_1^{ai} = \psi_1^{ai}(\xi^{ai}). \quad (9)$$

The description (9) does not fulfil material frame indifference in its current form. That is, the energy densities do not remain invariant with respect to superposed rigid body motions. To sufficiently satisfy material frame indifference, we express ψ_1^{ai} in terms of the objective scalar measure $|\xi^{ai}|$ as

$$\psi_1^{ai} = \psi_1^{ai}(|\xi^{ai}|).$$

The variation of Eq. (9) reads

$$\delta\psi_1^{ai} = \frac{\partial\psi_1^{ai}}{\partial\xi^{ai}} \cdot \delta\xi^{ai}. \quad (10)$$

Inserting Eq. (10) into Eq. (8) yields

$$\delta\Psi_1 = \sum_{a=1}^{\#\mathcal{P}} \sum_{i=1}^{\#\mathcal{N}} \frac{\partial\psi_1^{ai}}{\partial\xi^{ai}} \cdot \delta\xi^{ai} \mathcal{V}^i \mathcal{V}^a. \quad (11)$$

We define the force density per volume squared due to one-neighbour interactions by

$$\mathbf{p}_1^{ai} := \frac{\partial\psi_1^{ai}}{\partial\xi^{ai}},$$

and thus

$$\delta\Psi_1 = \sum_{a=1}^{\#\mathcal{P}} \sum_{i=1}^{\#\mathcal{N}} \mathbf{p}_1^{ai} \cdot \delta\xi^{ai} \mathcal{V}^i \mathcal{V}^a.$$

Note, $\mathbf{p}_1^{ai}$ has *two superscripts* and is therefore a (force) *density*

per volume squared. Since $\xi^{ai} = \mathbf{y}^i - \mathbf{y}^a$, the identity

$$\delta \xi^{ai} = \delta \mathbf{y}^i - \delta \mathbf{y}^a,$$

holds and therefore

$$\delta \Psi_1 = \sum_{a=1}^{\#\mathcal{P}} \sum_{i=1}^{\#\mathcal{N}} \mathbf{p}_1^{ai} \cdot [\delta \mathbf{y}^i - \delta \mathbf{y}^a] \mathcal{V}^i \mathcal{V}^a,$$

or alternatively

$$\delta \Psi_1 = \sum_{a=1}^{\#\mathcal{P}} \sum_{i=1}^{\#\mathcal{N}} \mathbf{p}_1^{ai} \cdot \delta \mathbf{y}^i \mathcal{V}^i \mathcal{V}^a - \sum_{a=1}^{\#\mathcal{P}} \text{int} \mathbf{b}_1^a \cdot \delta \mathbf{y}^a \mathcal{V}^a, \quad (12)$$

with $\text{int} \mathbf{b}_1^a$ the internal force density per volume in the material configuration due to one-neighbour interactions defined by

$$\text{int} \mathbf{b}_1^a := \sum_{i=1}^{\#\mathcal{N}} \mathbf{p}_1^{ai} \mathcal{V}^i.$$

Note that we identify $\text{int} \mathbf{b}_1^a$ as an internal force density since it is an energy conjugated quantity to $\delta \mathbf{y}^a$.

The intermediate steps to arrive at Eq. (12) for one-neighbour interactions are relatively straightforward. As will be demonstrated shortly, the counterparts of Eq. (12) for two- and three-neighbour interactions are obtained via a formally similar process. The intermediate steps for two- and three-neighbour interactions, however, are slightly more involved.

3.1.2. Two-neighbour interactions

The energy density per volume in the material configuration due to two-neighbour interactions ψ_2^a is a point-wise quantity composed of the summation of neighbour-wise energy densities. Let ψ_2^{aij} denote the two-neighbour interaction energy density per volume cubed in the material configuration. According to our convention, the number of superscripts identifies the nature of the interaction densities. That is, one superscript corresponds to the familiar energy density per volume and three su-

perscripts are associated with energy density per volume cubed. Consequently, the two-neighbour interaction energy density per volume ψ_2^a reads

$$\psi_2^a = \frac{1}{3} \sum_{i=1}^{\#\mathcal{N}} \sum_{\substack{j=1 \\ j \neq i}}^{\#\mathcal{N}} \psi_2^{aij} \mathcal{V}^{ij},$$

where the factor one-third prevents triple-counting since the combination of $\{a, i, j\}$ will eventually contribute three times to Ψ_2 , see Eq. (6)₂. The effective volume of the double-neighbour is denoted as $\mathcal{V}^{ij}$ and can be defined by

$$\mathcal{V}^{ij} := \frac{[\mathcal{V}_{\mathcal{H}}]^2}{[\#\mathcal{N}][\#\mathcal{N} - 1]},$$

where $[\#\mathcal{N}][\#\mathcal{N} - 1]$ is the total number of *double neighbours* within the horizon of collocation point $\mathcal{P}^a$. The effective volume of the double-neighbour is given by

$$\mathcal{V}^{ij} = \mathcal{V}^i \mathcal{V}^j \quad \text{with} \quad \mathcal{V}^j := \frac{\mathcal{V}_{\mathcal{H}}}{[\#\mathcal{N} - 1]}, \quad (13)$$

with $\mathcal{V}^i$ given by Eq. (7). Next, the variation of Ψ_2 is expressed as

$$\delta \Psi_2 = \delta \sum_{a=1}^{\#\mathcal{P}} \psi_2^a \mathcal{V}^a,$$

or

$$\delta \Psi_2 = \delta \sum_{a=1}^{\#\mathcal{P}} \frac{1}{3} \sum_{i=1}^{\#\mathcal{N}} \sum_{\substack{j=1 \\ j \neq i}}^{\#\mathcal{N}} \psi_2^{aij} \mathcal{V}^i \mathcal{V}^j \mathcal{V}^a. \quad (14)$$

Due to the variation rules on multiple sums, the factor one-third disappears and Eq. (14) reads eventually

$$\delta \Psi_2 = \sum_{a=1}^{\#\mathcal{P}} \sum_{i=1}^{\#\mathcal{N}} \sum_{\substack{j=1 \\ j \neq i}}^{\#\mathcal{N}} \delta \psi_2^{aij} \mathcal{V}^i \mathcal{V}^j \mathcal{V}^a.$$

The two-neighbour interactions energy density ψ_2^{aij} is ex-

pressed in terms of the *second relative deformation measure* $\mathbf{a}^{aj}$, see Eq. (3), as

$$\psi_2^{aj} = \psi_2^{aj}(\mathbf{a}^{aj}). \quad (15)$$

Again, the description (15) does not fulfil material frame indifference. To sufficiently satisfy material frame indifference, we express ψ_2^{aj} in terms of the objective measures $|\mathbf{a}^{aj}|$ instead of $\mathbf{a}^{aj}$. More precisely

$$\psi_2^{aj} = \psi_2^{aj}(|\mathbf{a}^{aj}|). \quad (16)$$

The variation of Eq. (15) reads

$$\delta\psi_2^{aj} = \frac{\partial\psi_2^{aj}}{\partial\mathbf{a}^{aj}} \cdot \delta\mathbf{a}^{aj},$$

and since $\mathbf{a}^{aj} = \boldsymbol{\xi}^{ai} \times \boldsymbol{\xi}^{aj}$, it follows that

$$\delta\psi_2^{aj} = \frac{\partial\psi_2^{aj}}{\partial\mathbf{a}^{aj}} \cdot [\delta\boldsymbol{\xi}^{ai} \times \boldsymbol{\xi}^{aj}] + \frac{\partial\psi_2^{aj}}{\partial\mathbf{a}^{aj}} \cdot [\boldsymbol{\xi}^{ai} \times \delta\boldsymbol{\xi}^{aj}]. \quad (17)$$

Inserting Eq. (17) into Eq. (14) yields

$$\begin{aligned} \delta\Psi_2 &= \sum_{a=1}^{\#\mathcal{P}} \sum_{i=1}^{\#N} \sum_{\substack{j=1 \\ j \neq i}}^{\#N} \frac{\partial\psi_2^{aj}}{\partial\mathbf{a}^{aj}} \cdot [\delta\boldsymbol{\xi}^{ai} \times \boldsymbol{\xi}^{aj}] \mathcal{V}^i \mathcal{V}^j \mathcal{V}^a \\ &+ \sum_{a=1}^{\#\mathcal{P}} \sum_{i=1}^{\#N} \sum_{\substack{j=1 \\ j \neq i}}^{\#N} \frac{\partial\psi_2^{aj}}{\partial\mathbf{a}^{aj}} \cdot [\boldsymbol{\xi}^{ai} \times \delta\boldsymbol{\xi}^{aj}] \mathcal{V}^i \mathcal{V}^j \mathcal{V}^a. \end{aligned}$$

To proceed, we exchange the order of summations over i and j in the second term and relabel the quantities, which yields

$$\begin{aligned} \delta\Psi_2 &= \sum_{a=1}^{\#\mathcal{P}} \sum_{i=1}^{\#N} \sum_{\substack{j=1 \\ j \neq i}}^{\#N} \frac{\partial\psi_2^{aj}}{\partial\mathbf{a}^{aj}} \cdot [\delta\boldsymbol{\xi}^{ai} \times \boldsymbol{\xi}^{aj}] \mathcal{V}^i \mathcal{V}^j \mathcal{V}^a \\ &- \sum_{a=1}^{\#\mathcal{P}} \sum_{i=1}^{\#N} \sum_{\substack{j=1 \\ j \neq i}}^{\#N} \frac{\partial\psi_2^{aj}}{\partial\mathbf{a}^{aj}} \cdot [\delta\boldsymbol{\xi}^{ai} \times \boldsymbol{\xi}^{aj}] \mathcal{V}^i \mathcal{V}^j \mathcal{V}^a. \end{aligned}$$

Due to the definition $\psi_2^{aj} = \psi_2^{aj}(|\mathbf{a}^{aj}|)$ in Eq. (16), the property

$$\frac{\partial\psi_2^{aj}}{\partial\mathbf{a}^{aj}} = -\frac{\partial\psi_2^{aj}}{\partial\mathbf{a}^{aji}},$$

holds leading to

$$\delta\Psi_2 = \sum_{a=1}^{\#\mathcal{P}} \sum_{i=1}^{\#N} \sum_{\substack{j=1 \\ j \neq i}}^{\#N} 2 \frac{\partial\psi_2^{aj}}{\partial\mathbf{a}^{aj}} \cdot [\delta\boldsymbol{\xi}^{ai} \times \boldsymbol{\xi}^{aj}] \mathcal{V}^i \mathcal{V}^j \mathcal{V}^a,$$

or alternatively

$$\delta\Psi_2 = \sum_{a=1}^{\#\mathcal{P}} \sum_{i=1}^{\#N} \sum_{\substack{j=1 \\ j \neq i}}^{\#N} \left[2 \boldsymbol{\xi}^{aj} \times \frac{\partial\psi_2^{aj}}{\partial\mathbf{a}^{aj}} \right] \cdot \delta\boldsymbol{\xi}^{ai} \mathcal{V}^i \mathcal{V}^j \mathcal{V}^a.$$

This should be compared with Eq. (11). Next, we define the force density per volume squared due to two-neighbour interactions as

$$\mathbf{p}_2^{ai} := \sum_{\substack{j=1 \\ j \neq i}}^{\#N} 2 \boldsymbol{\xi}^{aj} \times \frac{\partial\psi_2^{aj}}{\partial\mathbf{a}^{aj}} \mathcal{V}^j,$$

and thus

$$\delta\Psi_2 = \sum_{a=1}^{\#\mathcal{P}} \sum_{i=1}^{\#N} \mathbf{p}_2^{ai} \cdot \delta\boldsymbol{\xi}^{ai} \mathcal{V}^i \mathcal{V}^a. \quad (18)$$

Since $\delta\boldsymbol{\xi}^{ai} = \delta\mathbf{y}^i - \delta\mathbf{y}^a$, Eq. (18) can be expressed as

$$\delta\Psi_2 = \sum_{a=1}^{\#\mathcal{P}} \sum_{i=1}^{\#N} \mathbf{p}_2^{ai} \cdot \delta\mathbf{y}^i \mathcal{V}^i \mathcal{V}^a - \sum_{a=1}^{\#\mathcal{P}} \mathbf{b}_2^a \cdot \delta\mathbf{y}^a \mathcal{V}^a, \quad (19)$$

with $\mathbf{b}_2^a$ the internal force density per volume in the material configuration due to two-neighbour interactions defined by

$$\mathbf{b}_2^a := \sum_{i=1}^{\#N} \mathbf{p}_2^{ai} \mathcal{V}^i.$$

Note that, similar to $\mathbf{b}_1^a$, we identify $\mathbf{b}_2^a$ as an internal force density since it is an energy conjugated quantity to $\delta\mathbf{y}^a$.

3.1.3. Three-neighbour interactions

The point-wise energy density per volume in the material configuration due to three-neighbour interactions ψ_3^a is composed of the summation of neighbour-wise energy densities. Let ψ_3^{aijk} denote the three-neighbour interaction energy density per volume to the fourth power in the material configuration. Recall our convention that one superscript corresponds to the familiar energy density per volume and four superscripts are associated with an energy density per volume to the fourth power. Consequently, the three-neighbour interaction energy density per volume ψ_3^a reads

$$\psi_3^a = \frac{1}{4} \sum_{i=1}^{\#N} \sum_{\substack{j=1 \\ j \neq i}}^{\#N} \sum_{\substack{k=1 \\ k \neq j \\ k \neq i}}^{\#N} \psi_3^{aijk} \mathcal{V}^{ijk},$$

where the factor one-fourth is introduced to prevent quadruple-counting due to the combinations of $\{a, i, j, k\}$ that contribute four times to Ψ_3 , see Eq. (6)₃. The effective volume of the triple-neighbour is denoted as $\mathcal{V}^{ijk}$ is defined by

$$\mathcal{V}^{ijk} := \frac{[\mathcal{V}_H]^3}{[\#N][\#N-1][\#N-2]},$$

where $[\#N][\#N-1][\#N-2]$ corresponds to the total number of *triple neighbours* within the horizon of $\mathcal{P}^a$. The effective volume of the triple-neighbour $\mathcal{N}^{ijk}$ can also be written as

$$\mathcal{V}^{ijk} = \mathcal{V}^i \mathcal{V}^j \mathcal{V}^k \quad \text{with} \quad \mathcal{V}^k := \frac{\mathcal{V}_H}{[\#N-2]},$$

with $\mathcal{V}^i$ and $\mathcal{V}^j$ defined by Eqs. (7) and (13), respectively.

Next, the variation of Ψ_3 is expressed as

$$\begin{aligned} \delta\Psi_3 &= \delta \sum_{a=1}^{\#\mathcal{P}} \psi_3^a \mathcal{V}^a \\ &= \delta \sum_{a=1}^{\#\mathcal{P}} \frac{1}{4} \sum_{i=1}^{\#N} \sum_{\substack{j=1 \\ j \neq i}}^{\#N} \sum_{\substack{k=1 \\ k \neq j \\ k \neq i}}^{\#N} \psi_3^{aijk} \mathcal{V}^i \mathcal{V}^j \mathcal{V}^k \mathcal{V}^a. \end{aligned}$$

Due to the variation rules on multiple sums, the factor one-fourth disappears and yields

$$\delta\Psi_3 = \sum_{a=1}^{\#\mathcal{P}} \sum_{i=1}^{\#N} \sum_{\substack{j=1 \\ j \neq i}}^{\#N} \sum_{\substack{k=1 \\ k \neq j \\ k \neq i}}^{\#N} \delta\psi_3^{aijk} \mathcal{V}^i \mathcal{V}^j \mathcal{V}^k \mathcal{V}^a. \quad (20)$$

The three-neighbour interactions energy density ψ_3^{aijk} is expressed in terms of the *third relative deformation measure* v^{aijk} , see Eq. (4). That is,

$$\psi_3^{aijk} = \psi_3^{aijk}(v^{aijk}). \quad (21)$$

As before, since Eq. (21) does not fulfil material frame indifference, we express ψ_3^{aijk} in terms of the objective measures $|v^{aijk}|$ instead of v^{aijk} . That is,

$$\psi_3^{aijk} = \psi_3^{aijk}(|v^{aijk}|). \quad (22)$$

The variation of Eq. (21) reads

$$\delta\psi_3^{aijk} = \frac{\partial\psi_3^{aijk}}{\partial v^{aijk}} \delta v^{aijk},$$

and the definition $v^{aijk} = [\xi^{ai} \times \xi^{aj}] \cdot \xi^{ak}$ furnishes

$$\begin{aligned} \delta\psi_3^{aijk} &= \frac{\partial\psi_3^{aijk}}{\partial v^{aijk}} [\delta\xi^{ai} \times \xi^{aj}] \cdot \xi^{ak} \\ &\quad + \frac{\partial\psi_3^{aijk}}{\partial v^{aijk}} [\xi^{ai} \times \delta\xi^{aj}] \cdot \xi^{ak} \\ &\quad + \frac{\partial\psi_3^{aijk}}{\partial v^{aijk}} [\xi^{ai} \times \xi^{aj}] \cdot \delta\xi^{ak}. \end{aligned} \quad (23)$$

Inserting Eq. (23) into Eq. (20) yields

$$\begin{aligned}\delta\Psi_3 = & \sum_{a=1}^{\#P} \sum_{i=1}^{\#N} \sum_{j=1}^{\#N} \sum_{\substack{k=1 \\ k \neq j \\ k \neq i}}^{\#N} \frac{\partial\psi_3^{aijk}}{\partial v^{aijk}} [\delta\xi^{ai} \times \xi^{aj}] \cdot \xi^{ak} \mathcal{V}^{ijk} \mathcal{V}^a \\ & + \sum_{a=1}^{\#P} \sum_{i=1}^{\#N} \sum_{j=1}^{\#N} \sum_{\substack{k=1 \\ k \neq j \\ k \neq i}}^{\#N} \frac{\partial\psi_3^{aijk}}{\partial v^{aijk}} [\xi^{ai} \times \delta\xi^{aj}] \cdot \xi^{ak} \mathcal{V}^{ijk} \mathcal{V}^a \\ & + \sum_{a=1}^{\#P} \sum_{i=1}^{\#N} \sum_{j=1}^{\#N} \sum_{\substack{k=1 \\ k \neq j \\ k \neq i}}^{\#N} \frac{\partial\psi_3^{aijk}}{\partial v^{aijk}} [\xi^{ai} \times \xi^{aj}] \cdot \delta\xi^{ak} \mathcal{V}^{ijk} \mathcal{V}^a.\end{aligned}$$

To proceed, we exchange the order of summations over i and j on the second term and over i and k on the third term, and relabel the quantities accordingly, which yields

$$\begin{aligned}\delta\Psi_3 = & \sum_{a=1}^{\#P} \sum_{i=1}^{\#N} \sum_{j=1}^{\#N} \sum_{\substack{k=1 \\ k \neq j \\ k \neq i}}^{\#N} \frac{\partial\psi_3^{aijk}}{\partial v^{aijk}} [\delta\xi^{ai} \times \xi^{aj}] \cdot \xi^{ak} \mathcal{V}^{ijk} \mathcal{V}^a \\ & + \sum_{a=1}^{\#P} \sum_{i=1}^{\#N} \sum_{j=1}^{\#N} \sum_{\substack{k=1 \\ k \neq j \\ k \neq i}}^{\#N} \frac{\partial\psi_3^{aijk}}{\partial v^{ajik}} [\xi^{aj} \times \delta\xi^{ai}] \cdot \xi^{ak} \mathcal{V}^{ijk} \mathcal{V}^a \\ & + \sum_{a=1}^{\#P} \sum_{i=1}^{\#N} \sum_{j=1}^{\#N} \sum_{\substack{k=1 \\ k \neq j \\ k \neq i}}^{\#N} \frac{\partial\psi_3^{aijk}}{\partial v^{akji}} [\xi^{ak} \times \xi^{aj}] \cdot \delta\xi^{ai} \mathcal{V}^{ijk} \mathcal{V}^a,\end{aligned}$$

which can be expressed alternatively as

$$\begin{aligned}\delta\Psi_3 = & \sum_{a=1}^{\#P} \sum_{i=1}^{\#N} \sum_{j=1}^{\#N} \sum_{\substack{k=1 \\ k \neq j \\ k \neq i}}^{\#N} \frac{\partial\psi_3^{aijk}}{\partial v^{aijk}} [\delta\xi^{ai} \times \xi^{aj}] \cdot \xi^{ak} \mathcal{V}^{ijk} \mathcal{V}^a \\ & - \sum_{a=1}^{\#P} \sum_{i=1}^{\#N} \sum_{j=1}^{\#N} \sum_{\substack{k=1 \\ k \neq j \\ k \neq i}}^{\#N} \frac{\partial\psi_3^{aijk}}{\partial v^{ajik}} [\delta\xi^{ai} \times \xi^{aj}] \cdot \xi^{ak} \mathcal{V}^{ijk} \mathcal{V}^a \\ & - \sum_{a=1}^{\#P} \sum_{i=1}^{\#N} \sum_{j=1}^{\#N} \sum_{\substack{k=1 \\ k \neq j \\ k \neq i}}^{\#N} \frac{\partial\psi_3^{aijk}}{\partial v^{akji}} [\delta\xi^{ai} \times \xi^{aj}] \cdot \xi^{ak} \mathcal{V}^{ijk} \mathcal{V}^a.\end{aligned}$$

Due to the requirement $\psi_3^{aijk} = \psi_3^{aijk}(|v^{aijk}|)$, the property

$$\frac{\partial\psi_3^{aijk}}{\partial v^{aijk}} = -\frac{\partial\psi_3^{aijk}}{\partial v^{ajik}} = -\frac{\partial\psi_3^{aijk}}{\partial v^{akji}},$$

holds leading to

$$\delta\Psi_3 = \sum_{a=1}^{\#P} \sum_{i=1}^{\#N} \sum_{j=1}^{\#N} \sum_{\substack{k=1 \\ k \neq j \\ k \neq i}}^{\#N} 3 \frac{\partial\psi_3^{aijk}}{\partial v^{aijk}} [\delta\xi^{ai} \times \xi^{aj}] \cdot \xi^{ak} \mathcal{V}^{ijk} \mathcal{V}^a,$$

or alternatively

$$\delta\Psi_3 = \sum_{a=1}^{\#P} \sum_{i=1}^{\#N} \sum_{j=1}^{\#N} \sum_{\substack{k=1 \\ k \neq j \\ k \neq i}}^{\#N} \left[3 \frac{\partial\psi_3^{aijk}}{\partial v^{aijk}} [\xi^{aj} \times \xi^{ak}] \right] \cdot \delta\xi^{ai} \mathcal{V}^{ijk} \mathcal{V}^a.$$

Next, we define the force density per volume squared due to three-neighbour interactions as

$$\mathbf{p}_3^{ai} := \sum_{j=1}^{\#N} \sum_{\substack{k=1 \\ k \neq j \\ k \neq i}}^{\#N} 3 [\xi^{aj} \times \xi^{ak}] \frac{\partial\psi_3^{aijk}}{\partial v^{aijk}} \mathcal{V}^j \mathcal{V}^k,$$

and thus

$$\delta\Psi_3 = \sum_{a=1}^{\#P} \sum_{i=1}^{\#N} \mathbf{p}_3^{ai} \cdot \delta\xi^{ai} \mathcal{V}^i \mathcal{V}^a. \quad (24)$$

Since $\delta\xi^{ai} = \delta\mathbf{y}^i - \delta\mathbf{y}^a$, Eq. (24) can be expressed as

$$\delta\Psi_3 = \sum_{a=1}^{\#P} \sum_{i=1}^{\#N} \mathbf{p}_3^{ai} \cdot \delta\mathbf{y}^i \mathcal{V}^i \mathcal{V}^a - \sum_{a=1}^{\#P} \text{int} \mathbf{b}_3^a \cdot \delta\mathbf{y}^a \mathcal{V}^a, \quad (25)$$

with $\text{int} \mathbf{b}_3^a$ the internal force density per volume in the material configuration due to three-neighbour interactions defined by

$$\text{int} \mathbf{b}_3^a := \sum_{i=1}^{\#N} \mathbf{p}_3^{ai} \mathcal{V}^i.$$

Again, we identify $\text{int} \mathbf{b}_3^a$ as an internal force density since it is an energy conjugated quantity to $\delta\mathbf{y}^a$. Table 3.1.3 summarises the current discussion and gathers the key definitions and results associated with the internal potential energy.

3.2. External potential energy

The external potential energy consists of the contributions due to external loading applied to the system. The external

Table 2: Summary of the internal potential energy contributions and their variations.

one-neighbour interactions	two-neighbour interactions	three-neighbour interactions
internal potential energy in the material configuration with dimension N.m		
$\Psi_1 = \sum_{a=1}^{\#\mathcal{P}} \psi_1^a \mathcal{V}^a$	$\Psi_2 = \sum_{a=1}^{\#\mathcal{P}} \psi_2^a \mathcal{V}^a$	$\Psi_3 = \sum_{a=1}^{\#\mathcal{P}} \psi_3^a \mathcal{V}^a$
internal potential energy density per volume in the material configuration with dimension N.m/m ³		
$\psi_1^a = \frac{1}{2} \sum_{i=1}^{\#N} \psi_1^{ai} \mathcal{V}^i$	$\psi_2^a = \frac{1}{3} \sum_{i=1}^{\#N} \sum_{\substack{j=1 \\ j \neq i}}^{\#N} \psi_2^{aij} \mathcal{V}^{ij}$	$\psi_3^a = \frac{1}{4} \sum_{i=1}^{\#N} \sum_{\substack{j=1 \\ j \neq i}}^{\#N} \sum_{\substack{k=1 \\ k \neq j \\ k \neq i}}^{\#N} \psi_3^{aijk} \mathcal{V}^{ijk}$
with	with	with
$\psi_1^{ai} = \psi_1^{ai}(\xi^{ai})$, $[\psi_1^{ai}] = \text{N.m/m}^6$	$\psi_2^{aij} = \psi_2^{aij}(\mathbf{a}^{aij})$, $[\psi_2^{aij}] = \text{N.m/m}^9$	$\psi_3^{aijk} = \psi_3^{aijk}(\mathbf{v}^{aijk})$, $[\psi_3^{aijk}] = \text{N.m/m}^{12}$
internal force density per volume squared in the material configuration with dimension N/m ⁶		
$\mathbf{p}_1^{ai} := \frac{\partial \psi_1^{ai}}{\partial \xi^{ai}}$	$\mathbf{p}_2^{ai} := \sum_{\substack{j=1 \\ j \neq i}}^{\#N} 2 \xi^{aj} \times \frac{\partial \psi_2^{aij}}{\partial \mathbf{a}^{aij}} \mathcal{V}^j$	$\mathbf{p}_3^{ai} := \sum_{\substack{j=1 \\ j \neq i}}^{\#N} \sum_{\substack{k=1 \\ k \neq j \\ k \neq i}}^{\#N} 3 [\xi^{aj} \times \xi^{ak}] \frac{\partial \psi_3^{aijk}}{\partial \mathbf{v}^{aijk}} \mathcal{V}^j \mathcal{V}^k$
internal force density per volume in the material configuration with dimension N/m ³		
$\text{int} \mathbf{b}_1^a := \sum_{i=1}^{\#N} \mathbf{p}_1^{ai} \mathcal{V}^i$	$\text{int} \mathbf{b}_2^a := \sum_{i=1}^{\#N} \mathbf{p}_2^{ai} \mathcal{V}^i$	$\text{int} \mathbf{b}_3^a := \sum_{i=1}^{\#N} \mathbf{p}_3^{ai} \mathcal{V}^i$
internal potential energy variation in the material configuration with dimension N.m		
$\delta \Psi_1 = \sum_{a=1}^{\#\mathcal{P}} \sum_{i=1}^{\#N} \mathbf{p}_1^{ai} \cdot \delta \mathbf{y}^i \mathcal{V}^i \mathcal{V}^a$ $- \sum_{a=1}^{\#\mathcal{P}} \text{int} \mathbf{b}_1^a \cdot \delta \mathbf{y}^a \mathcal{V}^a$	$\delta \Psi_2 = \sum_{a=1}^{\#\mathcal{P}} \sum_{i=1}^{\#N} \mathbf{p}_2^{ai} \cdot \delta \mathbf{y}^i \mathcal{V}^i \mathcal{V}^a$ $- \sum_{a=1}^{\#\mathcal{P}} \text{int} \mathbf{b}_2^a \cdot \delta \mathbf{y}^a \mathcal{V}^a$	$\delta \Psi_3 = \sum_{a=1}^{\#\mathcal{P}} \sum_{i=1}^{\#N} \mathbf{p}_3^{ai} \cdot \delta \mathbf{y}^i \mathcal{V}^i \mathcal{V}^a$ $- \sum_{a=1}^{\#\mathcal{P}} \text{int} \mathbf{b}_3^a \cdot \delta \mathbf{y}^a \mathcal{V}^a$

loading can be divided into externally prescribed forces within the bulk and tractions on the surface of the body. We emphasize that externally prescribed tractions on the boundary of the body $\partial \mathcal{B}_0$ are also accommodated naturally in CPD, unlike PD. In CPD, the external potential energy Υ is given by

$$\Upsilon = - \sum_{a=1}^{\#\mathcal{P}} \text{ext} \mathbf{b}^a \cdot \mathbf{y}^a \mathcal{V}^a - \sum_{b=1}^{\#\partial \mathcal{P}} \text{ext} \mathbf{t}^b \cdot \mathbf{y}^b \mathcal{A}^b ,$$

where $\text{ext} \mathbf{b}^a$ denotes the point-wise external force density per volume in the material configuration with dimension N/m³. The point-wise external traction on the boundary in the material configuration with dimension N/m² is denoted as $\text{ext} \mathbf{t}^b$. Note that the second sum over b runs from 1 to the total number of boundary points $\#\partial \mathcal{P}$. $\mathcal{A}^b$ is the area of the support domain of the boundary collocation point $\mathcal{P}^b$ that, similar to $\mathcal{V}^a$, can be computed in accordance with the discretisation strategy. This format of the external potential energy follows from a more

general treatment applicable to higher gradient and non-local continua, see [71, 72]. The variation of the external potential energy reads

$$\delta\Upsilon = - \sum_{a=1}^{\#\mathcal{P}} \text{ext} \mathbf{b}^a \cdot \delta \mathbf{y}^a \mathcal{V}^a - \sum_{b=1}^{\#\partial\mathcal{P}} \text{ext} \mathbf{t}^b \cdot \delta \mathbf{y}^b \mathcal{A}^b. \quad (26)$$

3.3. Equilibrium

To derive the equations governing equilibrium, we set the variation of the total potential energy Π with respect to all admissible (spatial) variations $\delta \mathbf{y}$ at a fixed material placement to zero, see Eq. (5). That is

$$\delta\Psi + \delta\Upsilon = 0 \quad \forall \delta \mathbf{y}, \quad (27)$$

where $\delta\Psi = \delta\Psi_1 + \delta\Psi_2 + \delta\Psi_3$ is constructed from Eqs. (12), (19) and (25) as

$$\delta\Psi = \sum_{a=1}^{\#\mathcal{P}} \sum_{i=1}^{\#\mathcal{N}} \mathbf{p}^{ai} \cdot \delta \mathbf{y}^i \mathcal{V}^i \mathcal{V}^a - \sum_{a=1}^{\#\mathcal{P}} \text{int} \mathbf{b}^a \cdot \delta \mathbf{y}^a \mathcal{V}^a, \quad (28)$$

with

$$\mathbf{p}^{ai} := \mathbf{p}_1^{ai} + \mathbf{p}_2^{ai} + \mathbf{p}_3^{ai}, \quad \text{int} \mathbf{b}^a := \text{int} \mathbf{b}_1^a + \text{int} \mathbf{b}_2^a + \text{int} \mathbf{b}_3^a,$$

where $\mathbf{p}^{ai}$ is the total internal force density per volume squared in the material configuration. Similarly, $\text{int} \mathbf{b}^a$ is the total internal force density per volume in the material configuration. Note that $\text{int} \mathbf{b}^a$ can alternatively be expressed as

$$\text{int} \mathbf{b}^a = \sum_{i=1}^{\#\mathcal{N}} \mathbf{p}^{ai} \mathcal{V}^i.$$

Inserting the variation of internal and external potential energies Eq. (28) and Eq. (26), respectively, into the equilibrium

equation (27), yields

$$\begin{aligned} \sum_{a=1}^{\#\mathcal{P}} \sum_{i=1}^{\#\mathcal{N}} \mathbf{p}^{ai} \cdot \delta \mathbf{y}^i \mathcal{V}^i \mathcal{V}^a - \sum_{a=1}^{\#\mathcal{P}} \text{int} \mathbf{b}^a \cdot \delta \mathbf{y}^a \mathcal{V}^a \\ - \sum_{a=1}^{\#\mathcal{P}} \text{ext} \mathbf{b}^a \cdot \delta \mathbf{y}^a \mathcal{V}^a - \sum_{b=1}^{\#\partial\mathcal{P}} \text{ext} \mathbf{t}^b \cdot \delta \mathbf{y}^b \mathcal{A}^b = 0. \end{aligned} \quad (29)$$

Due to the arbitrariness of $\delta \mathbf{y}$, the equilibrium (29) can be expressed as a balance of forces

$$\text{int} \mathbf{b}^a + \text{ext} \mathbf{b}^a = \mathbf{0} \quad \forall \mathcal{P}^a, \quad (30)$$

together with the virtual power equivalence

$$\sum_{a=1}^{\#\mathcal{P}} \sum_{i=1}^{\#\mathcal{N}} \mathbf{p}^{ai} \cdot \delta \mathbf{y}^i \mathcal{V}^i \mathcal{V}^a - \sum_{b=1}^{\#\partial\mathcal{P}} \text{ext} \mathbf{t}^b \cdot \delta \mathbf{y}^b \mathcal{A}^b = 0. \quad (31)$$

The counterparts in classical continuum mechanics to the force balance (30) and the virtual power equivalence (31) read

$$\text{Div} \mathbf{P} + \text{ext} \mathbf{b} = \mathbf{0} \quad \forall \mathbf{X} \in \mathcal{B}_0,$$

and

$$\int_{\mathcal{B}_0} \text{Div}(\delta \mathbf{y} \cdot \mathbf{P}) dV - \int_{\partial\mathcal{B}_0} \text{ext} \mathbf{t} \cdot \delta \mathbf{y} dA = 0,$$

respectively, with $\mathbf{P}$ the Piola stress tensor. Note that the virtual power equivalence (31) is an underlying postulate of CPD since PD lacks the equivalent of Cauchy's fundamental theorem that is used in combination with the Gauss theorem. If the external boundary is traction free or if only displacement type boundary conditions are prescribed, the virtual power equivalence (31) reduces to

$$\sum_{a=1}^{\#\mathcal{P}} \sum_{i=1}^{\#\mathcal{N}} \mathbf{p}^{ai} \cdot \delta \mathbf{y}^i \mathcal{V}^i \mathcal{V}^a = 0.$$

4. Computational implementation

The underlying governing equation of CPD is the force balance (30) that is essentially the linear momentum balance. The angular momentum balance is a priori fulfilled if the internal potential energy densities satisfy material frame indifference or more precisely, if

$$\psi_1^{ai} = \psi_1^{ai}(|\xi^{ai}|), \quad \psi_2^{aij} = \psi_2^{aij}(|\mathbf{a}^{aij}|), \quad \psi_3^{aijk} = \psi_3^{aijk}(|\mathbf{v}^{aijk}|). \quad (32)$$

For the force balance (30), externally prescribed body forces are omitted henceforth since its incorporation into the framework is fairly straightforward and standard. That is, our point-wise non-local equilibrium equation and the point of departure for this section reads

$$\mathbf{R}^a = \mathbf{0} \quad \forall \mathcal{P}^a \quad \text{with} \quad \mathbf{R}^a := \sum_{i=1}^{\#N} \mathbf{p}_1^{ai} \mathcal{V}^i,$$

where the point-wise residual vector for collocation point $\mathcal{P}^a$ is denoted as $\mathbf{R}^a \equiv \text{int} \mathbf{b}^a$ and is composed of the contributions due to one-neighbour, two-neighbour and three-neighbour interactions defined by $\mathbf{R}_1^a$, $\mathbf{R}_2^a$ and $\mathbf{R}_3^a$, respectively. That is

$$\mathbf{R}^a = \mathbf{R}_1^a + \mathbf{R}_2^a + \mathbf{R}_3^a,$$

with

$$\mathbf{R}_1^a := \sum_{i=1}^{\#N} \mathbf{p}_1^{ai} \mathcal{V}^i, \quad \mathbf{R}_2^a := \sum_{i=1}^{\#N} \mathbf{p}_2^{ai} \mathcal{V}^i, \quad \mathbf{R}_3^a := \sum_{i=1}^{\#N} \mathbf{p}_3^{ai} \mathcal{V}^i.$$

After computing the point-wise residual vectors $\mathbf{R}^a$ at collocation point $\mathcal{P}^a$, we assemble them into a global residual vector $\mathbb{R}$.

For nonlinear problems and large deformations, the deformation is computed incrementally. The nonlinear system of governing equations at each increment is $\mathbb{R} = \mathbf{0}$ for which an approximate solution is achieved via an iterative Newton–

Raphson scheme. To do so, we establish a consistent linearization of the resulting system of equations at iteration k . That is

$$\mathbb{R}_{k+1} \stackrel{!}{=} \mathbf{0} \quad \text{with} \quad \mathbb{R}_{k+1} = \mathbb{R}_k + \mathbb{K}_k \cdot \Delta \mathbb{x}_k, \quad (33)$$

where $\mathbb{K}_k$ is the tangent at iteration k defined by

$$\mathbb{K}_k := \left. \frac{\partial \mathbb{R}}{\partial \mathbb{x}} \right|_k,$$

where $\mathbb{x}$ is the global deformation vector that consists of the point-wise deformation vectors as $\mathbb{x} := \{\mathbf{x}^1, \mathbf{x}^2, \dots, \mathbf{x}^a, \dots, \mathbf{x}^{\#P}\}$. The update of deformation $\Delta \mathbb{x}$ at iteration k is computed from Eq. (33). Then the global deformation vector $\mathbb{x}$ is updated at each iteration as $\mathbb{x}_{k+1} = \mathbb{x}_k + \Delta \mathbb{x}_k$. This iterative process is continued until the norm of the residual vector $\mathbb{R}$ is sufficiently small. Further details on computational aspects of the proposed framework are given in [69]. We will illustrate the key features of the proposed framework via a series of numerical examples in Section 6. Prior to that, we particularize the generic form of interaction potentials (32).

5. Harmonic potentials

In this section, we provide specific examples of harmonic potentials for one-neighbour, two-neighbour and three-neighbour interactions such that the requirement of material frame indifference is fulfilled. To do so, the interaction potentials ψ_1^{ai} , ψ_2^{aij} and ψ_3^{aijk} are expressed in terms of $|\xi^{ai}|$, $|\mathbf{a}^{aij}|$ and $|\mathbf{v}^{aijk}|$, respectively. Recall that we adopt a continuum-kinematics-inspired approach, where the deformation measures are common continuum descriptors, namely changes in length, area and volume. This leads to an intuitive description of the interaction energy densities. To aid understanding, one-neighbour interactions can be viewed as the resistance against the change of length between a point and its neighbours, reminiscent of the elastic

modulus in classical continuum mechanics. Two-neighbour interactions can be interpreted as the resistance against the change of the area of the triangle formed by a point and a pair of neighbours, analogous to Poisson-like effects of classical continuum mechanics in two dimensions. Finally, three-neighbour interactions are essentially the resistance against the change of the volume of the tetrahedron formed by each point and its triplet of neighbours, similar to Poisson-like effects in classical continuum mechanics in three dimensions. We define the elastic coefficients C_1 , C_2 and C_3 to characterise the resistance to the change of length, area and volume, respectively. The proposed harmonic potentials read

$$\begin{aligned}\psi_1^{ai} &= \frac{1}{2} C_1 L \left[\frac{l}{L} - 1 \right]^2, \\ \psi_2^{aij} &= \frac{1}{2} C_2 A \left[\frac{a}{A} - 1 \right]^2, \\ \psi_3^{aijk} &= \frac{1}{2} C_3 V \left[\frac{v}{V} - 1 \right]^2.\end{aligned}$$

See Table 2 for the definitions of the kinematic measures.

6. Examples

The main goal of this section is to demonstrate the presented theory via a series of numerical examples. The numerical investigation is devised such that the key features of the framework are illustrated. The numerical examples to demonstrate elasticity at large deformations are carried out on a unit square domain with and without a circular hole of radius $R = 0.2$ at its centre subject to uniaxial extension, as shown in Fig. 2.

Figure 2: Unit square without and with a hole subject to uniaxial extension.

The uniaxial extension is imposed on the square domain via prescribed displacements on its left and right edges, and the upper and lower edges remain free of external loading. An extension of 100% is prescribed in the horizontal direction. The deformation is imposed by displacements prescribed on additional patch layers on each side corresponding to a uniform displacement gradient. That is, the displacements of patch layers are not identical but the displacement gradient is constant throughout the patch layers. The parameter C_1 is fixed and the ratio C_2/C_1 is varied such that the influence of two-neighbour interactions are clearly observed. The domain is discretized uniformly with grid spacing of $\Delta = 0.005$; that is 200 grid points on the edges. The collocation points coincide with the grid points and the measure of the horizon is $\delta = 0.0151 \approx 3\Delta$. A comprehensive convergence study in terms of both grid spacing and horizon size has been carried out but is omitted here for the sake of brevity, see [69].

Figure 3 shows the deformation of the domain and the dependence on the ratio C_2/C_1 , with and without a hole in the middle of the specimen. A larger value of C_2/C_1 leads to more resistance to area change. That is, in the limit of $C_2/C_1 \rightarrow \infty$ the material behaviour will be incompressible. Therefore, the spectrum of the material response from compressible to nearly incompressible is obtained by increasing C_2/C_1 from 0 to 10^7 . The colour bars show the displacement in the vertical direction. Increasing C_2/C_1 results in a more pronounced lateral contraction so as to retain the initial area.

Figures 4 and 5 illustrate the evolution of the deformation for a specimen without and with a hole at its centre, respectively. The computational simulations are carried out for both compressible and nearly incompressible material with $C_2/C_1 = 0$ and $C_2/C_1 = 10^7$, respectively. At 100%, the deformations coincide with those shown in Fig. 3. The nearly incompressible material on the right resists considerably the change of area

Figure 3: Extension of a unit square with varying C_2/C_1 . Increasing C_2/C_1 results in more resistance to compressibility. A nearly incompressible material response is obtained for $C_2/C_1 = 10^7$.

and thus contracts significantly in the lateral direction. In addition, in Fig. 5, the hole expands far more than that for the compressible material on the left. Furthermore, the convergence behaviour associated with the Newton–Raphson scheme at various intermediate increments is given. The numbers in the convergence boxes are the L_2 -norm of the normalized residual at a Newton–Raphson iteration. It can be seen that the quadratic rate of convergence associated with a Newton–Raphson scheme is obtained. The computational simulations are carried out using our in-house code.

7. Outlook

As stated in the introduction, a key feature of the PD formulation is that it can inherently account for singularities such

as fracture. Fracture analysis in PD is commonly carried out by calculating a point-wise damage ratio as an indicator of possible crack formation, particularly relevant to brittle materials. The point-wise damage ratio d is defined as the ratio of the number of terminated interactions over the total number of initial interactions between a point and its neighbours within the horizon. As such, the damage ratio d ranges from 0 to 1. That is, $d = 0$ is associated with a virgin material where all interactions are intact, and $d = 1$ corresponds to a fully damaged material point. An interaction between a point and its neighbour is terminated if the stretch associated with that pair exceeds a certain threshold. Our current formulation also can capture damage and furthermore, increasing C_2/C_1 alternate the damage evolution in the material. This is in agreement with the fact that the

Figure 4: Unit square subject to uniaxial extension at large deformations for compressible (left) and nearly incompressible (right) material. The convergence behaviour corresponds to the L_2 -norm of the residual during the iterations of the Newton–Raphson scheme. At 100%, the compressible and nearly incompressible deformations are those illustrated in Fig. 3 associated with $C_2/C_1 = 0$ and $C_2/C_1 = 10^7$, respectively.

Figure 5: Perforated unit square subject to uniaxial extension at large deformations for compressible (left) and nearly incompressible (right) material. The convergence behaviour corresponds to the L_2 -norm of the residual during the iterations of the Newton–Raphson scheme. At 100%, the compressible and nearly incompressible deformations are those illustrated in Fig. 3 associated with $C_2/C_1 = 0$ and $C_2/C_1 = 10^7$, respectively.

Figure 6: Damage evolution in a unit square with a square hole subject to uniform expansion for compressible (top) and nearly incompressible (bottom) material. Damage is more diffuse in nearly incompressible material compared to a compressible material.

damage evolution is dependent on the stress state and hence the ratio C_2/C_1 .

Figure 6 shows the damage evolution in a unit square with a square hole subject to uniform expansion for compressible and nearly incompressible material. A uniform expansion of 5% is prescribed incrementally on the edges of the square. The deformation is suppressed for the sake of illustration. The domain is discretized uniformly with grid spacing of $\Delta = 0.01$; that is 100 grid points on the edges. The collocation points coincide with the grid points and the measure of the horizon is $\delta = 0.031 \approx 3\Delta$. The computational simulations for compressible and nearly incompressible material correspond to $C_2/C_1 = 0$ and $C_2/C_1 = 10^7$, respectively. A stretch based damage criterion is employed and the damage threshold is assumed 0.05. That is, the interaction between a point and its neighbour is terminated if the associated stretch reaches 0.05. In the absence of two-neighbour interactions, i.e. top row in Fig. 6, the damage evolution is intuitive and “localized” in contrast to the rather complex and diffuse damage pattern for the incompressible material at the bottom.

8. Conclusion

Continuum-kinematics-inspired peridynamics (CPD) was recently proposed by Javili et al. [68] as a geometrically exact

alternative to state-based peridynamics to formulate non-local continuum mechanics at finite deformations. In this manuscript the problem formulation and derivations of CPD have been presented in a discretized form from the onset, thereby providing a more accessible framework that can be readily adopted for computational implementation. The potential of the method has been made clear via a series of numerical examples. CPD is geometrically exact and does not suffer from displacement oscillations associated with non-ordinary state-based PD and furthermore, it can capture Poisson’s effect accurately unlike bond-based PD. It shall be noted, however, that due its non-local nature, CPD is computationally more expensive than its local counterparts such as FEM formulations of local elasticity, for example. A key feature of the proposed methodology is that it is fully implicit and the solution procedure shows the asymptotically quadratic rate of convergence associated with a Newton–Raphson scheme. Prediction of damage and fracture at large deformations using CPD is currently a work in progress and will be investigated separately in the near future.

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